

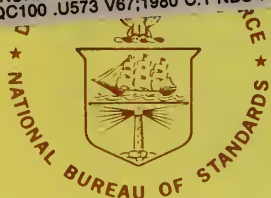
A11102 146399

NAT'L INST OF STANDARDS & TECH R.I.C.



A11102146399

/NSRDS-NBS
QC100 .U573 V67;1980 C.1 NBS-PUB-C 1964



NSRDS-NBS 67

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



Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion

QC
100
.U573
NO. 67
1980
C. 2

NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards¹ was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the Nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the Nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, and the Institute for Computer Sciences and Technology.

THE NATIONAL MEASUREMENT LABORATORY provides the national system of physical and chemical and materials measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; conducts materials research leading to improved methods of measurement, standards, and data on the properties of materials needed by industry, commerce, educational institutions, and Government; provides advisory and research services to other Government agencies; develops, produces, and distributes Standard Reference Materials; and provides calibration services. The Laboratory consists of the following centers:

Absolute Physical Quantities² — Radiation Research — Thermodynamics and Molecular Science — Analytical Chemistry — Materials Science.

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

Applied Mathematics — Electronics and Electrical Engineering² — Mechanical Engineering and Process Technology² — Building Technology — Fire Research — Consumer Product Technology — Field Methods.

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

Programming Science and Technology — Computer Systems Engineering.

¹Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Washington, DC 20234.

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

Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion

National Bureau of Standards
Library, E-01 Admin. Bldg.

NOV 24 1980

Doc 244 - 102

QC100

. 4573

110.67

1980

C 2

⁺ NSRDS-NBS

Francis Westley

Chemical Kinetics Information Center
National Measurement Laboratory
National Bureau of Standards
Washington, D.C. 20234

Sponsored by the

Department of Energy
Washington, D.C. 20545

and

Office of Standard Reference Data
National Bureau of Standards
Washington, D.C. 20234



U.S. DEPARTMENT OF COMMERCE, Philip M. Klutznick, Secretary

Luther H. Hodges, Jr., Deputy Secretary

Jordan J. Baruch, Assistant Secretary for Productivity, Technology, and Innovation

U.S. NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued April 1980

Library of Congress Cataloging in Publication Data

Westley, Francis.

Table of recommended rate constants for chemical reactions occurring in combustion.

(Nat. stand. ref. data ser. ; NSRDS-NBS 67)

"National standard reference data system."

Supt. of Docs. no.: C13.48:67

1. Chemical reaction, Rate of--Tables, etc. 2. Combustion--Tables, etc.

I. Title. II. Series: United States. National Bureau of Standards.

National standard reference data series ; NSRDS-NBS 67.

QC100.U573 no. 67 [QD502] 602'.1s [541.3'61'0212]

79-607159

NSRDS-NBS 67

Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 67, 119 pages (Apr. 1980)

CODEN: NSRDAP

© 1980 by the Secretary of Commerce on Behalf of the United States Government

U.S. GOVERNMENT PRINTING OFFICE

WASHINGTON: 1980

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

Price \$4.25

Foreword

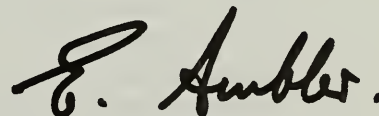
The National Standard Reference Data System provides access to the quantitative data of physical science, critically evaluated and compiled for convenience and readily accessible through a variety of distribution channels. The System was established in 1963 by action of the President's Office of Science and Technology and the Federal Council for Science and Technology, and responsibility to administer it was assigned to the National Bureau of Standards.

NSRDS receives advice and planning assistance from a Review Committee of the National Research Council of the National Academy of Sciences-National Academy of Engineering. A number of Advisory Panels, each concerned with a single technical area, meet regularly to examine major portions of the program, assign relative priorities, and identify specific key problems in need of further attention. For selected specific topics, the Advisory Panels sponsor subpanels which make detailed studies of users' needs, the present state of knowledge, and existing data resources as a basis for recommending one or more data compilation activities. This assembly of advisory services contributes greatly to the guidance of NSRDS activities.

The System now includes a complex of data centers and other activities in academic institutions and other laboratories. Components of the NSRDS produce compilations of critically evaluated data, reviews of the state of quantitative knowledge in specialized areas, and computations of useful functions derived from standard reference data. The centers and projects also establish criteria for evaluation and compilation of data and recommend improvements in experimental techniques. They are normally associated with research in the relevant field.

The technical scope of NSRDS is indicated by the categories of projects active or being planned: nuclear properties, atomic and molecular properties, solid state properties, thermodynamic and transport properties, chemical kinetics, and colloid and surface properties.

Reliable data on the properties of matter and materials are a major foundation of scientific and technical progress. Such important activities as basic scientific research, industrial quality control, development of new materials for building and other technologies, measuring and correcting environmental pollution depend on quality reference data. In NSRDS, the Bureau's responsibility to support American science, industry, and commerce is vitally fulfilled.

A handwritten signature in black ink, reading "E. Ambler." The signature is fluid and cursive, with a large initial "E" and a trailing flourish.

ERNEST AMBLER, *Director*

Contents

	Page
Foreword	III
1. Introduction	1
2. Guidelines for the User	2
Table of Arrhenius parameters for chemical reactions occurring in combustion	8
Reactions of: O	8
O ₂	14
O ₃	16
H	16
H ₂	22
OH	24
HO ₂	26
H ₂ O	28
H ₂ O ₂	28
S	28
S ₂	31
SO	31
SO ₂	32
SH	32
H ₂ S	33
N	33
N ₂	36
NO	37
NO ₂	39
NO ₃	40
N ₂ O	40
N ₂ O ₄	41
N ₂ O ₅	41
NH	41
NH ₂	42
NH ₃	42
NH ₂ NH ₂	42
HN ₃	43
HNO	43
HNO ₃	43
NS	44
C ₁ compounds	44
C ₂ compounds	72
C ₃ compounds	81
C ₄ compounds	86
C ₅ compounds	96
C ₆ compounds	100
C ₇ compounds	104
C ₈ compounds	106
C ₉ compounds	109
C ₁₀ compounds	109
3. Sources of Recommended Rate Constants	109
Appendix: Conversion Tables	110

Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion

Francis Westley

National Bureau of Standards, Chemical Kinetics Division, Center for Thermodynamics and Molecular Science, Washington, DC 20234

A table of recommended rate constants for gas phase chemical reactions occurring in combustion is presented. Specifically, it gives in tabular form the values of the parameters for the modified Arrhenius equation $k = AT^B \exp(-E/RT)$. The table covers reactions occurring in the combustion, oxidation and decomposition of aliphatic saturated or unsaturated C_1 to C_{10} hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides and their free radicals, as well as the reactions of O, O_2 , H, H_2 , OH, H_2O , H_2O_2 , N, N_2 , NO, N_2O , NO_2 , N_2O_4 , N_2O_5 , S, S_2 , SH, SO, SO_2 , SOH, NS, with each other. The table includes 169 first order reactions 782 second order reactions and 57 third order reactions. There are 1770 entries covering 1008 distinct chemical reactions. These recommendations have been taken from eleven evaluations and critical reviews published between 1970 and 1976. The papers examined by the evaluators extend from the nineteen fifties up to and including 1975.

Keywords: Arrhenius parameters; chemical kinetics; combustion; decomposition; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.

1. Introduction

This publication consists of a table of recommended reaction rate constants for the combustion, oxidation, and decomposition reactions of aliphatic saturated and unsaturated hydrocarbons, their oxygenated sulfur and amino derivatives, as well as for the reactions of hydrogen, nitrogen, oxygen, sulfur and their inorganic derivatives with each other. The table is a compilation of recommended rate constants given in eleven critical reviews on the kinetics of combustion, oxidation and decomposition reactions, published between 1970 and 1976. Its purpose is to provide the kineticists and kinetic modelers with a comprehensive and easy-to-consult reference book on the kinetic data for combustion and oxidation processes. The table gives 1008 recommended reaction rate constants from these eleven sources. A summary of the content of the table is given in the following listing of quotations from each source.

Source	No. of Recommended Rate Constants
Baulch et al. (1972)	40
Baulch et al. (1973)	64
Baulch et al. (1976)	36
Benson and O'Neal (1970)	167
Benson et al. (1975)	119

Engleman (1976)	123
Herron and Huie (1973)	46
Kerr and Parsonage (1972)	185
Kerr and Parsonage (1976)	181
Kondratiev (1970)	37
Lloyd (1974)	10
Total	1008

For ease of reference the bimolecular and termolecular reactions included in the table are listed separately under each reactant, so that a grouping of the reaction according to the first reactant is obtained. As a result, the total number of tabulated entries is 1770, although the real number of distinct chemical reactions is 1008.

The presentation of kinetic data is standardized and simplified as much as possible. Rate constants are expressed in the modified Arrhenius equation $k = AT^B \exp(-E/RT)$. In general uncertainties are given only for the rate constant k itself and not for the individual parameters in this equation. Sometimes an uncertainty is given for the value of E/R . This uncertainty is only of secondary importance and has been included in the uncertainty stated for the value of the rate constant. Rate constants are expressed in units of s^{-1} , $cm^3 mol^{-1} s^{-1}$, and $cm^6 mol^{-2} s^{-1}$ for reactions of first, second, and third order, respectively.

For the readers who prefer other kinetic units than the standard ones, two conversion tables for equivalent second and third order rate constant units are appended at the end of this publication.

*This work was supported by the Department of Energy and by the Office of Standard Reference Data of the National Bureau of Standards.

The arrangement of the tables is described in detail below, in the "Guidelines for the User."

It is hoped that this table of kinetic data will serve as a handy and easy to use reference book for all the kineticists and kinetic modelers interested in combustion and oxidation processes.

This publication is not the result of the effort of a single person, but of the whole staff of Chemical Kinetics Information Center. My thanks to all of them.

In particular, I wish to thank Dr. David Garvin, Chief of the Chemical Thermodynamics Division, and Dr. Robert F. Hampson, Jr., Director of the Chemical Kinetics Information Center, for their more than helpful suggestions and constant guidance; Dr. Wing Tsang, Chief of the Chemical Kinetics Division, for his encouragement in having this table published; Mr. James G. Koch, Supervisor, for putting the tables into a printable computer form; Mrs. Bettijoyce Molino and Mrs. Carla G. Messina from the Office of Standard Reference Data for applying the OMNIDATA and GPSDIC programs to the present tables; Mrs. Geraldine Zumwalt and Mrs. Janice L. Jones for punching and typing a difficult typescript, full of digits and numbers, with particular care.

2. Guidelines for the User

General

As pointed out above, the presentation of the kinetic data in this publication is an attempt to simplify and standardize them. In that respect, the choice of standard units for rate constants was easy; it was found that the most commonly used units for gas phase rate constants are the cubic centimeter, the mole and the second. The choice of a standard form for uncertainty limits is somewhat more complicated, but when a series of recommended rate constants is to be presented in a tabular form, the uncertainty limits cannot be omitted, for an uncertainty assigned to the recommended value of a rate constant is an estimate by the evaluator of the absolute accuracy of the preferred value. It is to be emphasized that in the present tables the concern is with the overall uncertainty of a reaction rate constant and not with the expression of precision of a set of experimental measurements. Most of the uncertainty limits included in this table are uniform within the respective temperature range indicated. However, for a limited number of reactions, the data warrant or require variable limits. In such cases, a note under the respective data indicates for which interval of the temperature range there is a change in the uncertainty limits.

It is thought that the uncertainty limits expressed in the form of lower and upper k factors, f and F , respectively, are the most suitable for tabulation. Thus, if k_0 is the

central value of a rate constant the limits of reliability for the rate constant k_0 are defined by the relationship:

$$fk_0 < k < Fk_0 \quad (1)$$

i.e., multiplication of the central value k_0 by f and F gives, respectively, the lower and upper reliability limits of the rate constant. In this standardized formulation of uncertainty limits, the value of f is less than unity and the value of F is greater than unity.

However the k factors are not the only way to express the uncertainty limits of a rate constant and different authors use different forms to indicate the degree of reliability of a recommended rate constant. It follows that certain mathematical relationships are needed to translate the different forms of uncertainty limits into the standard form used in this table (lower and upper k factors). The transformation formulas are given and discussed below.

In general there are two ways to state uncertainty limits: (1) by factors and by algebraic addends.

Uncertainty Expressed by Factors

Besides the standard form of uncertainty limits expressed by the lower and upper factors f and F , as defined by the above given relationship (1), there is another form which expresses the uncertainty limits by a unique factor. Thus, if k_0 is the central value of a rate constant, the statement that k_0 is uncertain to a factor of F means that the uncertainty limits are defined by the relationship:

$$k_0/F < k < k_0F \quad (2)$$

which shows that division and multiplication of the central value k_0 by F gives, respectively, the lower and upper reliability limits of the rate constant. By comparing relationships (1) and (2), it is obvious that in the case of an uncertainty expressed by a unique F the upper factor is equal to the unique factor itself, while the lower factor f is the reciprocal of F :

$$f = 1/F \quad (3)$$

Uncertainty Expressed by Algebraic Addends

There are three types of uncertainty limits for rate constants expressed as algebraic addends which are currently used by kineticists: (a) Uncertainty appended to one of the Arrhenius factors (A , B , or E/R), (b) Uncertainty appended to $\log_{10}k_0$, and (c) Uncertainty expressed as a percentage of k_0 . With respect to the type (a) uncertainties, the B factor uncertainties have been eliminated as being unimportant, while the uncertainties for

the E/R factor may be omitted because they are of secondary importance and are included in the k factors. Therefore, the only uncertainty of type (a) considered below is the one appended to the coefficient of the A factor.

(a) Uncertainty appended to the coefficient of A factor. In scientific notation, the A factor is of the form:

$$A = a \times 10^n \quad (4)$$

where a is a numerical coefficient less than 10 and n is the power of 10. If an uncertainty $\pm a'$ is appended to the coefficient a , the A factor takes the form:

$$A = (a \pm a') \times 10^n \quad (5)$$

If lower and upper factors (f and F) are wanted instead, the A factor takes the form:

$$A = fa \times 10^n \quad (6)$$

$$\text{or} \quad A = Fa \times 10^n \quad (7)$$

Comparison of (6) and (7) to (5) leads to the relationships: $fa = a - a'$ and $Fa = a + a'$ from which the following formulas are obtained:

$$f = 1 - a'/a \quad (8)$$

$$\text{and} \quad F = 1 + a'/a \quad (9)$$

Formulas (8) and (9) are the relationships needed to transform an uncertainty appended to the coefficient of the A factor into one using a k factor. A numerical example follows: $A = (2.0 \pm 0.5) \times 10^{14}$, therefore: $a = 2.0$ and $a' = 0.5$; $a'/a = 0.5/2.0 = 0.25$ and the k factors are: $f = 1 - 0.25 = 0.75$ and $F = 1 + 0.25 = 1.25$.

(b) Uncertainty appended to $\log_{10} k_0$. If k_0 is the central value of a rate constant, C its logarithm to the base 10 and D the uncertainty expressed as an algebraic addend to C , then the following relationship is true:

$$\log_{10} k = C \pm D \quad (10)$$

where $C = \log_{10} k_0$. If D is put in logarithmic form, say:

$$D = \log_{10} F \quad (11)$$

then relationship (10) becomes:

$$\log_{10} k = \log_{10} k_0 \pm \log_{10} F \quad (12)$$

which can take the form:

$$\log_{10} k_0 / F < \log_{10} k < \log_{10} F k_0$$

$$\text{or} \quad k_0 / F < k < F k_0 \quad (13)$$

Replacing $1/F$ by f , relationship (1) is obtained. It is obvious that the k factors f and F are the antilogarithms of $-D$ and D , respectively:

$$f = \text{antilog } (-D) = 10^{-D} \quad (14)$$

$$F = \text{antilog } D = 10^D \quad (15)$$

Formulas (14) and (15) are the relationships needed to transform the type b uncertainties into reliability limits expressed by k factors. A numerical example follows: $\log_{10} k = 14.23 \pm 0.3$, therefore: $f = 10^{-0.3} = 0.5$ and $F = 10^{0.3} = 2.0$.

(c) Uncertainty expressed in percentage of k_0 . Some kineticists prefer to use percentage for defining the uncertainty limits of a rate constant. Thus, the statement that a rate constant is $\pm p\%$ uncertain means that the uncertainty limits of k_0 are defined by the relationship:

$$k_0 - (p/100)k_0 < k < k_0 + (p/100)k_0$$

$$\text{or} \quad (1 - p/100)k_0 < k < (1 + p/100)k_0 \quad (16)$$

Replacing the percentage by the rate, defined as $r = p/100$, relationship (16) becomes:

$$(1 - r)k_0 < k < (1 + r)k_0 \quad (17)$$

Comparison of relationships (17) and (1) leads to the following formulas:

$$f = 1 - r \quad (18)$$

$$\text{and} \quad F = 1 + r \quad (19)$$

which are the relationships needed to transform the type c uncertainties into reliability limits expressed by k factors. A numerical example follows: $k = 3.7 \times 10^{12} \pm 20\%$, therefore $p = 20\%$ and $r = 0.2$. Thus: $f = 1 - 0.2 = 0.8$ and $F = 1 + 0.2 = 1.2$.

When a percent error has been stated as $> 100\%$, the F factor is determined first, according to relationship (19) then, instead of relationship (18), one simply sets: $f = 1/F$. E.g., for a 150% error, $r = 1.5$, $F = 1 + r = 2.5$ and $f = 1/F = 0.4$.

The above given relationships: (3), (8) and (9), (14) and (15), (18) and (19) can be used in reverse by the reader who prefers other types of uncertainty limits than the

standard k factors, f and F . However a word of caution is necessary. In contrast with the standard uncertainty limits, other types of uncertainties for rate constants using a unique factor or algebraic addend have a constraint imposed upon them. Thus, the uncertainties expressed by a unique algebraic addend are required to be symmetrical with respect to the central value to which they are appended, while the uncertainty expressed by a unique factor, F , indicates in fact that the upper factor F and the lower factor f are required to be inverse to each other ($f=1/F$). No such constraints are imposed on the standard uncertainty limits used here and for that reason this type of uncertainty has been found most suitable for tabulation purposed. Why some evaluators prefer uncertainty limits with constraints is not clear. It would seem more logical if the lower and upper uncertainty limits were studied independently from each other, without imposing any constraints on them. Probably it is a matter of convenience to express an uncertainty in the form, say: $\log_{10}k = C \pm D$ rather than by the inequality: $f k_0 < k < F k_0$.

If the transformation of the standard uncertainty limits into uncertainties with constraints is desired, some adjustments may be necessary according to the case. The following examples, for transformation of standard uncertainty into a unique factor uncertainty, are an illustration of the necessary adjustments:

(1) Standard factors: $f=0.5$ and $F=2.0$. It is obvious that $f=1/F$ and no adjustment is necessary.

(2) Standard factors: $f=0.8$ and $F=1.2$. In this case, f and F are not inverse to each other. Indeed $f'=1/F=0.83$ while $F'=1/f=1.25$.

The two pairs of factors ($f'=0.83$; $F=1.2$, and $f=0.8$; $F'=1.25$) are quite close. However, it is safer to choose the pair 0.8 and 1.25, by enlarging slightly the uncertainty range.

(3) Standard factors: $f=0.6$ and $F=1.4$. In this case, not only are the factors not inverse to each other, but the difference is significant: $f'=1/F=0.71$ and $F'=1/f=1.67$.

The two pairs of factors ($f'=0.71$; $F=1.4$, and $f=0.6$; $F'=1.67$) are significantly different. Again, it is safer to choose the pair 0.6 and 1.67 by enlarging the uncertainty range. And, since the concepts of uncertainty and reliability are opposite to each other, enlargement of the uncertainty range will result in a decrease in reliability.

The same adjustments may be necessary for transformation of k factors uncertainties into another type of uncertainties.

Arrangement of the Table

The table is arranged in six columns including the chemical reactions, temperature range, the parameters A ,

B , and E/R for the modified Arrhenius equation $k = AT^B \exp(-E/RT)$, and the uncertainty limits expressed as k factors f and F .

Section 3, the bibliography to the table includes the full references for the 11 critical reviews from which the present table was compiled. Following the bibliography, two conversion tables for equivalent second and third order rate constant units are appended.

Column 1 includes the chemical reactions indicating both the reactants and the products. In the same column, under each chemical reaction, the names of the reactants are given. The chemical nomenclature adopted is the one used in the Chemical Substance Indexes of Chemical Abstracts. Alternative names are not given. The chemical names of the products are not given. The line with chemical names is indented with respect to the line above it. Under the chemical names, the short reference of reviewer's book or article is given. It includes the last two digits of publication's year, followed by the first three letters of author's name. If two authors are given, a slash separates each author's three letters. Again, the short reference line is indented with respect to the line above it, e.g.,

73 HER/HUI indicates the review of rate constants for the reactions between aliphatic hydrocarbons and atomic oxygen, published by Herron and Huie in 1973.

In the same line with the short reference, but spaced out, the order of reaction is indicated by the words "Reaction order" followed by one of the digits 1, 2, or 3. As pointed out in the introduction, the order of reaction helps to establish the proper standard units for the reactions, as follows:

1 for first order reactions s^{-1}

2 for second order reactions $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$

3 for third order reactions $\text{cm}^6 \text{mol}^{-2} \text{s}^{-1}$

Following the reaction order, on the same line, the presence of an inert reaction partner "third body" is indicated by the letter M, followed by its chemical formula, e.g., M:Ar or M:CO₂. No indication is given if M is undefined, or if the reaction does not include M. In all, there are 112 reactions with M specified.

For 124 reactions, no Arrhenius parameters are indicated. Instead, for each of these 124 reactions, the ratio of the rate constant with respect to the rate of a reference reaction, taken as unity, is given. This information follows the reaction order information, on the same line, and is indicated by the symbol k/k_{ref} : followed by a number, e.g., k/k_{ref} : 0.59.

The last line of column 1, placed under the line including the short reference and reaction order information, begins with the heading Note:. It is given only when necessary and might include information about the dependence of k factors on temperature range, or the reaction taken as reference when the ratio k/k_{ref} is given in the previous line, or other information pertinent to the reaction indicated above. The rate constant, k_{ref} , for the reference reaction indicated in the note (by the same author) can be found in the table in the proper place. For a certain number of reactions taken from Baulch et al. (1972, 1973, and 1976) the relationship $k_1 = Kk_{-1}$ included in the note indicates that the respective rate constant was calculated from the equilibrium constant K and the rate constant k_{-1} of the reverse reaction. In such cases, the author usually gives the rate constant of the reverse reaction immediately after the data for the forward reaction. The arrangement of the present table (based on the standard order, as described below in the following paragraph) does not allow the forward rate constant of a reaction to be followed immediately by its reverse reaction data. The reader will have to locate the rate constant of a reverse reaction (by the same author) in its proper place in the table.

Column 2, with the heading T/K, indicates in kelvins the temperature range of validity of the recommended rate parameters. For some reactions only one temperature is given, meaning that the reaction was studied only at one temperature. If no temperature at all is indicated, it means that the kinetic parameters of the corresponding reaction are valid throughout the normal temperature range for combustion. The data estimated by Benson and Golden in their report "Estimating the Kinetics of Combustion" are in this category. The temperatures are aligned with the short reference and the reaction order information.

Column 3, with the heading A , gives the value of A for the equation $k = AT^B \exp(-E/RT)$ in short scientific notation. In other words, it appears as a number less than 10, followed by a parenthesis including an integer preceded by the sign + or -. The number less than 10 is the coefficient of the A factor, while the integer inside the parenthesis is the exponent of 10. Therefore, e.g., 3.5 (+14) should be read as $3.5 \times 10^{+14}$. The coefficient of the A factor has no more than one digit after the decimal point. The units of the A factor are the same as for the rate constant k_1 according to the order of the respective reaction, as shown above. For those cases when the recommended value is only for one temperature, the entry under this column is in fact the value of the rate constant k at this temperature. As for the temperatures, the data for the A factor are aligned with the short reference and reaction order information. If a dash appears in this

column, it means that no A factor value was reported by the evaluator for the corresponding reaction.

Column 4, with the heading B , gives the value of B for the equation $k = AT^B \exp(-E/RT)$. the value of B is usually low and varies from 0 to about 3 or 4. It may be negative or positive. The negative values of B are preceded by the sign -, while the positive values are without sign. No more than one digit is given after the decimal dot. If in this column a dash appears instead of a figure, it means that no B value was reported by the evaluator for the corresponding reaction. As for the temperature and A factor, the data for B are aligned with the short reference and reaction order information.

Column 5, with the heading E/R , indicates the value of E/R for the equation $k = AT^B \exp(-E/RT)$. Since E is the activation energy in cal mol^{-1} and R the gas constant with a value of $1.987 \text{ cal mol}^{-1} \text{K}^{-1}$, it follows that the units of E/R are kelvins. The values given in column 5 for E/R may vary from 0 to over 100000 kelvins. The E/R values may be positive or negative. The negative values are preceded by -, while the positive values are without sign. Some of the E/R values included in the table are followed by an uncertainty with plus or minus sign. As pointed out in the introduction, these uncertainties may be ignored, as being included in the lower and upper k factors indicated in the right column of the table. If in this column a dash appears instead of a figure, it means that no E/R value was reported by the evaluator. As for the data from the previous columns, the values for the E/R factor are aligned with the short reference and reaction order information.

Column 6, with the heading " k factors" and two subheadings, " f " and " F ", indicates the two uncertainty k factors, the lower factor f in the left subcolumn and the upper factor F in the right subcolumn. To find the uncertainty limits of a reaction, its rate constant is to be multiplied by the two factors, as shown above in relation (1): $fk_o < k < Fk_o$. The values of both factors are always positive. If no uncertainty limits are indicated by the evaluator, both subcolumns of the column 6 are left blank. As for the data from the previous columns, the k factors are aligned with the short reference and reaction order information.

Ordering of Chemical Reactions

The general rule for ordering the chemical equations of the reactions listed in column 1 of the table is the standard order of arrangement as described in NBS Technical Note 270-3 pp. 5, 6, and 22¹⁾. This rule is applied to the first reactants of the reactions listed in the table, as well as to the reactants following the first. The first reactant of a reaction takes precedence over the

following ones. The compounds listed as reactants may include the atoms O, H, S, N, and C, either each of them separately, or several, in any possible combination. The standard order of arrangement, when applied to these five atomic species, will result in the sequence O, H, S, N, C, each atom in it taking precedence over the following ones. When applied to the first reactants listed in the table, the standard order of arrangement will result in a sequence of five chemical systems, whose order of precedence is as follows:

(1) O system, (2) H-O system, (3) S-O-H system, (4) N-O-H-S system, and (5) C-O-H-S-N system.

In each system, the first atom is underlined to show that the compounds containing this atom only, should be listed first. It is to be noted that the atomic species following the underlined atom are in standard order, while the underlined atom itself should be put at the end if the standard order were to be followed. As it will be shown below, this exception to the standard rule, which is apparent only but not real, is due to the fact that all the compounds containing the atoms of a system with the exception of the underlined atom, are already listed in the previous systems. In each of these five chemical systems, the order of the compounds listed in the table as first reactants is as follows:

(1) O system: O, O₂, O₃.

(2) H-O system: H, H₂, OH, HO₂, H₂O, H₂O₂.

(3) S-O-H system: S, S₂, SO, SO₃, SH, SH₂, SOH.

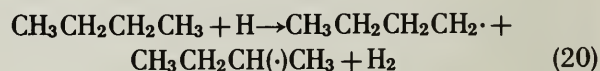
(4) N-O-H-S system: N, N₂, NO, NO₂, NO₃, N₂O, N₂O₄, N₂O₅, NH, NH₂, NH₃, N₂H₄, HN₃, HNO, HNO₃, NS.

(5) C-O-H-S-N system: C₁ compounds: C, CO, CO₂, CH, CH₂, CH₃, CH₄, CHO, HCHO, CH₃O·, CH₃OH, CH₃OOH, CS, CS₂, COS, CH₃S, CH₃SH, CN, C(NO₂)₄, CHN, CH₃NH₂, CH=N≡N, CH₃NHNH₂, CH₃NO, CH₃NO₂, CH₃NO₃, CH₃ONH₂. C₂ compounds: C₂, C₂O, CH=CH, CH₂=CH₂, CH₃CH₂·, CH₃CH₃, CH₂=C=O, etc. C₃ compounds, etc., up to C₁₀ compounds follow, being ordered according to the same pattern.

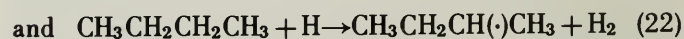
It is clear now that, for instance, the compounds included in the S-O-H system contain at least one sulfur atom, while the compounds containing only H, or O atoms, or both, are already listed in the previous two systems (O-system and H-O system). It is to be noted that for the C-O-H-S-N system the standard order is applied in a slightly different way: the compounds are first grouped according to the number of C atoms, then the rule for the standard order of arrangement is applied for each group apart. This is necessary as a result of the very large number of organic compounds.

The standard order is applied in the same way for the second, or third reactants of chemical reactions. Since the reactants of a chemical equation can be switched around, a number of bimolecular and termolecular reactions are inserted in the table in two and three places, respectively. E.g., reaction CH₄ + O → CH₃· + OH, is inserted in the C-O-H-S-N system. This reaction may also be written as O + CH₄ → OH + CH₃· and, as such, is listed in the O system. The advantage of such a procedure is obvious: referring to the example just given the reader will find the reaction between methane and oxygen listed with CH₄ as first reactant if he is interested in the reactions of methane, or listed with O as first reactant, if he is interested in the reactions of oxygen atom. The bimolecular reactions are the largest group of reactions included in the table. There are about 750 reactions listed in the table, having as reactants two distinct chemical compounds. Since each of these reactions is inserted twice, the number of entries for them will amount to about 1500. Only a small number of termolecular reactions has three distinct reactants. As an example, one of them is NO + NO₂ + O₂ → N₂O₅. This reaction will also be inserted under the forms: NO₂ + NO + O₂ → N₂O₅ and O₂ + NO + NO₂ → N₂O₅. A number of second and third order reactions includes a second and third body M, respectively. For this group of reactions, M will always be placed after all the other reactants, which means that the second order reactions with M as reactant will be inserted in the table only once, while the third order reactions with M as reactant will be inserted only twice. E.g., reaction O₃ + M → O + O₂ + M is inserted in the table only once, while reaction NO + O + M → NO₂ + M is inserted as such, and also under the form O + NO + M → NO₂ + M.

Most of the chemical reactions included in the table are balanced. A number of reactions are only apparently unbalanced. For instance, reaction



has a rate constant which is in fact the sum of the rate constants for the two reactions

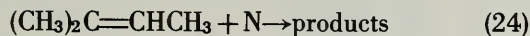


Since the Arrhenius parameters listed in the table refer to the total rate constant, the reaction is listed in the table under the form (20) rather than in two separate forms. In some instances, a reaction is balanced, but the alkyl radicals formed as products are not specified, e.g.:



¹ Wagman, D. D., Evans, W. H., Parker, V. B., Halow, I., Bailey, S. M., and Schumm, R. H., "Selected Values of Chemical Thermodynamic Properties," NBS Tech. Note 270-3 pp. 5, 16, 22 (1968).

The unspecified octyl radical inserted in square brackets as product in equation (23) represents all primary, secondary and tertiary octyl radicals that could be formed by abstraction of a H atom from the reactant 2,3,4-trimethyl-pentane. There are a number of reactions with the products totally unspecified. In such a case, the word "products" appears after the arrow:



Display of Chemical Reactions and Formulae

A chemical reaction equation should show as clearly as possible the formation of products from the reactants. For that reason, the reactions listed in the table are written on the basis of semi-structural formulas.

Straight chain hydrocarbons. All saturated normal hydrocarbons up to, and including *n*-pentane, are written so as to show separately each methyl and methylene group in the chain: CH_4 , CH_3CH_3 , $\text{CH}_3\text{CH}_2\text{CH}_3$, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$, $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$.

The higher hydrocarbons, from *n*-hexane to *n*-decane, are written in a more condensed form to facilitate the counting of the number of methylene groups in the chain: $\text{CH}_3(\text{CH}_2)_4\text{CH}_3$, $\text{CH}_3(\text{CH}_2)_5\text{CH}_3$, $\text{CH}_3(\text{CH}_2)_6\text{CH}_3$, $\text{CH}_3(\text{CH}_2)_7\text{CH}_3$, $\text{CH}_3(\text{CH}_2)_8\text{CH}_3$.

The unsaturated hydrocarbons are written so as to show the position of each double or triple bond in the molecule, e.g.:

Ethyne (Acetylene)	$\text{CH}\equiv\text{CH}$
1,2-Propadiene (Allene)	$\text{CH}_2=\text{C}=\text{CH}_2$
1,3-Butadiyne	$\text{CH}\equiv\text{CC}\equiv\text{CH}$
<i>cis</i> -2-Pentene	<i>cis</i> - $\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$
1-Heptene	$\text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2$

Alkyl radicals. The unpaired electron of each alkyl radical is always indicated, e.g.:

Methyl free radical	$\text{CH}_3\cdot$
Ethyl, 1-methyl-, free radical	
(Isopropyl)	$(\text{CH}_3)_2\text{CH}\cdot$
Methyl, hydroxy-, free radical	$\cdot\text{CH}_2\text{OH}$

If the unpaired electron of an alkyl radical belongs to a carbon in the middle of the chain, it is indicated inside a parenthesis following the carbon atom, e.g.:

Propyl, 1-methyl-, free radical	
(sec-Butyl)	$\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$
Butyl, 1,1-dimethyl-, free radical	
(2-Methyl-2-pentyl)	$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$
Methyl, oxo-, free radical	
(Formyl) is written:	$\cdot\text{CHO}$

Oxy free radicals. If the oxygen atom of an oxy radical is attached to the terminal carbon atom, the radical is written in the usual manner: $\text{CH}_3\text{O}\cdot$. If the oxygen atom of the oxy radical is attached to a C atom in the middle of the chain, then the oxygen atom, together with the unpaired electron, are inside a parenthesis following the C atom: $(\text{CH}_3)_2\text{C}(\text{O}\cdot)\text{CH}_2\text{CH}_3$.

Peroxo, and other free radicals. The rules for writing peroxo, and other free radicals are the same as for the oxy free radicals: $\text{CH}_3\text{O}_2\cdot$, $\text{CH}_3\text{S}\cdot$.

Atoms, like O, H, S, N, and simple radicals like OH, SH, NH, CH, CH_2 , are written without dot. Hydroperoxyl free radical is written $\text{HO}_2\cdot$ (with dot).

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$O + O + M \rightarrow O_2 + M$ OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: Ar NOTE: k FACTORS CHANGING TO: f = 0.4; F = 1.6 AT 4000K. M: N ₂ M: O ₂	190-4000	1.9(+13)	0	-900±175	0.8	1.2
NOTE: k ₁ = Kk ₋₁ . k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT ≈ 8000K.	190-400	1.0(+14)	0	-720	0.5	1.5
	2000-10000	4.7(+23)	-2.5	0	0.4	2.5
$O + O_2 \rightarrow O_2 + O$ OXYGEN ATOM + OXYGEN MOLECULE 76 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + O_2 + M \rightarrow O_3 + M$ OXYGEN ATOM + OXYGEN MOLECULE 76 BAU/DRY REACTION ORDER: 3. M: O ₂ NOTE: M eff: O ₂ (1.5) M: AR NOTE: M eff: Ar(1.0) M: N ₂ NOTE: M eff: N ₂ (1.4)	300	2.2(+14)	-	-	0.8	1.2
	300	1.5(+14)	-	-	0.8	1.3
	300	2.1(+14)	-	-	0.8	1.2
$O + O_3 \rightarrow O_2 + O_2$ OXYGEN ATOM + OZONE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.6; F = 3.0 AT ≈ 1000K	200-500	5.2(+12)	0	2090±260	0.5	1.5
$O + H + M \rightarrow OH + M$ OXYGEN + HYDROGEN ATOMS 76 ENG REACTION ORDER: 3.	1500-2500	7.9(+15)	0	0	0.1	10.
$O + H_2 \rightarrow OH + H$ OXYGEN ATOM + HYDROGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	400-2000	1.8(+10)	1.0	4480±150	0.7	1.3
$O + D_2 \rightarrow OD + D$ OXYGEN ATOM + DEUTERIUM MOLECULE 72 BAU/DRY REACTION ORDER: 2.	416-968	2.0(+13)	0	5500	0.5	2.0
$O + OH \rightarrow O_2 + H$ OXYGEN ATOM + HYDROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2. 76 ENG	300	2.3(+13)	-	-	0.6	1.4
	1500-2500	2.5(+13)	0	0	0.5	2.0
$O + OH \rightarrow O_2 + H$ OXYGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + OH + M \rightarrow HO_2 + M$ OXYGEN ATOM + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+17)	0	0	0.01	100.
$O + OH \rightarrow OH + O$ OXYGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$O + H_2O \rightarrow OH + OH$ OXYGEN ATOM + WATER 72 BAU/DRY REACTION ORDER: 2.	300-2000	6.8(+13)	0	9240±200	0.7	1.5
$O + S_2 \rightarrow SO + S$ OXYGEN ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + SO \rightarrow O_2 + S$ OXYGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	2770		
$O + SO \rightarrow SO + O$ OXYGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + SO + M \rightarrow SO_2 + M$ OXYGEN ATOM + SULFUR MONOXIDE 76 BAU/DRY REACTION ORDER: 3. M: Ar	298	6.7(+16)	-	-	0.7	1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$O + SO_2 \rightarrow O_2 + SO$ OXYGEN ATOM + SULFUR DIOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$	440-2100	1.3(+14)	-0.5	9980	0.3	1.7
$O + SH \rightarrow H + SO$ OXYGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + SH \rightarrow OH + S$ OXYGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0	4000		
$O + N + M \rightarrow NO + M$ OXYGEN ATOM + NITROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: N_2	200-400	6.4(+16)	-0.5	0		
$O + N_2 \rightarrow NO + N$ OXYGEN ATOM + NITROGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$	2000-5000	7.6(+13)	0	38000±150	0.5	2.0
$O + N_2 + M \rightarrow N_2O + M$ OXYGEN ATOM + NITROGEN MOLECULE 73 BAU/DRY REACTION ORDER: 3. M: Ar	1300-2500	1.4(+13)	0	10400±1500	0.7	1.5
$O + NO \rightarrow O_2 + N$ OXYGEN ATOM + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$. k FACTORS CHANGING TO: $f = 0.5$; $F = 2.0$ AT 3000K	1000-3000	1.5(+ 9)	1.0	19500±150	0.7	1.3
$O + NO \rightarrow NO + O$ OXYGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + NO + M \rightarrow NO_2 + M$ OXYGEN ATOM + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 3. M: O_2 NOTE: M eff: $O_2(1.0)$ AT 297K	200-500	1.1(+15)	0	-940±50	0.8	1.2
Ar(0.1) AT 297K	M: Ar 200-500	1.1(+14)	0	-940±50	0.8	1.2
H ₂ O(6.1) AT 297K	M: H ₂ O 200-500	6.7(+15)	0	-940±15	0.8	1.2
D ₂ O(5.0) AT 297K	M: D ₂ O 200-500	5.5(+15)	0	-940±50	0.8	1.2
SF ₆ (2.6) AT 297K	M: SF ₆ 200-500	2.9(+15)	0	-940±50	0.8	1.2
N ₂ (1.4) AT 297K	M: N ₂ 200-500	1.5(+15)	0	-940±50	0.8	1.2
N ₂ O(2.1) AT 297K	M: N ₂ O 200-500	2.3(+15)	0	-940±50	0.8	1.2
CO ₂ (2.1) AT 297K	M: CO ₂ 200-500	2.3(+15)	0	-940±50	0.8	1.2
CH ₄ (2.2) AT 297K	M: CH ₄ 200-500	2.4(+15)	0	-940±50	0.8	1.2
CF ₄ (2.2) AT 297K	M: CF ₄ 200-500	2.4(+15)	0	-940±50	0.8	1.2
$O + NO_2 \rightarrow O_2 + NO$ OXYGEN ATOM + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 2.	300-550	1.0(+13)	0	300±100	0.8	1.3
$O + NO_2 \rightarrow O_2 + NO$ OXYGEN ATOM + NITROGEN OXIDE(NO ₂) 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+13)	0	500±250	0.5	2.0
$O + NO_2 + M \rightarrow NO_3 + M$ OXYGEN ATOM + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 3. M: N ₂ NOTE: k ₀ (LOW PRESSURE).	295	2.3(+16)	-	-	0.4	2.5
NOTE: LIMITING HIGH PRESSURE k.	REACTION ORDER: 2. M: N ₂ 295	1.1(+13)	-	-	0.4	2.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$O + N_2O \rightarrow O_2 + N_2$ OXYGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2.	1200–2000	1.0(+14)	0	14100±2000	0.4 2.5
$O + N_2O \rightarrow NO + NO$ OXYGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2.	1200–2000	1.0(+14)	0	14100±1500	0.5 2.0
$O + NH \rightarrow OH + N$ OXYGEN ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$O + NH \rightarrow NO + H$ OXYGEN ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$O + NH + M \rightarrow HNO + M$ OXYGEN ATOM + IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 3.	1500–2500	1.0(+16)	–0.5	0±2500	0.3 3.2
$O + NH_3 \rightarrow OH + NH_2$ OXYGEN ATOM + AMMONIA 73 BAU/DRY REACTION ORDER: 2.	300–1000	1.5(+12)	0	3000±300	0.5 1.5
$O + HNO \rightarrow OH + NO$ OXYGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+11)	0.5	0±2500	0.3 3.2
$O + HNO \rightarrow O_2 + NH$ OXYGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	3500±2500	0.3 3.2
$O + HNO \rightarrow NO_2 + H$ OXYGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+10)	0.5	0±2500	0.3 3.2
$O + NS \rightarrow SO + N$ OXYGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$O + NS \rightarrow NO + S$ OXYGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$O + C + M \rightarrow CO + M$ OXYGEN ATOM + CARBON ATOM 76 BAU/DRY REACTION ORDER: 3. NOTE: M = Ar, OR CO $k_1 = Kk_{-1}$	7000–15000	3.3(+26)	–3.1	2114	0.3 1.8
$O + CO \rightarrow O_2 + C$ OXYGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	69300	
$O + CO \rightarrow CO + O$ OXYGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$O + CO + M \rightarrow CO_2 + M$ OXYGEN ATOM + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 3. M: CO NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.2 AT 500K.	250–500	2.4(+15)	0	2184±280	0.8 1.2
$O + CO_2 \rightarrow O_2 + CO$ OXYGEN ATOM + CARBON DIOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K. $k_1 = Kk_{-1}$	1500–3000	1.7(+13)	0	26500±2500	0.5 2.0
$O + CH \rightarrow OH + C$ OXYGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$O + CH \rightarrow CO + H$ OXYGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + CH + M \rightarrow CHO + M$ OXYGEN ATOM + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+16)	-0.5	0±2500	0.3	3.2
$O + :CH_2 \rightarrow H + \cdot CHO$ OXYGEN ATOM + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	2000±2500	0.3	3.2
$O + :CH_2 \rightarrow OH + CH$ OXYGEN ATOM + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.7	13100±2500	0.3	3.2
$O + CH_3 \cdot \rightarrow H + HCHO$ OXYGEN ATOM + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+13)	0	0	0.5	2.0
$O + CH_4 \rightarrow OH + CH_3 \cdot$ OXYGEN ATOM + METHANE 73 HER/HUI REACTION ORDER: 2. 76 ENG	350-1000 1500-2500	2.1(+13) 2.0(+13)	0 0	4550 4530±500	0.7 0.6	1.3 1.6
$O + \cdot CHO \rightarrow H + CO_2$ OXYGEN ATOM + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	0	0±1500		
$O + \cdot CHO \rightarrow OH + CO$ OXYGEN ATOM + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	1.0	250±1500		
$O + HCHO \rightarrow OH + \cdot CHO$ OXYGEN ATOM + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	1.0	1750±1000	0.5	1.2
$O + HCHO \rightarrow \text{products}$ OXYGEN ATOM + FORMALDEHYDE 73 HER/HUI REACTION ORDER: 2.	300	9.0(+10)	-	-	0.7	1.3
$O + HCDO \rightarrow \text{products}$ OXYGEN ATOM + FORMALDEHYDE-d 73 HER/HUI REACTION ORDER: 2.	300	4.9(+10)	-	-		
$O + CH_3O \cdot \rightarrow OH + HCHO$ OXYGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED	1500-2500	1.0(+14)	0	0±1500		
$O + CS \rightarrow C + SO$ OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	28940		
$O + CS \rightarrow CO + S$ OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. 75 BEN/GOL	300	1.3(+13) 6.3(+11)	- 0.5	- 0	0.5	1.5
$O + CS_2 \rightarrow S + COS$ OXYGEN ATOM + CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2.	302	2.2(+11)	-	-	0.5	1.5
$O + CS_2 \rightarrow SO + CS$ OXYGEN ATOM + CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2.	200-1000	2.2(+13)	0	700±150	0.7	1.3
$O + COS \rightarrow SO + CO$ OXYGEN ATOM + CARBON OXIDE SULFIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 ABOVE 600K.	190-1200	1.6(+13)	0	2250±250	0.5	1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$O + CN \rightarrow C + NO$ OXYGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	14545		
$O + CN \rightarrow CO + N$ OXYGEN ATOM + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+12)	0	0±2500	0.3	3.2
$O + C_2 \rightarrow CO + C$ OXYGEN ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O + CH=CH \rightarrow \text{products}$ OXYGEN ATOM + ETHYNE 73 HER/HUI REACTION ORDER: 2.	200-700	1.4(+13)	0	1500	0.8	1.2
$O + CH_2=CH_2 \rightarrow \text{cy-CH}_2\text{CH}_2O$ OXYGEN ATOM + ETHENE 73 HER/HUI REACTION ORDER: 2.	200-500	3.3(+12)	0	565	0.8	1.2
$O + CH_3CH_3 \rightarrow OH + CH_3CH_2\cdot$ OXYGEN ATOM + ETHANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.5(+13)	0	3200	0.7	1.3
$O + CH_2=C=O \rightarrow \text{products}$ OXYGEN ATOM + ETHENONE 73 HER/HUI REACTION ORDER: 2.	298	5.3(+11)	-	-	0.7	1.3
$O + CH_3CHO \rightarrow \text{products}$ OXYGEN ATOM + ACETALDEHYDE 73 HER/HUI REACTION ORDER: 2.	298-500	1.4(+13)	0	1140	0.5	2.0
$O + \text{cy-CH}_2\text{CH}_2O \rightarrow \text{products}$ OXYGEN ATOM + OXIRANE 73 HER/HUI REACTION ORDER: 2.	298	7.0(+ 8)	-	-	0.6	1.5
$O + CH_3CH_2OH \rightarrow \text{products}$ OXYGEN ATOM + ETHANOL 73 HER/HUI REACTION ORDER: 2.	298	8.7(+10)	-	-	0.6	1.5
$O + CH_3OCH_3 \rightarrow \text{products}$ OXYGEN ATOM + METHANE, OXYBIS- 73 HER/HUI REACTION ORDER: 2.	200-500	5.9(+12)	0	1520	0.7	1.3
$O + CH_3C\equiv CH \rightarrow \text{products}$ OXYGEN ATOM + PROPYNE 73 HER/HUI REACTION ORDER: 2.	298	4.0(+11)	-	-	0.5	2.0
$O + CH_3CH=CH_2 \rightarrow \text{cy-(CH}_3\text{)CHCH}_2O$ OXYGEN ATOM + 1-PROPENE 73 HER/HUI REACTION ORDER: 2.	200-500	2.5(+12)	0	38	0.8	1.2
$O + CH_3CH_2CH_3 \rightarrow OH + CH_3CH_2CH_2\cdot + (CH_3)_2CH\cdot$ OXYGEN ATOM + PROPANE 73 HER/HUI REACTION ORDER: 2.	298	9.0(+ 9)	-	-	0.7	2
$O + (CH_3)_2CHOH \rightarrow \text{products}$ OXYGEN ATOM + 2-PROPANOL 73 HER/HUI REACTION ORDER: 2.	298	1.3(+11)	-	-	0.6	1.5
$O + (CH_3)_2C=CH_2 \rightarrow \text{cy-(CH}_3\text{)}_2\text{CCH}_2O$ OXYGEN ATOM + 1-PROPENE, 2-METHYL- 73 HER/HUI REACTION ORDER: 2.	298	1.2(+13)	-	-	0.7	1.3
$O + CH\equiv CC\equiv CH \rightarrow \text{products}$ OXYGEN ATOM + 1,3-BUTADIENE 73 HER/HUI REACTION ORDER: 2.	300	9.0(+11)	-	-	0.7	1.4
$O + CH_2=CHCH=CH_2 \rightarrow \text{products}$ OXYGEN ATOM + 1,3-BUTADIENE 73 HER/HUI REACTION ORDER: 2.	298-400	3.4(+12)	0	-380	0.7	1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$0 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2)\text{CHCH}_2\text{O}$ OXYGEN ATOM + 1-BUTENE 73 HER/HUI REACTION ORDER: 2.	298	2.3(+12)	-	-	0.8 1.2
$0 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + cis-2-BUTENE 73 HER/HUI REACTION ORDER: 2.	250-500	5.9(+12)	0	-165	0.8 1.2
$0 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + trans-2-BUTENE 73 HER/HUI REACTION ORDER: 2.	298	1.4(+13)	-	-	0.7 1.3
$0 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ OXYGEN ATOM + BUTANE 73 HER/HUI REACTION ORDER: 2.	298-650	3.0(+13)	0	2920	0.7 1.3
$0 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ OXYGEN ATOM + BUTANE 73 HER/HUI REACTION ORDER: 2.	298-650	4.3(+13)	0	2410	0.7 1.3
$0 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2)\text{CHCH}_2\text{O}$ OXYGEN ATOM + 1-PENTENE 73 HER/HUI REACTION ORDER: 2.	298	2.8(+12)	-	-	0.7 1.3
$0 + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + cis-2-PENTENE 73 HER/HUI REACTION ORDER: 2.	298	1.1(+13)	-	-	0.7 1.3
$0 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + 2-BUTENE, 2-METHYL- 73 HER/HUI REACTION ORDER: 2.	298-400	3.9(+12)	0	-680	0.8 1.2
$0 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ OXYGEN ATOM + PENTANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$0 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ OXYGEN ATOM + PENTANE 73 HER/HUI REACTION ORDER: 2.	298-650	8.0(+13)	0	2320	0.7 1.3
$0 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{OH} + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ $+ (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ OXYGEN ATOM + BUTANE, 2-METHYL- 73 HER/HUI REACTION ORDER: 2.	307	8.0(+10)	-	-	0.7 1.4
$0 + (\text{CH}_3)_4\text{C} \rightarrow \text{OH} + (\text{CH}_3)_3\text{CCH}_2\cdot$ OXYGEN ATOM + PROPANE, 2,2-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.4
$0 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2)\text{CHCH}_2\text{O}$ OXYGEN ATOM + 1-HEXENE 73 HER/HUI REACTION ORDER: 2.	298	3.1(+12)	-	-	0.7 1.3
$0 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	298-400	3.4(+12)	0	-790	0.8 1.2
$0 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ OXYGEN ATOM + HEXANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$0 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ OXYGEN ATOM + HEXANE 73 HER/HUI REACTION ORDER: 2.	298-650	1.1(+14)	0	2250	0.8 1.3
$0 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{OH} + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ OXYGEN ATOM + BUTANE, 2,3-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.3
$0 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{OH} + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ OXYGEN ATOM + BUTANE, 2,3-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	298-650	3.1(+13)	0	1650	0.7 1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$O + CH_3(CH_2)_5CH_3 \rightarrow OH + CH_3(CH_2)_5CH_2\cdot$ OXYGEN ATOM + HEPTANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7	1.3
$O + CH_3(CH_2)_5CH_3 \rightarrow OH + CH_3(CH_2)_4CH(\cdot)CH_3$ $+ CH_3(CH_2)_3CH(\cdot)(CH_2)_2CH_3 + CH_3(CH_2)_2CH(\cdot)(CH_2)_2CH_3$ OXYGEN ATOM + HEPTANE 73 HER/HUI REACTION ORDER: 2.	298-650	1.2(+14)	0	2190	0.7	1.3
$O + (CH_3)_3C(CH_2)_2CH_3 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,2-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	6.5(+10)	-	-	0.7	1.4
$O + (CH_3)_2CHCH_2CH(CH_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,4-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	1.0(+11)	-	-	0.7	1.4
$O + CH_3(CH_2)_6CH_3 \rightarrow OH + CH_3(CH_2)_6CH_2\cdot$ OXYGEN ATOM + OCTANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7	1.3
$O + CH_3(CH_2)_6CH_3 \rightarrow OH + CH_3(CH_2)_5CH(\cdot)CH_3$ $+ CH_3(CH_2)_4CH(\cdot)CH_2CH_3 + CH_3(CH_2)_3CH(\cdot)(CH_2)_2CH_3$ OXYGEN ATOM + OCTANE 73 HER/HUI REACTION ORDER: 2.	298-650	9.3(+13)	0	2030	0.7	1.3
$O + (CH_3)_3CCH_2CH(CH_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,2,4-TRIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	5.5(+10)	-	-	0.6	1.5
$O + (CH_3)_2CHCH(CH_3)CH(CH_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,3,4-TRIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	3.0(+10)	-	-	0.6	1.5
$O + (CH_3)_3CC(CH_3)_3 \rightarrow \text{products}$ OXYGEN ATOM + BUTANE, 2,2,3,3-TETRAMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	8.0(+9)	-	-	0.6	1.5
$O_2 + O \rightarrow O + O_2$ OXYGEN MOLECULE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$O_2 + O + M \rightarrow O_3 + M$ OXYGEN MOLECULE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: O_2	300	2.2(+14)	-	-	0.8	1.2
NOTE: M eff: $O_2(1.5)$						
Ar(1.0)	300	1.5(+14)	-	-	0.8	1.3
$N_2(1.4)$	300	2.1(+14)	-	-	0.8	1.2
$O_2 + H \rightarrow O + OH$ OXYGEN MOLECULE + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2. 72 KON	700-2500 310-2060	2.2(+14) 1.5(+14)	0 0	8450±250 8420±125	0.7 0.9	1.3 1.2
$O_2 + D \rightarrow O + OD$ OXYGEN MOLECULE + DEUTERIUM ATOM 72 BAU/DRY REACTION ORDER: 2.	800-1000	8.9(+13)	-	7500		
$O_2 + H + M \rightarrow HO_2 + M$ OXYGEN MOLECULE + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 3. M: H_2	300-2000	5.0(+15)	0	-500±250	0.5	1.5
NOTE: M eff: $H_2(1.0)$						
$O_2(0.4)$	300-2000	2.0(+15)	0	-500±250	0.5	1.5
$H_2O(6.4)$	300-2000	3.2(+16)	0	-500±250	0.5	1.5
He(0.3). $k_1 = Kk_{-1}$	300-2000	1.5(+15)	0	-500±250	0.5	1.5
Ar(0.3). $k_1 = Kk_{-1}$	300-2000	1.5(+15)	0	-500±250	0.5	1.5
$N_2(0.4)$	300-2000	2.0(+15)	0	-500±250	0.5	1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
CO ₂ (1.5) M: CO ₂	300-2000	7.5(+15)	0	-500±250	0.5 1.5
O ₂ + H ₂ → OH + OH OXYGEN MOLECULE + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500-2500	2.5(+12)	0	19630±5000	0.1 10.
O ₂ + H ₂ → HO ₂ + H OXYGEN MOLECULE + HYDROGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	290-800	5.5(+13)	0	29100±350	0.4 2.5
O ₂ + S → O + SO OXYGEN MOLECULE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2.	250-450	1.4(+12)	0	0±50	0.3 1.7
O ₂ + SO → O + SO ₂ OXYGEN MOLECULE + SULFUR MONOXIDE 76 BAU/DRY REACTION ORDER: 2.	440-2100	4.5(+11)	0	3250±590	0.3 1.7
O ₂ + N → O + NO OXYGEN MOLECULE + NITROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 3000K.	300-3000	6.4(+ 9)	1.0	3150±150	0.7 1.3
O ₂ + N ₂ → O + N ₂ O OXYGEN MOLECULE + NITROGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: k ₁ = Kk ₋₁	1200-2000	6.3(+13)	0	55200±2000	0.4 2.5
O ₂ + NO → O + NO ₂ OXYGEN MOLECULE + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 2. NOTE: k ₁ = Kk ₋₁	300-550	1.7(+12)	0	23400	0.8 1.3
O ₂ + NO + NO → NO ₂ + NO ₂ OXYGEN MOLECULE + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 3.	273-660	1.2(+ 9)	0	-530±100	0.5 1.5
O ₂ + NO + NO ₂ → NO ₂ + NO ₃ OXYGEN MOLECULE + NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 3.	300-500	2.9(+ 7)	0	-400±500	0.4 2.5
O ₂ + C → O + CO OXYGEN MOLECULE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
O ₂ + CO → O + CO ₂ OXYGEN MOLECULE + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K.	1500-3000	2.5(+12)	0	24000±2500	0.5 2.0
O ₂ + CH → O + .CHO OXYGEN MOLECULE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3 3.2
O ₂ + CH ₂ → O + HCHO OXYGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.		5.0(+11)	0.5	3500±2500	0.3 3.2
O ₂ + CH ₃ → O + CH ₃ O. OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	15100±1500	
O ₂ + CH ₃ → OH + HCHO OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+13)	0	10000±5000	0.3 3.2
O ₂ + CH ₃ → HO ₂ + :CH ₂ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED	1500-2500	3.2(+12)	0	34975±1500	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F		
$O_2 + \cdot CHO \rightarrow HO_2 + CO$ OXYGEN MOLECULE + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.6(+12)	0	3500±1500			
$O_2 + CH_3O \cdot \rightarrow HO_2 + HCHO$ OXYGEN MOLECULE + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+12)	0	3000±1500			
$O_2 + CN \rightarrow CO + NO$ OXYGEN MOLECULE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0	0±5000	0.3	3.2	
$O_2 + M \rightarrow O + O + M$ OXYGEN MOLECULE 76 BAU/DRY REACTION ORDER: 2.	2500-8000 2000-10000	3.5(+25) 9.8(+24)	-2.5 -2.5	59380 59380	0.5 0.4	2.0 2.5	
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT $\approx 8000K$. M: O ₂ M: Ar	3000-18000	1.8(+18)	-1.0	59380±4900	0.5	2.0	
$O_3 + O \rightarrow O_2 + O_2$ OZONE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 AT $\approx 1000K$	200-500	5.2(+12)	0	2090±260	0.5	1.5	
$O_3 + H \rightarrow O_2 + OH$ OZONE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	300	1.6(+13)	-	-	0.5	2.0	
$O_3 + OH \rightarrow O_2 + HO_2$ OZONE + HYDROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2.	300	3.9(+10)	-	-	0.5	1.5	
$O_3 + HO_2 \rightarrow O_2 + O_2 + OH$ OZONE + HYDROPEROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2.	298	9.1(+ 8)	-	-	0.5	1.5	
$O_3 + H_2S \rightarrow SO_2 + H_2O$ OZONE + HYDROGEN SULFIDE 76 BAU/DRY REACTION ORDER: 2.	298	4.0(+ 2)	-	-	0.1	10.	
$O_3 + NO \rightarrow O_2 + NO_2$ OZONE + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 2.	200-350	8.9(+11)	0	1330±130	0.5	1.5	
$O_3 + NO_2 \rightarrow O_2 + NO_3$ OZONE + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 2.	286-302	5.9(+12)	0	3500	0.5	2.0	
$O_3 + M \rightarrow O + O_2 + M$ OZONE 76 BAU/DRY REACTION ORDER: 2. M: Ar	200-1000	2.48(+14)	0	11430±120	0.8	1.3	
$H + O + M \rightarrow OH + M$ HYDROGEN ATOM + OXYGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	7.9(+15)	0	0	0.1	10.	
$H + O_2 \rightarrow OH + O$ HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	700-2500	2.2(+14)	0	8450±250	0.7	1.3	
$D + O_2 \rightarrow OD + O$ DEUTERIUM ATOM + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	800-1000	8.9(+13)	0	7500			
$H + O_2 + M \rightarrow HO_2 + M$ HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 3. M: H ₂	300-2000	5.0(+15)	0	-500±250	0.5	1.5	
NOTE: M eff: H ₂ (1.0)							
	M: O ₂	300-2000	2.0(+15)	0	-500±250	0.5	1.5
O ₂ (0.4)							
	M: H ₂ O	300-2000	3.2(+16)	0	-500±250	0.5	1.5
H ₂ O(6.4)							

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions			T/K	A	B	E/R (in K)	k factors f F	
He(0.3). $k_1 = Kk_{-1}$	M: He	300-2000	1.5(+15)	0	-500±250	0.5	1.5	
Ar(0.3). $k_1 = Kk_{-1}$	M: Ar	300-2000	1.5(+15)	0	-500±250	0.5	1.5	
N ₂ (0.4)	M: N ₂	300-2000	2.0(+15)	0	-500±250	0.5	1.5	
CO ₂ (1.5)	M: CO ₂	300-2000	7.5(+15)	0	-500±250	0.5	1.5	
H + O ₃ → OH + O ₂ HYDROGEN ATOM + OZONE 76 BAU/DRY	REACTION ORDER: 2.	300	1.6(+13)	-	-	0.5	2.0	
H + H + M → H ₂ + M HYDROGEN ATOM 72 BAU/DRY	REACTION ORDER: 3.	M: H ₂ 300 M: H ₂ 2500-5000	3.0(+15) 2.6(+15)	- -1.0	- 0	0.5 0.4	1.5 2.5	
NOTE: M eff: H ₂ (1.0)	M: Ar	2500-5000	6.4(+17)	-1.0	0	0.4	2.5	
Ar(0.25). $k_1 = Kk_{-1}$								
H + H ₂ → H ₂ + H HYDROGEN ATOM + HYDROGEN MOLECULE 75 BEN/GOL	REACTION ORDER: 2.		6.3(+11)	0.5	4000			
H + D ₂ → DH + D HYDROGEN ATOM + DEUTERIUM MOLECULE 72 KON	REACTION ORDER: 2.	368-1000	3.1(+13)	0	4485±250	0.6	1.6	
D + H ₂ → DH + H DEUTERIUM ATOM + HYDROGEN MOLECULE 72 KON	REACTION ORDER: 2.	400-1000	5.0(+13)	0	3890±40	0.9	1.1	
H + OH → H ₂ + O HYDROGEN ATOM + HYDROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2.	400-2000	8.3(+9)	1.0	3500±150	0.7	1.3	
H + OH → OH + H HYDROGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL	REACTION ORDER: 2.		6.3(+11)	0.5	0			
H + OH + M → H ₂ O + M HYDROGEN ATOM + HYDROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 3.	M: H ₂ O 1000-3000	1.4(+23)	-2.0	0	0.7	1.5	
NOTE: M eff: H ₂ O(1.0). $k_1 = Kk_{-1}$	M: Ar	1000-3000	8.4(+21)	-2.0	0	0.5	2.0	
Ar(0.06)	M: N ₂	1000-3000	2.2(+22)	-2.0	0	0.5	2.0	
N ₂ (0.16)								
H + HO ₂ → O + H ₂ O HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 74 LLO	REACTION ORDER: 2.	300-1000	5. (+13)	0	500	0.3	3.2	
NOTE: E ESTIMATED. 76 ENG		1500-2500	1.0(+13)	0	500±500	0.1	1.0	
H + HO ₂ → H ₂ + O ₂ HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2.	290-800 1500-2500	2.5(+13) 2.5(+13)	0 0	350±350 350±350	0.4 0.5	2.5 2.0	
76 ENG								
H + HO ₂ → OH + OH HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2.	290-800 1500-2500	2.5(+14) 2.5(+14)	0 0	950±350 950±500	0.5 0.5	2.0 2.0	
76 ENG								
H + H ₂ O → OH + H ₂ HYDROGEN ATOM + WATER 72 BAU/DRY	REACTION ORDER: 2.	300-2500	9.3(+13)	0	10250±100	0.5	1.5	
NOTE: ERROR LIMITS ARE 50% FOR UPPER T'S.								
H + H ₂ O ₂ → H ₂ + HO ₂ HYDROGEN ATOM + HYDROGEN PEROXIDE 72 BAU/DRY	REACTION ORDER: 2.	300-800	1.7(+12)	0	1900±250	0.5	2.0	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A'	B	E/R (in K)	k factors f F	
$H + S_2 \rightarrow SH + S$ HYDROGEN ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		7.9(+12)	0.5	8355		
$H + SO \rightarrow OH + S$ HYDROGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	11200		
$H + SO \rightarrow SH + O$ HYDROGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	19930		
$H + SO_2 + M \rightarrow HSO_2 + M$ HYDROGEN ATOM + SULFUR DIOXIDE 76 BAU/DRY REACTION ORDER: 3.	1660-2120	5.1(+15)	-	-	0.5	1.5
$H + SH \rightarrow H_2 + S$ HYDROGEN ATOM + MERCAPTO FREE RADICAL 76 BAU/DRY REACTION ORDER: 2.	298	1.5(+13)	-	-	0.5	1.5
$H + SH \rightarrow SH + H$ HYDROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$H + H_2S \rightarrow H_2 + SH$ HYDROGEN ATOM + HYDROGEN SULFIDE 76 BAU/DRY REACTION ORDER: 2.	190-470	7.8(+12)	0	860±50	0.5	1.5
$H + N + M \rightarrow NH + M$ HYDROGEN ATOM + NITROGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	2.5(+17)	-0.5	0±1000	0.1	10.
$H + N_2 \rightarrow NH + N$ HYDROGEN ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	75945		
$H + NO \rightarrow OH + N$ HYDROGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	24460		
$H + NO \rightarrow NH + O$ HYDROGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	38200		
$H + NO + M \rightarrow HNO + M$ HYDROGEN ATOM + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 3.	230-700	5.4(+15)	0	-300±100	0.5	1.5
$H + NO + M \rightarrow HNO + M$ HYDROGEN ATOM + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 3. M: H ₂	1500-2500	5.0(+15)	0	-300±150	0.5	2.0
$H + NO_2 \rightarrow OH + NO$ HYDROGEN ATOM + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 2.	298-630	3.5(+14)	0	740±500	0.5	1.5
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT T = 633K.						
$H + NO_2 \rightarrow OH + NO$ HYDROGEN ATOM + NITROGEN OXIDE(NO ₂) 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+14)	0	750±500	0.5	2.0
$H + N_2O \rightarrow OH + N_2$ HYDROGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2.	700-2500	7.6(+13)	0	7600±500	0.5	1.5
$H + N_2O \rightarrow NH + NO$ HYDROGEN ATOM + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	15100±2500	0.3	3.2
$H + NH \rightarrow H_2 + N$ HYDROGEN ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$H + NH \rightarrow NH + H$ HYDROGEN ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$H + NH_2 + M \rightarrow NH_3 + M$ HYDROGEN ATOM + AMIDOGEN FREE RADICAL 73 BAU/DRY REACTION ORDER: 3. M: Ar NOTE: $k_1 = Kk_{-1}$	2000-3000	4.8(+14)	0	-8300±2500	0.5	2.0
$H + NH_2NH_2 \rightarrow H_2 + NH_2NH$ HYDROGEN ATOM + HYDRAZINE 73 BAU/DRY REACTION ORDER: 2.	250-500	1.3(+13)	0	1260±100	0.5	2.0
$H + HNO \rightarrow H_2 + NO$ HYDROGEN ATOM + NITROSYL HYDRIDE 73 BAU/DRY REACTION ORDER: 2.	2000	4.8(+12)	-	-	0.5	1.5
$H + HNO \rightarrow OH + NH$ HYDROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	11600±2500	0.3	3.2
$H + NS \rightarrow SH + N$ HYDROGEN ATOM + NITROGEN SULFIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	15700		
$H + NS \rightarrow NH + S$ HYDROGEN ATOM + NITROGEN SULFIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	20735		
$H + CO \rightarrow OH + C$ HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	77755		
$H + CO \rightarrow CH + O$ HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		2.5(+13)	0.5	88020		
$H + CO + M \rightarrow \cdot CHO + M$ HYDROGEN ATOM + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 3. M: H ₂ NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 773K.	298-773	6.9(+14)	0	850±500	0.7	1.3
76 ENG	1500-2500	1.6(+20)	-1.5	0	0.3	3.2
$H + CO_2 \rightarrow OH + CO$ HYDROGEN ATOM + CARBON DIOXIDE 76 BAU/DRY REACTION ORDER: 2.	1000-3000	1.5(+14)	0	13300±150	0.8	1.2
$H + CH \rightarrow H_2 + C$ HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$H + CH \rightarrow CH + H$ HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$H + CH + M \rightarrow CH_2 + M$ HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+19)	-1.0	0	0.3	3.2
$H + CH_2 \rightarrow H_2 + CH$ HYDROGEN ATOM + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.7	2500±2500	0.3	3.2
$H + CH_4 \rightarrow H_2 + CH_3$ HYDROGEN ATOM + METHANE 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+13)	0	5990±150	0.5	2.0
$D + CH_4 \rightarrow DH + CH_3$ DEUTERIUM ATOM + METHANE 72 KON REACTION ORDER: 2.	523-673	8.3(+12)	0	5100		
$H + \cdot CHO \rightarrow H_2 + CO$ HYDROGEN ATOM + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.6(+12)	0.5	0±2500	0.3	3.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{H} + \text{HCHO} \rightarrow \text{H}_2 + \cdot\text{CHO}$ HYDROGEN ATOM + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.3(+10)	1.0	1600	0.3 3.2
$\text{H} + \text{CH}_3\text{O} \cdot \rightarrow \text{H}_2 + \text{HCHO}$ HYDROGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	0±1500	
$\text{H} + \text{CS} \rightarrow \text{C} + \text{SH}$ HYDROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	48870	
$\text{H} + \text{CS} \rightarrow \text{CH} + \text{S}$ HYDROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+13)	0.5	50930	
$\text{H} + \text{COS} \rightarrow \text{HS} + \text{CO}$ HYDROGEN ATOM + CARBON OXIDE SULFIDE 76 BAU/DRY REACTION ORDER: 2.	298	1.3(+10)	—	—	0.8 1.3
$\text{H} + \text{CN} \rightarrow \text{C} + \text{NH}$ HYDROGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.0(+13)	0.5	52745	
$\text{H} + \text{CN} \rightarrow \text{CH} + \text{N}$ HYDROGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+12)	0.5	49775	
$\text{H} + \text{CN} + \text{M} \rightarrow \text{HCN} + \text{M}$ HYDROGEN ATOM + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	3.2(+16)	-0.5	0±2500	0.3 3.2
$\text{H} + \text{C}_2 \rightarrow \text{CH} + \text{C}$ HYDROGEN ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		1.6(+13)	0.5	30450	
$\text{H} + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\cdot$ HYDROGEN ATOM + ETHENE 72 KER/PAR REACTION ORDER: 2.	298	9.3(+13)	0	1410	
$\text{H} + \text{CH}_2=\text{CH}_2 + \text{M} \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{M}$ HYDROGEN ATOM + ETHENE 72 KON REACTION ORDER: 3.	298-813	5.6(+17)	0.5	495	
$\text{H} + \text{CH}_3\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\cdot$ HYDROGEN ATOM + ETHANE 72 KON REACTION ORDER: 2.	285-1440	1.0(+14)	0	4815±70	0.8 1.2
$\text{H} + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH} + \text{CH}_3\text{C}(\cdot)=\text{CH}_2$ HYDROGEN ATOM + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. NOTE: k TAKEN AS LOWER LIMIT.	298	0.5(+11)	—	—	
$\text{H} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ HYDROGEN ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	298	7.2(+12)	0	1460	
$\text{H} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_3$ HYDROGEN ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. NOTE: ARRHENIUS PARAMETERS ARE MINIMUM VALUES OF THEIR HIGH-PRESSURE LIMITS.	298	7.2(+12)	0	605	
$\text{H} + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CH}\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ HYDROGEN ATOM + PROPANE 72 KON REACTION ORDER: 2.	333-933	1.0(+13)	0	3130±180	0.7 1.4
$\text{H} + (\text{CH}_3)_2\text{CO} \rightarrow \text{H}_2 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\cdot$ HYDROGEN ATOM + 2-PROPANONE 72 KON REACTION ORDER: 2.	298-873	4.6(+13)	0	4220±20	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$H + CH_2=CHCH=CH_2 \rightarrow CH_2=CHCH(\cdot)CH_3 + CH_2=CHCH_2CH_2\cdot$ HYDROGEN ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGED RATE CONSTANT.	298	4.10(+13)	0	655	
$H + CH_2=CHCH=CH_2 \rightarrow CH_2=CHCH(\cdot)CH_3 + CH_2=CHCH_2CH_2\cdot$ HYDROGEN ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 4.9 NOTE: k_{ref} : $H + CH_3CH=CH_2$	300	-	-	-	
$H + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CH(\cdot)CH_3 + CH_3CH_2CH_2CH_2\cdot$ HYDROGEN ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.03 NOTE: k_{ref} : $H + CH_3CH=CH_2$	300	-	-	-	
	298	8.7(+11)	-	-	
$H + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CH_2CH_2\cdot$ HYDROGEN ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	5.0(+10)	-	-	
$H + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CH(\cdot)CH_3$ HYDROGEN ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	8.1(+11)	-	-	
$H + cis-CH_3CH=CHCH_3 \rightarrow CH_3CH_2CH(\cdot)CH_3$ HYDROGEN ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION. k/k_{ref} : 0.47	298	4.6(+11)	-	-	
	300	-	-	-	
$H + trans-CH_3CH=CHCH_3 \rightarrow CH_3CH_2CH(\cdot)CH_3$ HYDROGEN ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGE k k/k_{ref} : 0.59	298	5.6(+11)	-	-	
	300	-	-	-	
$H + (CH_3)_2C=CH_2 \rightarrow (CH_3)_3C\cdot$ HYDROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	3.10(+13)	0	755	
$H + (CH_3)_2C=CH_2 \rightarrow (CH_3)_2CHCH_2\cdot$ HYDROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 0.5% NON-TERMINAL ADDITION OF H TO $(CH_3)_2C=CH_2$.	298	1.3(+11)	-	-	
$H + (CH_3)_2C=CH_2 \rightarrow (CH_3)_3C\cdot + (CH_3)_2CHCH_2\cdot$ HYDROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.52 NOTE: k_{ref} : $H + CH_3CH=CH_2$	300	-	-	-	
$H + CH_3CH_2CH_2CH_3 \rightarrow H_2 + CH_3CH_2CH(\cdot)CH_3 + CH_3CH_2CH_2CH_2\cdot$ HYDROGEN ATOM + BUTANE 72 KON REACTION ORDER: 2.	320-930	4.1(+12)	0	2637±320	0.5 2.0
$H + (CH_3)_3CH \rightarrow H_2 + (CH_3)_3C\cdot + (CH_3)_2CHCH_2\cdot$ HYDROGEN ATOM + PROPANE, 2-METHYL- 72 KON REACTION ORDER: 2.	300-800	1.9(+13)	0	2680±85	0.8 1.2
$H + CH_3CH_2CH_2CH=CH_2 \rightarrow CH_3CH_2CH_2CH(\cdot)CH_3$ $+ CH_3CH_2CH_2CH_2CH_2\cdot$ HYDROGEN ATOM + 1-PENTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 0.89 NOTE: k_{ref} : $H + CH_3CH=CH_2$.	298 300	8.3(+11) -	- -	- -	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{H} + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ HYDROGEN ATOM + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.39$	298 300	3.8(+11) —	— —	— —		
NOTE: $k_{\text{ref}}: \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$.						
$\text{H} + \text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ HYDROGEN ATOM + trans-2-PENTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.44$	298 300	4.1(+11) —	— —	— —		
NOTE: $k_{\text{ref}}: \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$.						
$\text{H} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ HYDROGEN ATOM + 1-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	9.1(+11)	—	—		
$\text{D} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$ $+ \text{CH}_3\text{CH}_2\text{CD}(\text{CH}_3)\text{CH}_2\cdot$ DEUTERIUM ATOM + 1-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	2.0(+12)	—	—		
$\text{H} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ $+ (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ HYDROGEN ATOM + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	7.4(+11)	—	—		
$\text{D} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{D}$ $+ (\text{CH}_3)_2\text{CHCHDCH}_2\cdot$ DEUTERIUM ATOM + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	7.6(+11)	—	—		
$\text{H} + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ $+ (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ HYDROGEN ATOM + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.03$	298 300	9.1(+11) —	— —	— —		
NOTE: $k_{\text{ref}}: \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$						
$\text{H} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHC}(\cdot)(\text{CH}_3)_2$ HYDROGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.84$	298 300	7.8(+11) —	— —	— —		
NOTE: $k_{\text{ref}}: \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$						
$\text{H} + (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2\cdot$ $+ (\text{CH}_3)_3\text{CC}(\cdot)(\text{CH}_3)_2$ HYDROGEN ATOM + 1-BUTENE, 2,3,3-TRIMETHYL- 72 KER/PAR REACTION ORDER: 2.	298	1.6(+12)	—	—		
NOTE: TENTATIVE VALUE BASED ON REACTION: $\text{H} + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
$\text{H}_2 + \text{O} \rightarrow \text{H} + \text{OH}$ HYDROGEN MOLECULE + OXYGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	400–2000	1.8(+10)	1.0	4480±150	0.7	1.3
$\text{D}_2 + \text{O} \rightarrow \text{D} + \text{OD}$ DEUTERIUM MOLECULE + OXYGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	416–968	2.0(+13)	0	5500	0.5	2.0
$\text{H}_2 + \text{O}_2 \rightarrow \text{H} + \text{HO}_2\cdot$ HYDROGEN MOLECULE + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	290–800	5.5(+13)	0	29100±350	0.4	2.5
$\text{H}_2 + \text{O}_2 \rightarrow \text{OH} + \text{OH}$ HYDROGEN MOLECULE + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500–2500	2.5(+12)	0	19630±5000	0.1	10.
$\text{H}_2 + \text{H} \rightarrow \text{H} + \text{H}_2$ HYDROGEN MOLECULE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{H}_2 + \text{D} \rightarrow \text{H} + \text{HD}$ HYDROGEN MOLECULE + DEUTERIUM ATOM 72 KON REACTION ORDER: 2.	400-1000	5.0(+13)	0	3890±40	0.9	1.1
$\text{D}_2 + \text{H} \rightarrow \text{D} + \text{DH}$ DEUTERIUM MOLECULE + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	1000	3.1(+13)	0	4485±250	0.6	1.6
$\text{H}_2 + \text{OH} \rightarrow \text{H} + \text{H}_2\text{O}$ HYDROGEN MOLECULE + HYDROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 FOR T :300K T >300K	300-2500	2.2(+13)	0	2590±100	0.8	1.2
$\text{D}_2 + \text{OH} \rightarrow \text{D} + \text{DHO}$ DEUTERIUM MOLECULE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-623	1.9(+13)	0	2904±280	0.5	2.0
$\text{H}_2 + \text{HO}_2 \rightarrow \text{H} + \text{H}_2\text{O}_2$ HYDROGEN MOLECULE + HYDROPEROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2.	300-800	7.3(+11)	0	9400±250	0.5	2.0
$\text{H}_2 + \text{S} \rightarrow \text{H} + \text{SH}$ HYDROGEN MOLECULE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$ 75 BEN/GOL	298	1.3(- 1)	-	-	0.5	1.5
		2.5(+12)	0.5	13640		
$\text{H}_2 + \text{N} \rightarrow \text{H} + \text{NH}$ HYDROGEN MOLECULE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	18700		
$\text{H}_2 + \text{C} \rightarrow \text{H} + \text{CH}$ HYDROGEN MOLECULE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	15700		
$\text{H}_2 + \text{CO}_2 \rightarrow \text{H}_2\text{O} + \text{CO}$ HYDROGEN MOLECULE + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+ 9)	0.5	7550±2500	0.3	3.2
$\text{H}_2 + \text{CH}_2 \rightarrow \text{H} + \text{CH}_3$ HYDROGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	3525±1500		
$\text{H}_2 + \text{CH}_3 \rightarrow \text{H} + \text{CH}_4$ HYDROGEN MOLECULE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	370-700	8.5(+11)	0	5500±500	0.7	1.3
$\text{H}_2 + \text{CD}_3 \rightarrow \text{H} + \text{CD}_3\text{H}$ HYDROGEN MOLECULE + METHYL-D ₃ -FREE RADICAL 72 KON REACTION ORDER: 2.	400-570	7.4(+11)	0	5250±235	0.6	1.7
$\text{DH} + \text{CH}_3 \rightarrow \text{H} + \text{CH}_3\text{D}$ DEUTERIUM HYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-700	2.4(+11)	0	5635±500	0.5	1.5
$\text{DH} + \text{CH}_3 \rightarrow \text{D} + \text{CH}_4$ DEUTERIUM HYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-700	2.1(+11)	0	5300±500	0.5	1.5
$\text{D}_2 + \text{CH}_3 \rightarrow \text{D} + \text{CH}_3\text{D}$ DEUTERIUM MOLECULE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-700	7.1(+11)	0	5990±250	0.7	1.3
$\text{H}_2 + \text{CN} \rightarrow \text{H} + \text{HCN}$ HYDROGEN MOLECULE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	2500±1500		
$\text{H}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{H} + \text{CH}_3\text{CH}_3$ HYDROGEN MOLECULE + ETHYL FREE RADICAL 72 KON REACTION ORDER: 2.	473-823	3.0(+11)	0	5435		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{H}_2 + \text{M} \rightarrow \text{H} + \text{H} + \text{M}$ HYDROGEN MOLECULE 72 BAU/DRY NOTE: $k_1 = Kk_{-1}$ REACTION ORDER: 2. M: Ar	2500-5000	2.2(+14)	0	48300±2000	0.5 2.0
$\text{OH} + \text{O} \rightarrow \text{O} + \text{OH}$ HYDROXYL FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{OH} + \text{O} \rightarrow \text{H} + \text{O}_2$ HYDROXYL FREE RADICAL + OXYGEN ATOM 72 BAU/DRY NOTE: k_1 CALCULATED FROM $k_{-1}K$ IS: $1.3 \times 10^{13} \text{cc.mole}^{-1}\text{s}^{-1}$ REACTION ORDER: 2.	300	2.3(+13)	-	-	0.6 1.4
$\text{OH} + \text{O} \rightarrow \text{H} + \text{O}_2$ HYDROXYL FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	2.5(+13)	0	0	0.5 2.0
$\text{OH} + \text{O} + \text{M} \rightarrow \text{HO}_2 + \text{M}$ HYDROXYL FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+17)	0	0	0.01 100.
$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$ HYDROXYL FREE RADICAL + OZONE 76 BAU/DRY REACTION ORDER: 2.	300	3.9(+10)	-	-	0.5 1.5
$\text{OH} + \text{H} \rightarrow \text{O} + \text{H}_2$ HYDROXYL FREE RADICAL + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	400-2000	8.3(+ 9)	1.0	3500±150	0.7 1.3
$\text{OH} + \text{H} \rightarrow \text{H} + \text{OH}$ HYDROXYL FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{OH} + \text{H} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M}$ HYDROXYL FREE RADICAL + HYDROGEN ATOM 72 BAU/DRY NOTE: M eff: $\text{H}_2\text{O}(1.0)$. $k_1 = Kk_{-1}$ Ar(0.06) $\text{N}_2(0.16)$ REACTION ORDER: 3. M: H_2O	1000-3000	1.4(+23)	-2.0	0	0.7 1.5
	1000-3000	8.4(+21)	-2.0	0	0.5 2.0
	1000-3000	2.2(+22)	-2.0	0	0.5 2.0
$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$ HYDROXYL FREE RADICAL + HYDROGEN MOLECULE 72 BAU/DRY NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 FOR T > 300K REACTION ORDER: 2.	300-2500	2.2(+13)	0	2590±100	0.8 1.2
$\text{OH} + \text{D}_2 \rightarrow \text{DHO} + \text{D}$ HYDROXYL FREE RADICAL + DEUTERIUM MOLECULE 72 KON REACTION ORDER: 2.	300-623	1.9(+13)	0	2904±280	0.5 2.0
$\text{OH} + \text{OH} \rightarrow \text{HO}_2 + \text{H}$ HYDROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2.	290-800	1.2(+13)	0	20200±350	0.5 2.0
$\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$ HYDROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2.	300-2000	6.3(+12)	0	550±200	0.7 1.5
$\text{OH} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O}_2 + \text{M}$ HYDROXYL FREE RADICAL 72 BAU/DRY NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 1500K. REACTION ORDER: 3. M: N_2	700-1500	9.1(+14)	0	2550±1000	0.8 1.3
$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{HO}_2$ HYDROXYL FREE RADICAL + HYDROGEN PEROXIDE 72 BAU/DRY REACTION ORDER: 2.	300-800	1.0(+13)	0	910±150	0.5 1.5
$\text{OH} + \text{S} \rightarrow \text{O} + \text{SH}$ HYDROXYL FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	12700	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{OH} + \text{S} \rightarrow \text{H} + \text{SO}$ HYDROXYL FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{OH} + \text{H}_2\text{S} \rightarrow \text{H}_2\text{O} + \text{HS}$ HYDROXYL FREE RADICAL + HYDROGEN SULFIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS INCREASING TO: f = 0.5; F = 1.5 AT 900K.	298-900	6.3(+12)	0	200±150	0.7	1.3
$\text{OH} + \text{N} \rightarrow \text{O} + \text{NH}$ HYDROXYL FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	17765		
$\text{OH} + \text{N} \rightarrow \text{H} + \text{NO}$ HYDROXYL FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{OH} + \text{N} + \text{M} \rightarrow \text{HNO} + \text{M}$ HYDROXYL FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+15)	-0.5	0		
$\text{OH} + \text{NO}_2 + \text{M} \rightarrow \text{HNO}_3 + \text{M}$ HYDROXYL FREE RADICAL + NITROGEN OXIDE(NO_2) 73 BAU/DRY REACTION ORDER: 3.	300	5.0(+17)	-	-	0.4	1.6
$\text{OH} + \text{N}_2\text{O} \rightarrow \text{HO}_2 + \text{N}_2$ HYDROXYL FREE RADICAL + NITROGEN OXIDE(N_2O) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+13)	0	7550		
$\text{OH} + \text{NH} \rightarrow \text{H}_2\text{O} + \text{N}$ HYDROXYL FREE RADICAL AND IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	1000±2500	0.3	3.2
$\text{OH} + \text{HNO} \rightarrow \text{H}_2\text{O} + \text{NO}$ HYDROXYL FREE RADICAL + NITROSYL HYDRIDE 73 BAU/DRY REACTION ORDER: 2.	2000	3.6(+13)	-	-	0.5	1.5
$\text{OH} + \text{HNO}_3 \rightarrow \text{H}_2\text{O} + \text{NO}_3$ HYDROXYL FREE RADICAL + NITRIC ACID 73 BAU/DRY REACTION ORDER: 2.	300	8.0(+10)	-	-	0.5	2.0
$\text{OH} + \text{C} \rightarrow \text{O} + \text{CH}$ HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		7.9(+11)	0.5	14800		
$\text{OH} + \text{C} \rightarrow \text{H} + \text{CO}$ HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{OH} + \text{CO} \rightarrow \text{H} + \text{CO}_2$ HYDROXYL FREE RADICAL + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS OVER 1000K: f = 0.5; F = 1.5. RECOMMENDED k FOR 250-2500K: $\log(k) \text{ccmol}^{-1}\text{s}^{-1} = 10.83 + 3.94^{-4}T$	250-2000	1.5(+ 7)	1.3	- 385	0.8	1.2
$\text{OH} + \text{CH} \rightarrow \text{H} + \text{.CHO}$ HYDROXYL FREE RADICAL AND METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.		5.0(+11)	0.5	5000±2500	0.3	3.2
$\text{OH} + \text{CH}_2 \rightarrow \text{O} + \text{CH}_3$ HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
$\text{OH} + \text{CH}_2 \rightarrow \text{H} + \text{HCHO}$ HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+13)	0	2517		
$\text{OH} + \text{CH}_2 \rightarrow \text{H}_2\text{O} + \text{CH}$ HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{OH} + \text{CH}_3 \rightarrow \text{H} + \text{CH}_3\text{O}$ HYDROXYL FREE RADICAL AND METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+12)	0	0		
$\text{OH} + \text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2$ HYDROXYL FREE RADICAL AND METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+10)	0.7	1000±2500	0.3	3.2
$\text{OH} + \text{CH}_4 \rightarrow \text{H}_2\text{O} + \text{CH}_3$ HYDROXYL FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+13)	0	2500±250	0.5	2.0
$\text{OH} + \text{CHO} \rightarrow \text{H}_2\text{O} + \text{CO}$ HYDROXYL FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+10)	1.0	0±1500		
$\text{OH} + \text{CH}_3\text{O} \rightarrow \text{H}_2\text{O} + \text{HCHO}$ HYDROXYL FREE RADICAL + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+13)	0	0±1500		
$\text{OH} + \text{HCHO} \rightarrow \text{H}_2\text{O} + \text{CHO}$ HYDROXYL FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+10)	1.0	0±1500	0.5	2.0
$\text{OH} + \text{CN} \rightarrow \text{O} + \text{HCN}$ HYDROXYL FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+12)	0	1500±1500		
$\text{OH} + \text{HCN} \rightarrow \text{H}_2\text{O} + \text{CN}$ HYDROXYL FREE RADICAL + HYDROCYANIC ACID 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.6	2500±2500	0.3	3.2
$\text{OH} + \text{CH}=\text{CH} \rightarrow \text{H}_2\text{O} + \text{CH}=\text{CH}$ HYDROXYL FREE RADICAL + ETHYNE 72 KON REACTION ORDER: 2.	300-2000	7.6(+12)	0	2335±400	0.5	2.1
$\text{OH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{H}_2\text{O} + \text{CH}_2=\text{CH}$ HYDROXYL FREE RADICAL + ETHENE 72 KON REACTION ORDER: 2.	3500-1400	1.6(+14)	0	2831±445	0.4	2.4
$\text{OH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2\text{CH}_2\text{OH}$ HYDROXYL FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	300	1.1(+12)	-	-	0.8	1.3
$\text{OH} + \text{CH}_3\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2$ HYDROXYL FREE RADICAL + ETHANE 72 KON REACTION ORDER: 2.	302-793	1.3(+14)	0	1998		
$\text{OH} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{OH} + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2$ HYDROXYL FREE RADICAL + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. NOTE: ADDITION TO TERMINAL CARBON OF DOUBLE BOND IS PROBABLY 95%	300	6.6(+12)	-	-		
$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + \text{O}_2 + \text{O}_2$ HYDROPEROXYL FREE RADICAL + OZONE 76 BAU/DRY REACTION ORDER: 2.	298	9.1(+ 8)	-	-	0.5	1.5
$\text{HO}_2 + \text{H} \rightarrow \text{O}_2 + \text{H}_2$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2. 76 ENG	290-800 1500-2500	2.5(+13) 2.5(+13)	0 0	350±350 350±500	0.4 0.5	2.5 2.0
$\text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{O}$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 74 LLO REACTION ORDER: 2. NOTE: E ESTIMATED.	300-1000	5. (+13)	0	500	0.3	3.2
$\text{HO}_2 + \text{H} \rightarrow \text{OH} + \text{OH}$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2. 76 ENG	290-800 1500-2500	2.5(+14) 2.5(+14)	0 0	950±350 956±500	0.5 0.5	2.0 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{O}$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+13)	0	500±500	0.1	10.
$\text{HO}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O}_2 + \text{H}$ HYDROPEROXYL FREE RADICAL + HYDROGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	300-800	7.3(+11)	0	9400±250	0.5	2.0
$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$ HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: E ESTIMATED. k FACTORS ARE LARGER AT T>300K.	300-1000	1.0(+13)	0	500	0.5	2.0
$\text{HO}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{O}_2 + \text{OH}$ HYDROPEROXYL FREE RADICAL + WATER 72 BAU/DRY REACTION ORDER: 2.	300-800	2.8(+13)	0	16500±500	0.5	1.5
$\text{HO}_2 + \text{SO}_2 \rightarrow \text{OH} + \text{SO}_3$ HYDROPEROXYL FREE RADICAL + SULFUR DIOXIDE 74 LLO REACTION ORDER: 2.	300	5.2(+ 8)	-	-	0.9	1.2
$\text{HO}_2 + \text{N} \rightarrow \text{O}_2 + \text{NH}$ HYDROPEROXYL FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0	0±2500	0.3	3.2
$\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$ HYDROPEROXYL FREE RADICAL + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2.	700-1000	1.5(+14)	0	11900±1000	0.3	3.0
$\text{HO}_2 + \text{CH} \rightarrow \text{O}_2 + \text{CH}_2$ HYDROPEROXYL FREE RADICAL AND METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+10)	0.5	7550±2500	0.3	3.2
$\text{HO}_2 + \text{CH} \rightarrow \text{OH} + \text{.CHO}$ HYDROPEROXYL FREE RADICAL AND METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
$\text{HO}_2 + \text{CH}_3 \cdot \rightarrow \text{O}_2 + \text{CH}_4$ HYDROPEROXYL FREE RADICAL AND METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	3000±2500	0.3	3.2
$\text{HO}_2 + \text{.CHO} \rightarrow \text{O}_2 + \text{HCHO}$ HYDROPEROXYL FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	1500±1500		
$\text{HO}_2 + \text{HCHO} \rightarrow \text{H}_2\text{O}_2 + \text{.CHO}$ HYDROPEROXYL FREE RADICAL + FORMALDEHYDE 74 LLO REACTION ORDER: 2. NOTE: k FACTORS ARE: f = 0.1; F = 10. AT 300 K.	300-800	1.0(+12)	0	4000	0.7	1.5
$\text{HO}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{products}$ HYDROPEROXYL FREE RADICAL + ETHENE 74 LLO REACTION ORDER: 2. NOTE: RATIO DATA VERSUS k_{ref} FOR $\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$. k FACTORS MIGHT BE HIGHER.	300	1.0(+ 7)	-	-	0.1	10.
$\text{HO}_2 + \text{CH}_3\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2 \cdot$ HYDROPEROXYL RADICAL + ETHANE 74 LLO REACTION ORDER: 2. NOTE: E ESTIMATED. UPPER LIMIT RECOMMENDED. k_{ref} IS FOR $\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$.	300-1000	1.0(+12)	0	7000	0.1	10.
$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_2\text{CH} \cdot$ HYDROPEROXYL FREE RADICAL + PROPANE 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} FOR $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300-1000	2.0(+11)	0	5300	0.1	10.
$\text{HO}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{products}$ HYDROPEROXYL FREE RADICAL + 1-PROPENE, 2-METHYL- 74 LLO REACTION ORDER: 2. NOTE: SUGGESTED k VALUE.	300	1.0(+ 8)	-	-	0.1	10.

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ HYDROPEROXYL FREE RADICAL + BUTANE 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} FOR $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300-1000	5.0(+11)	0	5285	0.1 10.
$\text{HO}_2 + (\text{CHO})_3\text{CH} \rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_3\text{C}\cdot$ HYDROPEROXYL FREE RADICAL + PROPANE, 2-METHYL 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} FOR $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300-1000	1.0(+11)	0	3500	0.1 10.
$\text{HO}_2 + \text{M} \rightarrow \text{H} + \text{O}_2 + \text{M}$ HYDROPEROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2. NOTE: M = AR, OR He. $k_1 = Kk_{-1}$	300-2000	2.1(+15)	0	23000±250	0.5 1.5
$\text{H}_2\text{O} + \text{O} \rightarrow \text{OH} + \text{OH}$ WATER + OXYGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	300-2000	6.8(+13)	0	9240±200	0.7 1.5
$\text{H}_2\text{O} + \text{H} \rightarrow \text{H}_2 + \text{OH}$ WATER + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2. NOTE: GIVEN k FACTORS ARE FOR HIGH T'S.	300-2500	9.3(+13)	0	10250±100	0.5 1.5
$\text{H}_2\text{O} + \text{HO}_2 \rightarrow \text{OH} + \text{H}_2\text{O}_2$ WATER + HYDROPEROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2.	300-800	2.8(+13)	0	16500±500	0.5 1.5
$\text{H}_2\text{O} + \text{NH} \rightarrow \text{H}_2 + \text{HNO}$ WATER + IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	1500±2500	0.3 3.2
$\text{H}_2\text{O} + \text{CH}_3\cdot \rightarrow \text{OH} + \text{CH}_4$ WATER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	1273-1773	7.1(+12)	0	12900±1000	0.5 2.0
$\text{H}_2\text{O} + \text{M} \rightarrow \text{H} + \text{OH} + \text{M}$ WATER 72 BAU/DRY REACTION ORDER: 2. M: H_2O	2000-6000	2.2(+16)	0	52900±2500	0.7 1.5
NOTE: M eff: $\text{H}_2\text{O}(1.0)$. $k_1 = Kk_{-1}$					
Ar(0.06)					
M: Ar	2000-6000	1.3(+15)	0	52900±2500	0.5 2.0
M: N_2	2000-6000	3.5(+15)	0	52900±2500	0.5 2.0
$\text{N}_2(0.16)$					
$\text{H}_2\text{O}_2 + \text{H} \rightarrow \text{HO}_2 + \text{H}_2$ HYDROGEN PEROXIDE + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	300-800	1.7(+12)	0	1900±250	0.5 2.0
$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{HO}_2 + \text{H}_2\text{O}$ HYDROGEN PEROXIDE + HYDROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2.	300-800	1.0(+13)	0	910±150	0.5 1.5
$\text{H}_2\text{O}_2 + \text{M} \rightarrow \text{OH} + \text{OH} + \text{M}$ HYDROGEN PEROXIDE 72 BAU/DRY REACTION ORDER: 2. M: N_2	700-1500	1.20(+17)	0	22900±1000	0.8 1.3
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 1500K.					
$\text{S} + \text{O}_2 \rightarrow \text{SO} + \text{O}$ SULFUR ATOM + OXYGEN MOLECULE 76 BAU/DRY REACTION ORDER: 2.	250-450	1.4(+12)	0	0.0±50	0.5 1.5
$\text{S} + \text{H}_2 \rightarrow \text{SH} + \text{H}$ SULFUR ATOM + HYDROGEN MOLECULE 76 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$	298	1.3(-1)	-	-	0.5 1.5
75 BEN/GOL		2.5(+12)	0.5	13640	
$\text{S} + \text{OH} \rightarrow \text{SO} + \text{H}$ SULFUR ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$S + OH \rightarrow SH + O$ SULFUR ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	12700	
$S + S_2 \rightarrow S_2 + S$ SULFUR ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$S + SO \rightarrow S_2 + O$ SULFUR ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	11500	
$S + SO \rightarrow SO + S$ SULFUR ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$S + SH \rightarrow S_2 + H$ SULFUR ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$S + SH \rightarrow SH + S$ SULFUR ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$S + N_2 \rightarrow NS + N$ SULFUR ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	55200	
$S + NO \rightarrow SO + N$ SULFUR ATOM + NITROGEN OXIDE (NO) 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	17260	
$S + NO \rightarrow NS + O$ SULFUR ATOM + NITROGEN OXIDE (NO) 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	17465	
$S + NH \rightarrow SH + N$ SULFUR ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$S + NH \rightarrow NS + H$ SULFUR ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$S + NS \rightarrow S_2 + N$ SULFUR ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	10870	
$S + NS \rightarrow NS + S$ SULFUR ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$S + CO \rightarrow SO + C$ SULFUR ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	66530	
$S + CO \rightarrow CS + O$ SULFUR ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	37600	
$S + CH \rightarrow SH + C$ SULFUR ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$S + CH \rightarrow CS + H$ SULFUR ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$S + CS \rightarrow S_2 + C$ SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	40463	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
S + CS → CS + S SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
S + CS + M → CS ₂ + M SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 76 BAU/DRY REACTION ORDER: 3. NOTE: k ₁ = Kk ₋₁	1800-3700	8.7(+13)	0	4370	0.5	1.5
S + CS ₂ → S ₂ + CS SULFUR ATOM + CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2.	298	3.9(+11)	-	-	0.5	1.5
S + COS → S ₂ + CO SULFUR ATOM + CARBON OXIDE SULFIDE 76 BAU/DRY REACTION ORDER: 2.	230-2600	1.7(+12)	0	2050±230	0.3	3.0
S + CN → NS + C SULFUR ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		2.0(+12)	0.5	32010		
S + CN → CS + N SULFUR ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
S + C ₂ → CS + C SULFUR ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
S + CH≡CH → cy-CH=CHS SULFUR ATOM + ETHYNE 72 KER/PAR REACTION ORDER: 2.	298	1.7(+11)	-	-		
S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S SULFUR ATOM + ETHENE 72 KER/PAR REACTION ORDER: 2.	298	8.1(+11)	-	-		
S + CH ₃ C≡CH → cy-(CH ₃)C=CHS SULFUR ATOM + 1-PROPYLENE 72 KER/PAR REACTION ORDER: 2.	298	1.1(+12)	-	-		
S + CH ₃ CH=CH ₂ → cy-(CH ₃)CHCH ₂ S SULFUR ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 6.9	298 298	5.8(+12) -	- -	- -		
NOTE: k _{ref} : S + CH ₂ =CH ₂						
S* (¹ D) + CH ₃ CH=CH ₂ → cy-(CH ₃)CHCH ₂ S SULFUR ATOM (¹ D) + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 1.7 NOTE: k _{ref} : S* (¹ D) + CH ₂ =CH ₂	300	-	-	-		
S + CH ₃ C≡CCH ₃ → cy-(CH ₃)C=C(CH ₃)S SULFUR ATOM + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2.	298	1.9(+13)	-	-		
S + CH ₂ =CHCH=CH ₂ → cy-(CH ₂ =CH)CHCH ₂ S SULFUR ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2.	298	6.0(+13)	-	-		
S + CH ₃ CH ₂ CH=CH ₂ → cy-(CH ₃ CH ₂)CHCH ₂ S SULFUR ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 10.0	298 298	9.3(+12) -	- -	- -		
NOTE: k _{ref} : S + CH ₂ =CH ₂						
S + cis-CH ₃ CH=CHCH ₃ → cy-(CH ₃)CHCH(CH ₃)S SULFUR ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 16.0	298 298	1.4(+13) -	- -	- -		
NOTE: k _{ref} : S + CH ₂ =CH ₂						

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$S + \text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow \text{cy-(CH}_3\text{)CHCH(CH}_3\text{)S}$ SULFUR ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 20.0	298 298	1.4(+13) -	- -	- -		
NOTE: k _{ref} : S + CH ₂ =CH ₂						
$S + (\text{CH}_3)_2\text{C=CH}_2 \rightarrow \text{cy-(CH}_3)_2\text{CCH}_2\text{S}$ SULFUR ATOM + 1-PROPENE, 2-METHYL 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 50.0	298 298	4.0(+13) -	- -	- -		
NOTE: k _{ref} : S + CH ₂ =CH ₂						
$S^*(^1\text{D}) + (\text{CH}_3)_2\text{C=CH}_2 \rightarrow \text{cy-(CH}_3)_2\text{CCH}_2\text{S}$ SULFUR ATOM (¹ D) + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 3.5	300	-	-	-		
NOTE: k _{ref} : S [*] (¹ D) + CH ₂ =CH ₂						
$S + \text{CH}_3(\text{CH}_2)_2\text{CH=CH}_2 \rightarrow \text{cy-CH}_3(\text{CH}_2)\text{CHCH}_2\text{S}$ SULFUR ATOM + 1-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	8.1(+12)	-	-		
$S + \text{CH}_3\text{CH}_2\text{C(CH}_3\text{)=CH}_2 \rightarrow \text{cy-CH}_3\text{CH}_2\text{C(CH}_3\text{)CH}_2\text{S}$ SULFUR ATOM + 1-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	7.4(+13)	-	-		
$S + (\text{CH}_3)_2\text{C=CHCH}_3 \rightarrow \text{cy-(CH}_3)_2\text{CCH(CH}_3\text{)S}$ SULFUR ATOM + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 56.	298 298	6.5(+13) -	- -	- -		
NOTE: k _{ref} : S + CH ₂ =CH ₂						
$S + (\text{CH}_3)_2\text{C=C(CH}_3)_2 \rightarrow \text{cy-(CH}_3)_2\text{CC(CH}_3)_2\text{S}$ SULFUR ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.	298	8.5(+13)	-	-		
$S_2 + O \rightarrow S + SO$ SULFUR DIMER + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$S_2 + H \rightarrow S + SH$ SULFUR DIMER + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		7.9(+12)	0.5	8355		
$S_2 + S \rightarrow S + S_2$ SULFUR DIMER + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$S_2 + N \rightarrow S + NS$ SULFUR DIMER + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$S_2 + C \rightarrow S + CS$ SULFUR DIMER + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$SO + O \rightarrow O + SO$ SULFUR MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$SO + O \rightarrow S + O_2$ SULFUR MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	2770		
$SO + O + M \rightarrow SO_2 + M$ SULFUR MONOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3.	298	6.7(+13)	-	-	0.7	1.3
$SO + O_2 \rightarrow SO_2 + O$ SULFUR MONOXIDE + OXYGEN MOLECULE 76 BAU/DRY REACTION ORDER: 2.	440-2100	4.5(+11)	0	3250±590	0.3	1.7
$SO + H \rightarrow O + SH$ SULFUR MONOXIDE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	19930		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{SO} + \text{H} \rightarrow \text{S} + \text{OH}$ SULFUR MONOXIDE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	11200	
$\text{SO} + \text{S} \rightarrow \text{O} + \text{S}_2$ SULFUR MONOXIDE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	11500	
$\text{SO} + \text{S} \rightarrow \text{S} + \text{SO}$ SULFUR MONOXIDE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{SO} + \text{N} \rightarrow \text{O} + \text{NS}$ SULFUR MONOXIDE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	8254	
$\text{SO} + \text{N} \rightarrow \text{S} + \text{NO}$ SULFUR MONOXIDE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{SO} + \text{C} \rightarrow \text{O} + \text{CS}$ SULFUR MONOXIDE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{SO} + \text{C} \rightarrow \text{S} + \text{CO}$ SULFUR MONOXIDE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{SO}_2 + \text{O} \rightarrow \text{SO} + \text{O}_2$ SULFUR DIOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$	440-2100	1.3(+14)	-0.5	9980	0.3 1.7
$\text{SO}_2 + \text{H} + \text{M} \rightarrow \text{HSO}_2 + \text{M}$ SULFUR DIOXIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 3.	1660-2120	5.1(+15)	-	-	0.5 1.5
$\text{SO}_2 + \text{HO}_2 \rightarrow \text{SO}_3 + \text{OH}$ SULFUR DIOXIDE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: RATIO DATA VERSUS k_{ref} FOR REACTION $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300	5.2(+ 8)	-	-	0.9 1.2
$\text{SH} + \text{O} \rightarrow \text{S} + \text{OH}$ MERCAPTO FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{SH} + \text{O} \rightarrow \text{SO} + \text{H}$ MERCAPTO FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{SH} + \text{H} \rightarrow \text{S} + \text{H}_2$ MERCAPTO FREE RADICAL + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	298	1.5(+13)	-	-	0.5 1.5
$\text{SH} + \text{H} \rightarrow \text{H} + \text{SH}$ MERCAPTO FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{SH} + \text{S} \rightarrow \text{H} + \text{S}_2$ MERCAPTO FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{SH} + \text{S} \rightarrow \text{S} + \text{SH}$ MERCAPTO FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(P11)	0.5	4000	
$\text{SH} + \text{SH} \rightarrow \text{H}_2\text{S} + \text{S}$ MERCAPTO FREE RADICAL 76 BAU/DRY REACTION ORDER: 2.	295	7.8(+12)	-	-	0.5 1.5
$\text{SH} + \text{N} \rightarrow \text{H} + \text{NS}$ MERCAPTO FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	403	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{SH} + \text{N} \rightarrow \text{S} + \text{NH}$ MERCAPTO FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	9060		
$\text{SH} + \text{C} \rightarrow \text{H} + \text{CS}$ MERCAPTO FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{SH} + \text{C} \rightarrow \text{S} + \text{CH}$ MERCAPTO FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	6090		
$\text{H}_2\text{S} + \text{O}_3 \rightarrow \text{H}_2\text{O} + \text{SO}_2$ HYDROGEN SULFIDE + OZONE 76 BAU/DRY REACTION ORDER: 2.	298	4.0(+ 2)	-	-	0.1	10.
$\text{H}_2\text{S} + \text{H} \rightarrow \text{SH} + \text{H}_2$ HYDROGEN SULFIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	190-470	7.8(+12)	0	860±50	0.5	1.5
$\text{H}_2\text{S} + \text{OH} \rightarrow \text{SH} + \text{H}_2\text{O}$ HYDROGEN SULFIDE + HYDROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 900K.	298-900	6.3(+12)	0	200±150	0.7	1.3
$\text{H}_2\text{S} + \text{CH}_3 \cdot \rightarrow \text{SH} + \text{CH}_4$ HYDROGEN SULFIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-600	2.00(+11)	0	2065±150	0.4	2.5
$\text{N} + \text{O} + \text{M} \rightarrow \text{NO} + \text{M}$ NITROGEN ATOM + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: N ₂	200-400	6.4(+16)	-0.5	0	0.5	1.5
$\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$ NITROGEN ATOM + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 3000K.	300-3000	6.4(+ 9)	1.0	3150±150	0.7	1.3
$\text{N} + \text{H} + \text{M} \rightarrow \text{NH} + \text{M}$ NITROGEN ATOM + HYDROGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	2.5(+17)	-0.5	0±1000		
$\text{N} + \text{H}_2 \rightarrow \text{NH} + \text{H}$ NITROGEN ATOM + HYDROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	18700		
$\text{N} + \text{OH} \rightarrow \text{NO} + \text{H}$ NITROGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{N} + \text{OH} \rightarrow \text{NH} + \text{O}$ NITROGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	17765		
$\text{N} + \text{OH} + \text{M} \rightarrow \text{HNO} + \text{M}$ NITROGEN ATOM + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	1.00(+15)	-0.5	0		
$\text{N} + \text{HO}_2 \rightarrow \text{NH} + \text{O}_2$ NITROGEN ATOM + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.00(+11)	0	0±2500	0.3	3.2
$\text{N} + \text{S}_2 \rightarrow \text{NS} + \text{S}$ NITROGEN ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{N} + \text{SO} \rightarrow \text{NO} + \text{S}$ NITROGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{N} + \text{SO} \rightarrow \text{NS} + \text{O}$ NITROGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	8254		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$N + SH \rightarrow NH + S$ NITROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	9060		
$N + SH \rightarrow NS + H$ NITROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	403		
$N + N + M \rightarrow N_2 + M$ NITROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: N_2 NOTE: k FACTORS RANGE: 200-600K, BUT MIGHT INCREASE AT LOWER T'S.	100-600	3.0(+14)	0	- 500±50	0.5	1.5
$N + N_2 \rightarrow N_2 + N$ NITROGEN ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$N + NO \rightarrow N_2 + O$ NITROGEN ATOM + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGE TO: f = 0.5; F = 2.0 ABOVE 2000K.	300-5000	1.6(+13)	0	0	0.8	1.2
$N + NO \rightarrow NO + N$ NITROGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$N + NO_2 \rightarrow N_2 + O_2$ NITROGEN ATOM + NITROGEN OXIDE(NO ₂) 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+12)	0	0±1500		
$N + NO_2 \rightarrow NO + NO$ NITROGEN ATOM + NITROGEN OXIDE(NO ₂) 76 ENG REACTION ORDER: 2.	1500-2500	4.0(+12)	0	0±1500	0.2	5.0
$N + NO_2 \rightarrow N_2O + O$ NITROGEN ATOM + NITROGEN OXIDE(NO ₂) 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+12)	0	0±1500	0.5	2.0
$N + N_2O \rightarrow NO + N_2$ NITROGEN ATOM + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+ 8)	0	5000±2500	0.3	3.2
$N + NH \rightarrow N_2 + H$ NITROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$N + NH \rightarrow NH + N$ NITROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$N + HNO \rightarrow H + N_2O$ NITROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+10)	0.5	1500±2500		
$N + HNO \rightarrow NH + NO$ NITROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	1000±2500		
$N + NS \rightarrow N_2 + S$ NITROGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$N + NS \rightarrow NS + N$ NITROGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$N + CO \rightarrow NO + C$ NITROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	57300		
$N + CO \rightarrow CN + O$ NITROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		3.2(+12)	0.5	38800		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{N} + \text{CO}_2 \rightarrow \text{NO} + \text{CO}$ NITROGEN ATOM + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500–2500	2.00(+11)	0.5	1500±10000	0.1 10.
$\text{N} + \text{CH} \rightarrow \text{NH} + \text{C}$ NITROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	6995	
$\text{N} + \text{CH} \rightarrow \text{CN} + \text{H}$ NITROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{N} + \text{CH}_2 \rightarrow \text{NH} + \text{CH}$ NITROGEN ATOM + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	6.3(+11)	0.67	20400±2500	0.3 3.2
$\text{N} + \text{CHO} \rightarrow \text{O} + \text{HCN}$ NITROGEN ATOM + FORMYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.0(+14)	0	0	
$\text{N} + \text{CHO} \rightarrow \text{NH} + \text{CO}$ NITROGEN ATOM + FORMYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	2.0(+11)	0.5	1000±2500	
$\text{N} + \text{CH}_3\text{O} \cdot \rightarrow \text{NH} + \text{HCHO}$ NITROGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+14)	0	0±1500	
$\text{N} + \text{CS} \rightarrow \text{C} + \text{NS}$ NITROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	37200	
$\text{N} + \text{CS} \rightarrow \text{CN} + \text{S}$ NITROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	1160	
$\text{N} + \text{CN} \rightarrow \text{N}_2 + \text{C}$ NITROGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{N} + \text{C}_2 \rightarrow \text{CN} + \text{C}$ NITROGEN ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{N} + \text{CH}=\text{CH} \rightarrow \text{C}_2\text{H}_2\text{N}$ NITROGEN ATOM + ETHYNE 72 KER/PAR REACTION ORDER: 2. NOTE: UPPER LIMIT.	440	2.0(+ 9)	–	–	
$\text{N} + \text{CH}_2=\text{CH}_2 \rightarrow \text{products}$ NITROGEN ATOM + ETHENE 72 KER/PAR REACTION ORDER: 2.	320–550	2.0(+10)	0	353	
$\text{N} + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow \text{products}$ NITROGEN ATOM + 1-PROPYLE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 6.5	320–550 435	6.9(+10) –	0 –	745 –	
NOTE: k _{ref} : N + CH=CH					
$\text{N} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}$ NITROGEN ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 2.8	320–550 435	1.2(+11) –	0 –	655 –	
NOTE: k _{ref} : N + CH ₂ =CH ₂					
$\text{N} + \text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{products}$ NITROGEN ATOM + 1-BUTYNE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 13.0	320–550 435	3.5(+11) –	0 –	1125 –	
NOTE: k _{ref} : N + CH≡CH					

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{N} + \text{CH}_3\text{C}\equiv\text{CCH}_3 \rightarrow \text{products}$ NITROGEN ATOM + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 12.0	320-550 435	1.9(+11) -	0 -	926 -		
NOTE: k_{ref} : $\text{N} + \text{CH}\equiv\text{CH}$.						
$\text{N} + \text{CH}_2=\text{CHCH}=\text{CH}_2 \rightarrow \text{products}$ NITROGEN ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2.	340	3.5(+10)	-	-		
$\text{N} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$ NITROGEN ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 3.4	320-550 435	1.6(+11) -	0 -	660 -		
NOTE: k_{ref} : $\text{N} + \text{CH}_2=\text{CH}_2$.						
$\text{N} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ NITROGEN ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.4	320-550 435	2.3(+11) -	0 -	995 -		
NOTE: k_{ref} : $\text{N} + \text{CH}_2=\text{CH}_2$						
$\text{N} + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ NITROGEN ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 3.0	320-550 435	3.4(+11) -	0 -	1055 -		
NOTE: k_{ref} : $\text{N} + \text{CH}_2=\text{CH}_2$						
$\text{N} + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{products}$ NITROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 4.1	320-550 435	7.8(+10) -	0 -	277 -		
NOTE: k_{ref} : $\text{N} + \text{CH}_2=\text{CH}_2$						
$\text{N} + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{products}$ NITROGEN ATOM + 1-PENTYNE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 14.0	320-550 435	3.0(+11) -	0 -	1047 -		
NOTE: k_{ref} : $\text{N} + \text{CH}\equiv\text{CH}$						
$\text{N} + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{products}$ NITROGEN ATOM + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 3.5	320-550 435	9.3(+10) -	0 -	433 -		
NOTE: k_{ref} : $\text{N} + \text{CH}_2=\text{CH}_2$						
$\text{N} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{products}$ NITROGEN ATOM + 1-HEXYNE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 14.0	320-55 435	4.6(+11) -	0 -	1233 -		
NOTE: k_{ref} : $\text{N} + \text{CH}\equiv\text{CH}$						
$\text{N} + \text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_2\text{CH}_3 \rightarrow \text{products}$ NITROGEN ATOM + 3-HEXYNE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 14.0	320-550 435	3.4(+11) -	0 -	1102 -		
NOTE: k_{ref} : $\text{N} + \text{CH}\equiv\text{CH}$						
$\text{N} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$ NITROGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 3.5	320-550 435	1.7(+11) -	0 -	690 -		
NOTE: k_{ref} : $\text{N} + \text{CH}_2=\text{CH}_2$						
$\text{N}_2 + \text{O} \rightarrow \text{N} + \text{NO}$ NITROGEN MOLECULE + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	2000-5000	7.6(+13)	0	38000±150	0.5	2.0
NOTE: $k_1 = Kk_{-1}$						
$\text{N}_2 + \text{O} + \text{M} \rightarrow \text{N}_2\text{O} + \text{M}$ NITROGEN MOLECULE + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: Ar	1300-2500	1.4(+13)	0	10400±1500	0.7	1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$N_2 + O_2 \rightarrow N_2O + O$ NITROGEN MOLECULE + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$	1200–2000	6.3(+13)	0	55200±2000	0.4 2.5
$N_2 + H \rightarrow N + NH$ NITROGEN MOLECULE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	75945	
$N_2 + S \rightarrow N + NS$ NITROGEN MOLECULE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	55200	
$N_2 + N \rightarrow N + N_2$ NITROGEN MOLECULE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$N_2 + C \rightarrow N + CN$ NITROGEN MOLECULE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	22750	
$N_2 + CH \rightarrow N + HCN$ NITROGEN MOLECULE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: REVISED ESTIMATE.	1500–2500	1.0(+11)	0	9560	
$N_2 + CH \rightarrow NH + CN$ NITROGEN MOLECULE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+14)	0	46300±10000	
$N_2 + CH_2 \rightarrow NH + HCN$ NITROGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.0(+14)	0	35230±10000	
$N_2 + M \rightarrow N + N + M$ NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. M: N_2 73 BAU/DRY	1500–2500 6000–15000	4.0(+21) 3.7(+21)	–1.6 –1.6	13240±500 113200±500	0.3 3.0
$NO + O \rightarrow O + NO$ NITROGEN OXIDE(NO) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$NO + O \rightarrow N + O_2$ NITROGEN OXIDE(NO) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS INCREASING TO: f = 0.5; F = 2.0 AT 3000K. $k_1 = Kk_{-1}$	1000–3000	1.5(+ 9)	1.0	19500±150	0.7 1.3
$NO + O + M \rightarrow NO_2 + M$ NITROGEN OXIDE(NO) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: O_2 NOTE: M eff: $O_2(1.0)$ AT 297K	200–500	1.1(+15)	0	–940±50	0.8 1.2
Ar(0.1) AT 297K	M: Ar 200–500	1.1(+14)	0	–940±50	0.8 1.2
H ₂ O(6.1) AT 297K	M: H ₂ O 200–500	6.7(+15)	0	–940±50	0.8 1.2
D ₂ O(5.0) AT 297K	M: D ₂ O 200–500	5.5(+15)	0	–940±50	0.8 1.2
SF ₆ (2.6) AT 297K	M: SF ₆ 200–500	2.9(+15)	0	–940±50	0.8 1.2
N ₂ (1.4) AT 297K	M: N ₂ 200–500	1.5(+15)	0	–940±50	0.8 1.2
N ₂ O(2.1) AT 297K	M: N ₂ O 200–500	2.3(+15)	0	–940±50	0.8 1.2
CO ₂ (2.1) AT 297K	M: CO ₂ 200–500	2.3(+15)	0	–940±50	0.8 1.2
CH ₄ (2.2) AT 297K	M: CH ₄ 200–500	2.4(+15)	0	–940±50	0.8 1.2
CF ₄ (2.2) AT 297K	M: CF ₄ 200–500	2.4(+15)	0	–940±50	0.8 1.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{NO} + \text{O}_2 \rightarrow \text{NO}_2 + \text{O}$ NITROGEN OXIDE(NO) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = Kk_{-1}$	300-550	1.7(+12)	0	23400	0.8	1.3
$\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$ NITROGEN OXIDE(NO) + OZONE 73 BAU/DRY REACTION ORDER: 2.	200-350	8.9(+11)	0	1330±130	0.5	1.5
$\text{NO} + \text{H} \rightarrow \text{O} + \text{NH}$ NITROGEN OXIDE(NO) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	38200		
$\text{NO} + \text{H} \rightarrow \text{N} + \text{OH}$ NITROGEN OXIDE(NO) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	24460		
$\text{NO} + \text{H} + \text{M} \rightarrow \text{HNO} + \text{M}$ NITROGEN OXIDE(NO) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: H_2 76 ENG M: H_2	230-700 1500-2500	5.4(+15) 5.0(+15)	0 0	-300±100 -300±150	0.5 0.5	1.5 2.0
$\text{NO} + \text{S} \rightarrow \text{O} + \text{NS}$ NITROGEN OXIDE(NO) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	17465		
$\text{NO} + \text{S} \rightarrow \text{N} + \text{SO}$ NITROGEN OXIDE(NO) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	17260		
$\text{NO} + \text{N} \rightarrow \text{O} + \text{N}_2$ NITROGEN OXIDE(NO) + NITROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 ABOVE 2000K	300-5000	1.6(+13)	-	-	0.8	1.2
$\text{NO} + \text{N} \rightarrow \text{N} + \text{NO}$ NITROGEN OXIDE(NO) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NO} + \text{NO} \rightarrow \text{N}_2 + \text{O}_2$ NITROGEN OXIDE(NO_2) + OXYGEN MOLECULE 72 KON REACTION ORDER: 2.	1370-4300	1.3(+14)	0	38060±720	0.7	1.5
$\text{NO} + \text{NO} \rightarrow \text{N}_2\text{O} + \text{O}$ NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 2.	1200-2000	1.3(+12)	0	32100±1500	0.5	2.0
$\text{NO} + \text{NO} + \text{O}_2 \rightarrow \text{NO}_2 + \text{NO}_2$ NITROGEN OXIDE(NO) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 3.	273-660	1.2(+ 9)	0	-530±100	0.5	1.5
$\text{NO} + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{O}_2$ NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO_2) 76 ENG REACTION ORDER: 2.	1500-2500	1.0 (+12)	0	30200	0.01	100.
$\text{NO} + \text{NO}_2 + \text{O}_2 \rightarrow \text{NO}_2 + \text{NO}_3$ NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO_2) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 3.	300-500	2.9(+ 7)	0	-400±500	0.4	2.5
$\text{NO} + \text{NO}_3 \rightarrow \text{NO}_2 + \text{NO}_2$ NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO_3) 72 KON REACTION ORDER: 2.	298-547	1.5(+14)	0	1163±115	0.7	1.4
$\text{NO} + \text{N}_2\text{O} \rightarrow \text{NO}_2 + \text{N}_2$ NITROGEN OXIDE(NO) + NITROGEN OXIDE(N_2O) 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+14)	0	25000	0.1	1.0
$\text{NO} + \text{HNO} \rightarrow \text{N}_2\text{O} + \text{OH}$ NITROGEN OXIDE(NO) + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+12)	0	13000±2500	0.5	2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{NO} + \text{C} \rightarrow \text{O} + \text{CN}$ NITROGEN OXIDE(NO) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{NO} + \text{C} \rightarrow \text{N} + \text{CO}$ NITROGEN OXIDE(NO) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NO} + \text{CH} \rightarrow \text{O} + \text{HCN}$ NITROGEN OXIDE(NO) + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	2.0(+12)	0	0±1000		
$\text{NO} + \text{CH} \rightarrow \text{N} + \text{CHO}$ NITROGEN OXIDE(NO) + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.6(+13)	0	5000±3000		
$\text{NO} + \text{CH}_2 \rightarrow \text{N} + \text{HCHO}$ NITROGEN OXIDE(NO) + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.6(+12)	0	3500±2000		
$\text{NO} + \text{CHO} \rightarrow \text{HNO} + \text{CO}$ NITROGEN OXIDE(NO) + FORMYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	1000±2500	0.3	3.2
$\text{NO} + \text{CN} \rightarrow \text{N}_2 + \text{CO}$ NITROGEN OXIDE(NO) + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0	0±2500	0.3	3.2
$\text{NO} + \text{M} \rightarrow \text{N} + \text{O} + \text{M}$ NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: M = Ar, OR N ₂ OR O ₂ . GIVEN WITH CAUTION. 72 KON	1500-2500	4.0(+20)	-1.5	75500±2500	0.3	3.2
	M: Ar 3000-8000	8.00(+2)	-1.5	75500		
$\text{NO}_2 + \text{O} \rightarrow \text{NO} + \text{O}_2$ NITROGEN OXIDE(NO ₂) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2. 76 ENG	300-550 1500-2500	1.0(+13) 1.0(+13)	0 0	300±100 500±250	0.8 0.5	1.3 2.0
$\text{NO}_2 + \text{O} + \text{M} \rightarrow \text{NO}_3 + \text{M}$ NITROGEN OXIDE(NO ₂) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2. M: N ₂ NOTE: LIMITING HIGH PRESSURE k REACTION ORDER: 3. k ₀ (LOW PRESSURE).	295 295	1.1(+13) 2.3(+16)	- -	- -	0.4 0.4	2.5 2.5
$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$ NITROGEN OXIDE(NO ₂) + OZONE 73 BAU/DRY REACTION ORDER: 2.	286-302	5.9(+12)	0	3500	0.5	2.0
$\text{NO}_2 + \text{H} \rightarrow \text{NO} + \text{OH}$ NITROGEN OXIDE(NO ₂) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 633K. 76 ENG	298-630 1500-2500	3.5(+14) 3.2(+14)	0 0	740±500 750±500	0.5 0.5	1.5 2.0
$\text{NO}_2 + \text{OH} + \text{M} \rightarrow \text{HNO}_3 + \text{M}$ NITROGEN OXIDE(NO ₂) + HYDROXYL FREE RADICAL 73 BAU/DRY REACTION ORDER: 3. M: He	300	5.0(+17)	-	-	0.4	1.6
$\text{NO}_2 + \text{N} \rightarrow \text{O} + \text{N}_2\text{O}$ NITROGEN OXIDE(NO ₂) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+12)	0	0±1500	0.5	2.0
$\text{NO}_2 + \text{N} \rightarrow \text{O}_2 + \text{N}_2$ NITROGEN OXIDE(NO ₂) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+12)	0	0±1500	0.5	2.0
$\text{NO}_2 + \text{N} \rightarrow \text{NO} + \text{NO}$ NITROGEN OXIDE(NO ₂) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	4.0(+12)	0	0±1500	0.2	5.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{NO}_2 + \text{NO} \rightarrow \text{O}_2 + \text{N}_2\text{O}$ NITROGEN OXIDE(NO_2) + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+12)	0	30200	0.01 100.
$\text{NO}_2 + \text{NO} + \text{O}_2 \rightarrow \text{NO}_3 + \text{NO}_2$ NITROGEN OXIDE(NO_2) + NITROGEN OXIDE(NO) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 3.	300-500	2.9(+7)	0	-400±500	0.4 2.5
$\text{NO}_2 + \text{NO}_2 \rightarrow \text{NO} + \text{NO} + \text{O}_2$ NITROGEN OXIDE(NO_2) 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS INCREASING SLIGHTLY ABOVE 1000K.	600-2000	2.0(+12)	0	13500±100	0.7 1.3
$\text{NO}_2 + \text{NO}_2 + \text{M} \rightarrow \text{N}_2\text{O}_4 + \text{M}$ NITROGEN OXIDE(NO_2) 73 BAU/DRY REACTION ORDER: 3. M: N_2 NOTE: CORRECTED k VALUE (PERSONAL COMMUNICATION FROM DR. BAULCH TO DR. HAMPSON). $k_1 = Kk_{-1}$	250-350	1.1(+13)	0	-1040	0.7 1.3
$\text{NO}_2 + \text{NO}_3 \rightarrow \text{NO} + \text{NO}_2 + \text{O}_2$ NITROGEN OXIDE(NO_2) + NITROGEN OXIDE(NO_3) 73 BAU/DRY REACTION ORDER: 2.	300-850	1.4(+11)	0	1610±500	0.4 2.5
$\text{NO}_2 + \text{NO}_3 + \text{M} \rightarrow \text{N}_2\text{O}_5 + \text{M}$ NITROGEN OXIDE(NO_2) + NITROGEN OXIDE(NO_3) 73 BAU/DRY REACTION ORDER: 2.	300	2.3(+12)	-	-	0.4 2.5
NOTE: LIMITING HIGH PRESSURE k M IS A N_2O_5 + NO MIXTURE REACTION ORDER: 3. k_0 (LOW PRESSURE). M IS A N_2O_5 + NO MIXTURE.	300	1.0(+18)	-	-	0.5 2.0
$\text{NO}_2 + \text{NH} \rightarrow \text{NO} + \text{HNO}$ NITROGEN OXIDE(NO_2) + IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	2500±2500	0.3 3.2
$\text{NO}_2 + \text{CO} \rightarrow \text{NO} + \text{CO}_2$ NITROGEN OXIDE(NO_2) + CARBON MONOXIDE 72 KON REACTION ORDER: 2. 76 ENG	500-800 1500-2500	1.9(+12) 2.00(+12)	0 0	14726±385 15000±1500	0.5 1.9 0.5 2.0
$\text{NO}_2 + \text{M} \rightarrow \text{NO} + \text{O} + \text{M}$ NITROGEN OXIDE(NO_2) 73 BAU/DRY REACTION ORDER: 2. M: Ar	1400-2400	1.1(+16)	0	33000±750	0.8 1.3
$\text{NO}_3 + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2$ NITROGEN OXIDE(NO_3) + NITROGEN OXIDE(NO) 72 KON REACTION ORDER: 2.	298-547	1.5(+14)	0	1160±120	0.7 1.4
$\text{NO}_3 + \text{NO}_2 \rightarrow \text{NO}_2 + \text{NO} + \text{O}_2$ NITROGEN OXIDE(NO_3) + NITROGEN OXIDE(NO_2) 73 BAU/DRY REACTION ORDER: 2.	300-850	1.4(+11)	0	1600±500	0.4 2.5
$\text{NO}_3 + \text{NO}_2 + \text{M} \rightarrow \text{N}_2\text{O}_5 + \text{M}$ NITROGEN OXIDE(NO_3) + NITROGEN OXIDE(NO_2) 72 BAU/DRY REACTION ORDER: 2.	300	2.3(+12)	-	-	0.4 2.5
NOTE: LIMITING HIGH-PRESSURE k. M IS A N_2O_5 + NO MIXTURE. $k_1 = Kk_{-1}$ REACTION ORDER: 3. k_0 (LOW PRESSURE). M IS A N_2O_5 + NO MIXTURE.	300	1.0(+18)	-	-	0.5 2.0
$\text{NO}_3 + \text{M} \rightarrow \text{NO} + \text{O}_2 + \text{M}$ NITROGEN OXIDE(NO_3) 72 KON REACTION ORDER: 2. M: NO_2	500-1100	1.9(+11)	0	1990±110	0.8 1.3
$\text{N}_2\text{O} + \text{O} \rightarrow \text{N}_2 + \text{O}_2$ NITROGEN OXIDE(N_2O) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	1200-2000	1.0(+14)	0	14100±2000	0.4 2.5
$\text{N}_2\text{O} + \text{O} \rightarrow \text{NO} + \text{NO}$ NITROGEN OXIDE(N_2O) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2. 72 KON	1200-2000 900-2300	1.0(+14) 3.6(+13)	0 0	14000±1500 13700	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{N}_2\text{O} + \text{H} \rightarrow \text{N}_2 + \text{OH}$ NITROGEN OXIDE(N_2O) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	700-2500	7.6(+13)	0	7600±500	0.5	1.5
$\text{N}_2\text{O} + \text{H} \rightarrow \text{NO} + \text{NH}$ NITROGEN OXIDE(N_2O) + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	15100±2500	0.3	3.2
$\text{N}_2\text{O} + \text{OH} \rightarrow \text{N}_2 + \text{HO}_2$ NITROGEN OXIDE(N_2O) + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+13)	0	7550		
$\text{N}_2\text{O} + \text{N} \rightarrow \text{N}_2 + \text{NO}$ NITROGEN OXIDE(N_2O) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+ 8)	0	5000±2500	0.3	3.2
$\text{N}_2\text{O} + \text{NO} \rightarrow \text{N}_2 + \text{NO}_2$ NITROGEN OXIDE(N_2O) + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+14)	0	25165	0.1	10.
$\text{N}_2\text{O} + \text{CO} \rightarrow \text{N}_2 + \text{CO}_2$ NITROGEN OXIDE(N_2O) + CARBON MONOXIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0	10000±1500	0.5	2.0
$\text{N}_2\text{O} + \text{M} \rightarrow \text{N}_2 + \text{O} + \text{M}$ NITROGEN OXIDE(N_2O) 73 BAU/DRY REACTION ORDER: 2.	1300-2500	5.0(+14)	0	29000±1500	0.7	1.5
$\text{N}_2\text{O}_4 \rightarrow \text{NO}_2 + \text{NO}_2$ NITROGEN OXIDE(N_2O_4) 70 BEN/O'N REACTION ORDER: 1.	253-301	1.0(+16)	0	6600		
$\text{N}_2\text{O}_4 + \text{M} \rightarrow \text{NO}_2 + \text{NO}_2 + \text{M}$ NITROGEN OXIDE(N_2O_4) 73 BAU/DRY REACTION ORDER: 2. M: N_2	250-350	2.5(+17)	0	5550±500	0.7	1.3
$\text{N}_2\text{O}_5 + \text{M} \rightarrow \text{NO}_2 + \text{NO}_3 + \text{M}$ NITROGEN OXIDE (N_2O_5) 73 BAU/DRY REACTION ORDER: 1. NOTE: LIMITING HIGH-PRESSURE k. M IS A N_2O_5 + NO MIXTURE. REACTION ORDER: 2. k_0 (LOW PRESSURE). M IS A N_2O_5 + NO MIXTURE.	300-340	5.7(+14)	0	10600	0.4	2.5
		1.3(+19)	0	9700	0.5	2.0
$\text{NH} + \text{O} \rightarrow \text{H} + \text{NO}$ IMIDOGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{NH} + \text{O} \rightarrow \text{N} + \text{OH}$ IMIDOGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NH} + \text{O} + \text{M} \rightarrow \text{HNO} + \text{M}$ IMIDOGEN FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+16)	-0.5	0±2500	0.3	3.2
$\text{NH} + \text{H} \rightarrow \text{H} + \text{NH}$ IMIDOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{NH} + \text{H} \rightarrow \text{N} + \text{H}_2$ IMIDOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NH} + \text{OH} \rightarrow \text{N} + \text{H}_2\text{O}$ IMIDOGEN FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	1000±2500	0.3	3.2
$\text{NH} + \text{H}_2\text{O} \rightarrow \text{HNO} + \text{H}_2$ IMIDOGEN FREE RADICAL + WATER 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	1500±2500	0.3	3.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{NH} + \text{S} \rightarrow \text{H} + \text{NS}$ IMIDOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{NH} + \text{S} \rightarrow \text{N} + \text{SH}$ IMIDOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NH} + \text{N} \rightarrow \text{H} + \text{N}_2$ IMIDOGEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{NH} + \text{N} \rightarrow \text{N} + \text{NH}$ IMIDOGEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NH} + \text{NO}_2 \rightarrow \text{HNO} + \text{NO}$ IMIDOGEN FREE RADICAL + NITROGEN OXIDE(NO_2) 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	2500±2500	0.3	3.2
$\text{NH} + \text{NH} \rightarrow \text{H}_2 + \text{N}_2$ IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+13)	0	0	0.1	10.
$\text{NH} + \text{C} \rightarrow \text{H} + \text{CN}$ IMIDOGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{NH} + \text{C} \rightarrow \text{N} + \text{CH}$ IMIDOGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{NH} + \text{CN} \rightarrow \text{N} + \text{HCN}$ IMIDOGEN FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	1000±25000		
$\text{NH}_2 + \text{H} + \text{M} \rightarrow \text{NH}_3 + \text{M}$ AMIDOGEN FREE RADICAL + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: Ar NOTE: $k_1 = Kk_{-1}$	2000-3000	4.8(+14)	0	-8300±2500	0.5	2.0
$\text{NH}_3 + \text{O} \rightarrow \text{NH}_2 + \text{OH}$ AMMONIA + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	300-1000	1.5(+12)	0	3020±300	0.5	1.5
$\text{NH}_3 + \text{CH}_3 \cdot \rightarrow \text{NH}_2 + \text{CH}_4$ AMMONIA + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	1.0(+11)	0	5100±500	0.3	1.3
$\text{ND}_3 + \text{CH}_3 \cdot \rightarrow \text{ND}_2 + \text{CH}_3\text{D}$ AMMONIA-D ₃ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	5535±500	0.3	1.3
$\text{NH}_3 + \text{M} \rightarrow \text{H} + \text{NH}_2 + \text{M}$ AMMONIA 73 BAU/DRY REACTION ORDER: 2. M: Ar	2000-3000	9.2(+15)	0	42400±2500	0.5	2.0
$\text{NH}_2\text{NH}_2 + \text{H} \rightarrow \text{NH}_2\text{NH} \cdot + \text{H}_2$ HYDRAZINE + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	250-500	1.3(+13)	0	1260±100	0.5	2.0
$\text{NH}_2\text{NH}_2 + \text{CH}_3 \cdot \rightarrow \text{NH}_2\text{NH} \cdot + \text{CH}_4$ HYDRAZINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	2515±500	0.5	2.0
$\text{ND}_2\text{ND}_2 + \text{CH}_3 \cdot \rightarrow \text{ND}_2\text{ND} \cdot + \text{CH}_3\text{D}$ HYDRAZINE-D ₄ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	7.2(+10)	0	3200±500	0.5	2.0
$\text{NH}_2\text{NH}_2 + \text{M} \rightarrow \text{NH}_2 \cdot + \text{NH}_2 \cdot + \text{M}$ HYDRAZINE 73 BAU/DRY REACTION ORDER: 2. M: Ar NOTE: LIMITING HIGH PRESSURE k.	1250-1400	8.0(+13)	0	27700±1000	0.3	3.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{NH}_2\text{NH}_2 + \text{M} \rightarrow \text{NH}_2 + \text{NH}_2 + \text{M}$ HYDRAZINE 73 BAU/DRY NOTE: k_0 (LOW PRESSURE). REACTION ORDER: 2. M: Ar	1250-1400	4.0(+15)	0	20600±1000	0.3	3.0
$\text{HN}_3 + \text{CH}_3 \cdot \rightarrow \text{N}_3 \cdot + \text{CH}_4$ HYDRAZOIC ACID + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE. REACTION ORDER: 2.	300-400	1.0(+11)	0	2100±500	0.5	2.0
$\text{HNO} + \text{O} \rightarrow \text{H} + \text{NO}_2$ NITROSYL HYDRIDE + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+10)	0.5	0±2500	0.3	3.2
$\text{HNO} + \text{O} \rightarrow \text{NO} + \text{OH}$ NITROSYL HYDRIDE + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	0±2500	0.3	3.2
$\text{HNO} + \text{O} \rightarrow \text{NH} + \text{O}_2$ NITROSYL HYDRIDE + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	3500±2500	0.3	3.2
$\text{HNO} + \text{H} \rightarrow \text{NO} + \text{H}_2$ NITROSYL HYDRIDE + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	2000	4.8(+12)	-	-	0.5	1.5
$\text{HNO} + \text{H} \rightarrow \text{NH} + \text{OH}$ NITROSYL HYDRIDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	11600±2500	0.3	3.2
$\text{HNO} + \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$ NITROSYL HYDRIDE + HYDROXYL FREE RADICAL 73 BAU/DRY REACTION ORDER: 2.	2000	3.6(+13)	-	-	0.5	1.5
$\text{HNO} + \text{N} \rightarrow \text{NO} + \text{NH}$ NITROSYL HYDRIDE + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	1000±2500	0.3	3.2
$\text{HNO} + \text{N} \rightarrow \text{N}_2\text{O} + \text{H}$ NITROSYL HYDRIDE + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+10)	0.5	1500±2500	0.3	3.2
$\text{HNO} + \text{NO} \rightarrow \text{OH} + \text{N}_2\text{O}$ NITROSYL HYDRIDE + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+12)	0	13100±2500	0.5	2.0
$\text{HNO} + \text{CO} \rightarrow \text{NH} + \text{CO}_2$ NITROSYL HYDRIDE + CARBON MONOXIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	3500±2500	0.3	3.2
$\text{HNO} + \text{CH} \rightarrow \text{NO} + \text{CH}_2$ NITROSYL HYDRIDE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+11)	0.5	0±2500	0.3	3.2
$\text{HNO} + \text{CH}_2 \rightarrow \text{NO} + \text{CH}_3 \cdot$ NITROSYL HYDRIDE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+11)	0.5	0±2500	0.3	3.2
$\text{HNO} + \text{CH}_3 \cdot \rightarrow \text{NO} + \text{CH}_4$ NITROSYL HYDRIDE + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	0±2500	0.3	3.2
$\text{HNO} + \cdot\text{CHO} \rightarrow \text{NO} + \text{HCHO}$ NITROSYL HYDRIDE + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.5	0±2500	0.3	3.2
$\text{HNO} + \text{CN} \rightarrow \text{NO} + \text{HCN}$ NITROSYL HYDRIDE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	4.00(+11)	0.5	0±2500	0.3	3.2
$\text{HNO}_3 + \text{OH} \rightarrow \text{NO}_3 + \text{H}_2\text{O}$ NITRIC ACID + HYDROXYL FREE RADICAL 73 BAU/DRY REACTION ORDER: 2.	300	8.0(+10)	-	-	0.5	2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{HNO}_3 + \text{M} \rightarrow \text{NO}_2 + \text{OH} + \text{M}$ NITRIC ACID 73 BAU/DRY REACTION ORDER: 2. M: Ar	800-1200	1.6(+15)	0	15400±1500	0.4 2.5
$\text{NS} + \text{O} \rightarrow \text{S} + \text{NO}$ NITROGEN SULFIDE(NS) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{NS} + \text{O} \rightarrow \text{N} + \text{SO}$ NITROGEN SULFIDE(NS) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{NS} + \text{H} \rightarrow \text{S} + \text{NH}$ NITROGEN SULFIDE(NS) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	20735	
$\text{NS} + \text{H} \rightarrow \text{N} + \text{SH}$ NITROGEN SULFIDE(NS) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	15700	
$\text{NS} + \text{S} \rightarrow \text{S} + \text{NS}$ NITROGEN SULFIDE(NS) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{NS} + \text{S} \rightarrow \text{N} + \text{S}_2$ NITROGEN SULFIDE(NS) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	10870	
$\text{NS} + \text{N} \rightarrow \text{S} + \text{N}_2$ NITROGEN SULFIDE(NS) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{NS} + \text{N} \rightarrow \text{N} + \text{NS}$ NITROGEN SULFIDE(NS) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{NS} + \text{C} \rightarrow \text{S} + \text{CN}$ NITROGEN SULFIDE(NS) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{NS} + \text{C} \rightarrow \text{N} + \text{CS}$ NITROGEN SULFIDE(NS) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{C} + \text{O} + \text{M} \rightarrow \text{CO} + \text{M}$ CARBON ATOM + OXYGEN ATOM 76 BAU/DRY NOTE: M = Ar, OR CO $k_1 = Kk_{-1}$ REACTION ORDER: 3.	7000-14000	3.3(+26)	-3.1	-2114	0.3 1.8
$\text{C} + \text{O}_2 \rightarrow \text{CO} + \text{O}$ CARBON ATOM + OXYGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{C} + \text{H}_2 \rightarrow \text{CH} + \text{H}$ CARBON ATOM + HYDROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	15700	
$\text{C} + \text{OH} \rightarrow \text{CO} + \text{H}$ CARBON ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{C} + \text{OH} \rightarrow \text{CH} + \text{O}$ CARBON ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		7.9(+11)	0.5	14800	
$\text{C} + \text{S}_2 \rightarrow \text{CS} + \text{S}$ CARBON ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{C} + \text{SO} \rightarrow \text{CO} + \text{S}$ CARBON ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$C + SO \rightarrow CS + O$ CARBON ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + SH \rightarrow CH + S$ CARBON ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	6090	
$C + SH \rightarrow CS + H$ CARBON ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + N_2 \rightarrow CN + N$ CARBON ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	22750	
$C + NO \rightarrow CO + N$ CARBON ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$C + NO \rightarrow CN + O$ CARBON ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + NH \rightarrow CH + N$ CARBON ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$C + NH \rightarrow CN + H$ CARBON ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + NS \rightarrow CS + N$ CARBON ATOM + NITRIC SULFIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$C + NS \rightarrow CN + S$ CARBON ATOM + NITRIC SULFIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + CO \rightarrow C_2 + O$ CARBON ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	58025	
$C + CH \rightarrow CH + C$ CARBON ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$C + CH \rightarrow C_2 + H$ CARBON ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + CS \rightarrow CS + C$ CARBON ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + CS \rightarrow C_2 + S$ CARBON ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		5.0(+11)	0.5	20435	
$C + CN \rightarrow CN + C$ CARBON ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$C + CN \rightarrow C_2 + N$ CARBON ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		2.5(+11)	0.5	19300	
$C + C_2 \rightarrow C_2 + C$ CARBON ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CO} + \text{O} \rightarrow \text{O} + \text{CO}$ CARBON MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CO} + \text{O} + \text{M} \rightarrow \text{CO}_2 + \text{M}$ CARBON MONOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: CO NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 500K.	250-500	2.4(+15)	0	2180±280	0.8	1.2
$\text{CO} + \text{O} \rightarrow \text{C} + \text{O}_2$ CARBON MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	69300		
$\text{CO} + \text{O}_2 \rightarrow \text{CO}_2 + \text{O}$ CARBON MONOXIDE + OXYGEN MOLECULE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K.	1500-3000	2.5(+12)	0	24000±2500	0.5	2.0
$\text{CO} + \text{H} \rightarrow \text{O} + \text{CH}$ CARBON MONOXIDE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+13)	0.5	88020		
$\text{CO} + \text{H} \rightarrow \text{C} + \text{OH}$ CARBON MONOXIDE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	77755		
$\text{CO} + \text{H} + \text{M} \rightarrow \text{CHO} + \text{M}$ CARBON MONOXIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: H ₂ NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 773K.	298-773	7.2(+14)	0	850±500	0.7	1.3
$\text{CO} + \text{H} + \text{M} \rightarrow \text{CHO} + \text{M}$ CARBON MONOXIDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	1.6(+20)	-1.5	0	0.3	3.2
$\text{CO} + \text{OH} \rightarrow \text{CO}_2 + \text{H}$ CARBON MONOXIDE + HYDROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS OVER 1000K: f = 0.5; F = 1.5. RECOMMENDED k FOR 250-2500K: $\log k(\text{cm}^3 \text{mole}^{-1} \text{s}^{-1}) = 10.83 + 3.94 \times 10^{-4} T$	250-2000	1.5(+7)	1.3	-385	0.8	1.2
$\text{CO} + \text{HO}_2 \rightarrow \text{CO}_2 + \text{OH}$ CARBON MONOXIDE + HYDROPEROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2.	700-1000	1.5(+14)	0	11900±1000	0.3	3.0
$\text{CO} + \text{S} \rightarrow \text{O} + \text{CS}$ CARBON MONOXIDE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	37600		
$\text{CO} + \text{S} \rightarrow \text{C} + \text{SO}$ CARBON MONOXIDE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	66530		
$\text{CO} + \text{N} \rightarrow \text{O} + \text{CN}$ CARBON MONOXIDE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		3.2(+12)	0.5	38800		
$\text{CO} + \text{N} \rightarrow \text{C} + \text{NO}$ CARBON MONOXIDE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	57300		
$\text{CO} + \text{NO}_2 \rightarrow \text{CO}_2 + \text{NO}$ CARBON MONOXIDE + NITROGEN OXIDE(NO ₂) 72 KON REACTION ORDER: 2. 76 ENG	500-800 1500-2500	1.9(+12) 2.0(+12)	0 0	14726±385 15000±1500	0.5 0.5	1.9 2.0
$\text{CO} + \text{N}_2\text{O} \rightarrow \text{CO}_2 + \text{N}_2$ CARBON MONOXIDE + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0	10000±1500	0.5	2.0
$\text{CO} + \text{HNO} \rightarrow \text{CO}_2 + \text{NH}$ CARBON MONOXIDE + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	3500±2500	0.3	3.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CO} + \text{C} \rightarrow \text{O} + \text{C}_2$ CARBON MONOXIDE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	58025		
$\text{CO} + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{C}(\text{O}) \cdot$ CARBON MONOXIDE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	273-400	3.8(+ 8)	0	1965		
$\text{CO} + \text{M} \rightarrow \text{C} + \text{O} + \text{M}$ CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: $f = 0.5$; $F = 1.5$ OVER 10000K. M = Ar OR CO	7000-15000	8.8(+29)	-3.5	128700±1800	0.3	1.8
$\text{CO}_2 + \text{O} \rightarrow \text{CO} + \text{O}_2$ CARBON DIOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: $f = 0.5$; $F = 1.5$ AT 3000K. $k_1 = Kk_{-1}$	1500-3000	1.7(+13)	0	26500±2500	0.5	2.0
$\text{CO}_2 + \text{H} \rightarrow \text{CO} + \text{OH}$ CARBON DIOXIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	1000-3000	1.5(+14)	0	13300±150	0.8	1.2
$\text{CO}_2 + \text{H}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$ CARBON DIOXIDE + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+ 9)	0.5	7550±2500	0.3	3.2
$\text{CO}_2 + \text{N} \rightarrow \text{CO} + \text{NO}$ CARBON DIOXIDE + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	15000±10000	0.1	1.0
$\text{CO}_2 + \text{CH} \rightarrow \text{CO} + \cdot\text{CHO}$ CARBON DIOXIDE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+10)	0.5	3000±2500	0.3	3.2
$\text{CO}_2 + \text{M} \rightarrow \text{CO} + \text{O} + \text{M}$ CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+15)	0	50000±2500	0.5	2.0
$\text{CH} + \text{O} \rightarrow \text{H} + \text{CO}$ METHYLIDYNE FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CH} + \text{O} \rightarrow \text{C} + \text{OH}$ METHYLIDYNE FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{CH} + \text{O} + \text{M} \rightarrow \cdot\text{CHO} + \text{M}$ METHYLIDYNE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+16)	-0.5	0±2500	0.3	3.2
$\text{CH} + \text{O}_2 \rightarrow \cdot\text{CHO} + \text{O}$ METHYLIDYNE FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
$\text{CH} + \text{H} \rightarrow \text{H} + \text{CH}$ METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CH} + \text{H} \rightarrow \text{C} + \text{H}_2$ METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
$\text{CH} + \text{H} + \text{M} \rightarrow \text{CH}_2 + \text{M}$ METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	1.00(+19)	-1.0	0	0.3	3.2
$\text{CH} + \text{OH} \rightarrow \cdot\text{CHO} + \text{H}$ METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	5000±2500	0.3	3.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH} + \text{HO}_2 \rightarrow \text{CH}_2 + \text{O}_2$ METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+10)	0.5	7550±2500	0.3 3.2
$\text{CH} + \text{HO}_2 \rightarrow \text{CHO} + \text{OH}$ METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+11)	0.5	3000±2500	0.3 3.2
$\text{CH} + \text{S} \rightarrow \text{H} + \text{CS}$ METHYLIDYNE FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{CH} + \text{S} \rightarrow \text{C} + \text{SH}$ METHYLIDYNE FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{CH} + \text{N} \rightarrow \text{H} + \text{CN}$ METHYLIDYNE FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{CH} + \text{N} \rightarrow \text{C} + \text{NH}$ METHYLIDYNE FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	6995	
$\text{CH} + \text{N}_2 \rightarrow \text{CN} + \text{NH}$ METHYLIDYNE FREE RADICAL + NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+14)	0	46300±10000	
$\text{CH} + \text{N}_2 \rightarrow \text{HCN} + \text{N}$ METHYLIDYNE FREE RADICAL + NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: REVISED ESTIMATE.	1500–2500	1.0(+11)	0	9560	
$\text{CH} + \text{NO} \rightarrow \text{CHO} + \text{N}$ METHYLIDYNE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.6(+13)	0	5000±3000	
$\text{CH} + \text{NO} \rightarrow \text{HCN} + \text{O}$ METHYLIDYNE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	2.0(+12)	0	0±1000	
$\text{CH} + \text{HNO} \rightarrow \text{CH}_2 + \text{NO}$ METHYLIDYNE FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	6.3(+11)	0.5	0±2500	0.3 3.2
$\text{CH} + \text{C} \rightarrow \text{H} + \text{C}_2$ METHYLIDYNE FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{CH} + \text{C} \rightarrow \text{C} + \text{CH}$ METHYLIDYNE FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$\text{CH} + \text{CO}_2 \rightarrow \text{CHO} + \text{CO}$ METHYLIDYNE FREE RADICAL + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+10)	0.5	3000±2500	0.3 3.2
$\text{CH} + \text{CH}_4 \rightarrow \text{CH}_2 + \text{CH}_3$ METHYLIDYNE FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2.	1500–2500	2.5(+11)	0.7	3000±2500	0.3 3.2
$\text{CH} + \text{CHO} \rightarrow \text{CH}_2 + \text{CO}$ METHYLIDYNE FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+10)	0.7	500±2500	0.3 3.2
$\text{CH} + \text{HCHO} \rightarrow \text{CH}_2 + \text{CHO}$ METHYLIDYNE FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.7	2000±2500	0.3 3.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_2 + \text{O} \rightarrow \text{CH} + \text{OH}$ METHYLENE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.7	13000±2500	0.3	3.2
$\text{CH}_2 + \text{O} \rightarrow \cdot\text{CHO} + \text{H}$ METHYLENE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	2000±2500	0.3	3.2
$\text{CH}_2 + \text{O}_2 \rightarrow \text{HCHO} + \text{O}$ METHYLENE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3500±2500	0.3	3.2
$\text{CH}_2 + \text{H} \rightarrow \text{CH} + \text{H}_2$ METHYLENE FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.7	2500±2500	0.3	3.2
$\text{CH}_2 + \text{H}_2 \rightarrow \text{CH}_3 \cdot + \text{H}$ METHYLENE FREE RADICAL + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	3525±1500		
$\text{CH}_2 + \text{OH} \rightarrow \text{CH} + \text{H}_2\text{O}$ METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
$\text{CH}_2 + \text{OH} \rightarrow \text{CH}_3 \cdot + \text{O}$ METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
$\text{CH}_2 + \text{OH} \rightarrow \text{HCHO} + \text{H}$ METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+13)	0	2500		
$\text{CH}_2 + \text{N} \rightarrow \text{CH} + \text{NH}$ METHYLENE FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+11)	0.67	20400±2500	0.3	3.2
$\text{CH}_2 + \text{N}_2 \rightarrow \text{HCN} + \text{NH}$ METHYLENE FREE RADICAL + NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	35230±10000		
$\text{CH}_2 + \text{NO} \rightarrow \text{HCHO} + \text{N}$ METHYLENE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.6(+12)	0	3500±2000		
$\text{CH}_2 + \text{HNO} \rightarrow \text{CH}_3 \cdot + \text{NO}$ METHYLENE FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+11)	0.5	0±2500	0.3	3.2
$\text{CH}_2 + \text{CH}_2 \rightarrow \text{CH} + \text{CH}_3 \cdot$ METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
$\text{CH}_2 + \text{CH}_4 \rightarrow \text{CH}_3 \cdot + \text{CH}_3 \cdot$ METHYLENE FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2.	1500-2500	1.3(+12)	0.7	10000±2500	0.3	3.2
$\text{CH}_2 + \cdot\text{CHO} \rightarrow \text{CH}_3 \cdot + \text{CO}$ METHYLENE FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+10)	0.7	500±2500	0.3	3.2
$\text{CH}_2 + \text{HCHO} \rightarrow \text{CH}_3 \cdot + \text{CHO}$ METHYLENE FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	2.0(+11)	0	3270±1500		
$\text{CH}_2 + \text{CN} \rightarrow \text{CH} + \text{HCN}$ METHYLENE FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	2500±1500		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$^1\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.27 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.0 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.63 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.6 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.37 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 0.94 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.39 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 0.89 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.96 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.86 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.12 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.83 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.16 NOTE: k_{ref} : $^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.74 NOTE: k_{ref} : $^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$\text{CH}_3 + \text{O} \rightarrow \text{HCHO} + \text{H}$ METHYL FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+13)	0	0	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3 \cdot + \text{O}_2 \rightarrow \text{CH}_2 + \text{HO}_2$ METHYL FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	34975±1500		
$\text{CH}_3 \cdot + \text{O}_2 \rightarrow \text{HCHO} + \text{OH}$ METHYL FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+13)	0	10000±5000	0.3	3.2
$\text{CH}_3 \cdot + \text{O}_2 \rightarrow \text{CH}_3\text{O} \cdot + \text{O}$ METHYL FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	15100±1500		
$\text{CH}_3 \cdot + \text{H}_2 \rightarrow \text{CH}_4 + \text{H} \cdot$ METHYL FREE RADICAL + HYDROGEN MOLECULE 72 KER/PAR REACTION ORDER: 2.	370–700	8.5(+11)	0	5500±500	0.7	1.3
$\text{CH}_3 \cdot + \text{HD} \rightarrow \text{CH}_3\text{D} + \text{H} \cdot$ METHYL FREE RADICAL + DEUTERIUM HYDRIDE 76 KER/PAR REACTION ORDER: 2.	400–700	2.4(+11)	0	5635±500	0.5	1.5
$\text{CH}_3 \cdot + \text{HD} \rightarrow \text{CH}_4 + \text{D} \cdot$ METHYL FREE RADICAL + DEUTERIUM HYDRIDE 76 KER/PAR REACTION ORDER: 2.	400–700	2.1(+11)	0	5300±500	0.5	1.5
$\text{CH}_3 \cdot + \text{D}_2 \rightarrow \text{CH}_3\text{D} + \text{D} \cdot$ METHYL FREE RADICAL + DEUTERIUM MOLECULE 76 KER/PAR REACTION ORDER: 2.	300–700	7.1(+11)	0	5990±250	0.7	1.3
$\text{CD}_3 \cdot + \text{H}_2 \rightarrow \text{CD}_3\text{H} + \text{H} \cdot$ METHYL-D ₃ FREE RADICAL + HYDROGEN MOLECULE 72 KON REACTION ORDER: 2.	400–570	7.4(+11)	0	5250±235	0.6	1.7
$\text{CH}_3 \cdot + \text{OH} \rightarrow \text{CH}_2 + \text{H}_2\text{O}$ METHYL FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	6.3(+10)	0.7	1000±2500	0.3	3.2
$\text{CH}_3 \cdot + \text{OH} \rightarrow \text{CH}_3\text{O} \cdot + \text{H}$ METHYL FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	6.3(+12)	0	0		
$\text{CH}_3 \cdot + \text{HO}_2 \rightarrow \text{CH}_4 + \text{O}_2$ METHYL FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	3000±2500	0.3	3.2
$\text{CH}_3 \cdot + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \cdot\text{OH}$ METHYL FREE RADICAL + WATER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	1273–1773	7.1(+12)	0	12900±1000	0.5	2.0
$\text{CH}_3 \cdot + \text{H}_2\text{S} \rightarrow \text{CH}_4 + \text{SH}$ METHYL FREE RADICAL + HYDROGEN SULFIDE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300–600	2.0(+11)	0	2065±750	0.4	2.5
$\text{CH}_3 \cdot + \text{NH}_3 \rightarrow \text{CH}_4 + \text{NH}_2$ METHYL FREE RADICAL + AMMONIA 76 KER/PAR REACTION ORDER: 2.	350–650	1.0(+11)	0	5100±500	0.3	1.8
$\text{CH}_3 \cdot + \text{ND}_3 \rightarrow \text{CH}_3\text{D} + \text{ND}_2$ METHYL FREE RADICAL + AMMONIA-d ₃ 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+11)	0	5535±500	0.3	1.8
$\text{CH}_3 \cdot + \text{NH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{NH}_2\text{NH} \cdot$ METHYL FREE RADICAL + HYDRAZINE 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+11)	0	2500±500	0.5	2.0
$\text{CH}_3 \cdot + \text{ND}_2\text{ND}_2 \rightarrow \text{CH}_3\text{D} + \text{ND}_2\text{ND} \cdot$ METHYL FREE RADICAL + HYDRAZINE-d ₄ 76 KER/PAR REACTION ORDER: 2.	350–500	7.2(+10)	0	3200±500	0.5	2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + \text{HN}_3 \rightarrow \text{CH}_4 + \text{N}_3$ METHYL FREE RADICAL + HYDRAZOIC ACID 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-400	1.0(+11)	0	2100±500	0.5 2.0
$\text{CH}_3\cdot + \text{HNO} \rightarrow \text{CH}_4 + \text{NO}$ METHYL FREE RADICAL + NITROSYL HYDRIDE 76 KER/PAR REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	0±2500	0.3 3.2
$\text{CH}_3\cdot + \text{CO} \rightarrow \text{CH}_3\text{C(0)}\cdot$ METHYL FREE RADICAL + CARBON MONOXIDE 72 KON REACTION ORDER: 2.	273-400	3.8(+8)	0	1968	
$\text{CH}_3\cdot + \text{CH}_4 \rightarrow \text{CH}_4 + \text{CH}_3\cdot$ METHYL FREE RADICAL + METHANE 76 KER/PAR REACTION ORDER: 2.	450-800	4.0(+11)	0	7045±250	0.7 1.3
$\text{CH}_3\cdot + \text{CHD}_3 \rightarrow \text{CH}_4 + \text{CD}_3\cdot$ METHYL FREE RADICAL + METHANE-d ₃ 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-650	1.1(+11)	0	6995±250	0.7 1.3
$\text{CH}_3\cdot + \text{CD}_4 \rightarrow \text{CH}_3\text{D} + \text{CD}_3\cdot$ METHYL FREE RADICAL + METHANE-d ₄ 76 KER/PAR REACTION ORDER: 2.	400-650	2.5(+11)	0	7700±500	0.5 1.5
$\text{CD}_3\cdot + \text{CH}_3\text{D} \rightarrow \text{CD}_4 + \text{CH}_3\cdot$ METHYL-d ₃ -FREE RADICAL + METHANE-d 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-650	5.0(+10)	0	7200±500	0.5 1.5
$\text{CD}_3\cdot + \text{CD}_4 \rightarrow \text{CD}_4 + \text{CD}_3\cdot$ METHYL-d ₃ -FREE RADICAL + METHANE-d ₄ 72 KON REACTION ORDER: 2.	473-623	4.1(+12)	0	8960±250	
$\text{CH}_3\cdot + \cdot\text{CHO} \rightarrow \text{CH}_4 + \text{CO}$ METHYL FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.5	0±2500	0.3 3.2
$\text{CH}_3\cdot + \text{HCHO} \rightarrow \text{CH}_4 + \cdot\text{CHO}$ METHYL FREE RADICAL + FORMALDEHYDE 76 KER/PAR REACTION ORDER: 2.	300-500	1.1(+11)	0	3070±500	0.5 1.5
$\text{CH}_3\cdot + \text{HCHO} \rightarrow \text{CH}_4 + \cdot\text{CHO}$ METHYL FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+10)	0.5	3000±2500	0.3 3.2
$\text{CH}_3\cdot + \text{DCDO} \rightarrow \text{CH}_3\text{D} + \cdot\text{CDO}$ METHYL FREE RADICAL + FORMALDEHYDE-d ₂ 76 KER/PAR REACTION ORDER: 2.	300-500	1.4(+11)	0	3975±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{O}\cdot$ METHYL FREE RADICAL + METHANOL 76 KER/PAR REACTION ORDER: 2.	350-550	6.2(+10)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{OH}$ METHYL FREE RADICAL + METHANOL 76 KER/PAR REACTION ORDER: 2.	350-500	1.9(+11)	0	5035±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{O}\cdot + \cdot\text{CH}_2\text{OH}$ METHYL FREE RADICAL + METHANOL 76 KER/PAR REACTION ORDER: 2.	350-550	2.3(+11)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CD}_3\text{OH} \rightarrow \text{CH}_3\text{D} + \cdot\text{CD}_2\text{OH}$ METHYL FREE RADICAL + METHAN-d ₃ -OL 76 KER/PAR REACTION ORDER: 2.	370-550	2.0(+11)	0	5940±500	0.6 1.4
$\text{CH}_3\cdot + \text{CD}_3\text{OH} \rightarrow \text{CH}_4 + \text{CD}_3\text{O}\cdot$ METHYL FREE RADICAL + METHAN-d ₃ -OL 76 KER/PAR REACTION ORDER: 2.	370-550	6.2(+10)	0	4900±500	0.6 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{OD} \rightarrow \text{CD}_3\text{H} + \cdot\text{CH}_2\text{OD}$ METHYL-d ₃ FREE RADICAL + METHANOL-d 76 KER/PAR REACTION ORDER: 2.	400-500	1.9(+11)	0	5000±500	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CD}_3\cdot + \text{CH}_3\text{OD} \rightarrow \text{CD}_4 + \text{CH}_3\text{O}\cdot$ METHYL-d ₃ FREE RADICAL + METHANOL-d 76 KER/PAR REACTION ORDER: 2. NOTE: GIVEN WITH CAUTION	400-500	3.2(+10)	0	5700±1000	0.5	2.0
$\text{CH}_3\cdot + \text{CH}_3\text{SH} \rightarrow \text{CH}_4 + \text{CH}_3\text{S}\cdot + \cdot\text{CH}_2\text{SH}$ METHYL FREE RADICAL + METHANETHIOL 76 KER/PAR REACTION ORDER: 2.	303	1.2(+ 8)	-	-	0.5	2.0
$\text{CH}_3\cdot + \text{CD}_3\text{SH} \rightarrow \text{CH}_4 + \text{CD}_3\text{S}\cdot$ METHYL FREE RADICAL + METHANE-d ₃ -THIOL 76 KER/PAR REACTION ORDER: 2.	400-500	1.1(+11)	0	2050±500	0.5	2.0
$\text{CH}_3\cdot + \text{CD}_3\text{SH} \rightarrow \text{CH}_3\text{D} + \cdot\text{CD}_2\text{SH}$ METHYL FREE RADICAL + METHANE-d ₃ -THIOL 76 KER/PAR REACTION ORDER: 2.	400-500	7.6(+10)	0	4200±250	0.5	2.0
$\text{CH}_3\cdot + \text{CN} \rightarrow \text{CH}_2 + \text{HCN}$ METHYL FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.7	1500±2500	0.3	3.2
$\text{CH}_3\cdot + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + METHANAMINE 72 KON REACTION ORDER: 2.	388-617	5.4(+11)	0	5020±500	0.3	3.0
$\text{CH}_3\cdot + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{NH}\cdot + \cdot\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + METHANAMINE 76 KER/PAR REACTION ORDER: 2.	350-650	2.1(+11)	0	4330±500	0.7	1.3
$\text{CH}_3\cdot + \text{CH}_3\text{ND}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{ND}_2$ METHYL FREE RADICAL + METHANAMINE-d ₂ 76 KER/PAR REACTION ORDER: 2.	350-450	1.4(+11)	0	4530±500	0.7	1.3
$\text{CH}_3\cdot + \text{CH}_3\text{ND}_2 \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{ND}$ METHYL FREE RADICAL + METHANAMINE-d ₂ 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-450	2.0(+11)	0	5135±1000	0.5	1.5
$\text{CH}_3\cdot + \text{CD}_3\text{NH}_2 \rightarrow \text{CH}_4 + \text{CD}_3\text{NH}\cdot$ METHYL FREE RADICAL + METHAN-d ₃ -AMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-500	2.0(+11)	0	4530±750	0.5	2.0
$\text{CH}_3\cdot + \text{CD}_3\text{NH}_2 \rightarrow \text{CH}_3\text{D} + \cdot\text{CD}_2\text{NH}_2$ METHYL FREE RADICAL + METHAN-d ₃ -AMINE 76 KER/PAR REACTION ORDER: 2.	400-500	7.2(+10)	0	5100±500	0.5	1.5
$\text{CH}_3\cdot + \text{CH}_3\text{NHNH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}(\cdot)\text{NH}_2 + \text{CH}_3\text{NHNH}\cdot$ $+ \cdot\text{CH}_2\text{NHNH}_2$ METHYL FREE RADICAL + HYDRAZINE, METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	420	6.3(+ 8)	-	-		
$\text{CH}_3\cdot + \text{HCONH}_2 \rightarrow \text{CH}_4 + \text{HCONH}\cdot + \cdot\text{CONH}_2$ METHYL FREE RADICAL + FORMAMIDE 76 KER/PAR REACTION ORDER: 2.	350-500	3.6(+10)	0	3300±500	0.5	1.5
$\text{CH}_3\cdot + \text{HCOND}_2 \rightarrow \text{CH}_4 + \cdot\text{COND}_2$ METHYL FREE RADICAL + FORMAMIDE-N,N-d ₂ 76 KER/PAR REACTION ORDER: 2.	350-500	5.5(+10)	0	3575±500	0.5	2.0
$\text{CH}_3\cdot + \text{HCOND}_2 \rightarrow \text{CH}_3\text{D} + \text{HCOND}$ METHYL FREE RADICAL + FORMAMIDE-N,N-d ₂ 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	4900±500	0.5	2.0
$\text{CH}_3\cdot + \text{CH}_3\text{NO}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{NO}_2$ METHYL FREE RADICAL + METHANE, NITRO- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-500	1.0(+11)	0	5100±750	0.5	2.5
$\text{CH}_3\cdot + \text{CH}_3\text{ONH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{ONH}\cdot$ METHYL FREE RADICAL + HYDROXYLAMINE, O-METHYL- 76 KER/PAR REACTION ORDER: 2.	300-500	5.0(+10)	0	2265±500	0.5	1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + \text{CH}_3\text{OND}_2 \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{OND}$ METHYL FREE RADICAL + HYDROXYLAMINE-N,N-d ₂ , O-METHYL- 76 KER/PAR REACTION ORDER: 2.	300-500	3.5(+10)	0	2970±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}=\text{CH} \rightarrow \text{CH}_4 + \text{CH}=\text{C}$ METHYL FREE RADICAL + ETHYNE 76 KER/PAR REACTION ORDER: 2. NOTE: GIVEN WITH CAUTION.	473-773	-	-	7100	
$\text{CH}_3\cdot + \text{CH}=\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}$ METHYL FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2.	371-479	2.5(+11)	0	3900	
$\text{CH}_3\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2=\text{CH}$ METHYL FREE RADICAL + ETHENE 76 KER/PAR REACTION ORDER: 2.	350-650	4.2(+11)	0	5600±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	353-453	3.3(+11)	0	3900	
$\text{CH}_3\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot + (\text{CH}_3)_2\text{CH}$ METHYL FREE RADICAL + ETHENE 72 KON REACTION ORDER: 2.	350-705	2.0(+11)	0	3575±105	0.8 1.3
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\cdot$ METHYL FREE RADICAL + ETHANE 76 KER/PAR REACTION ORDER: 2.	400-800	5.6(+11)	0	5840±250	0.7 1.3
$\text{CH}_3\cdot + \text{CD}_3\text{CD}_3 \rightarrow \text{CH}_3\text{D} + \text{CD}_3\text{CD}_2\cdot$ METHYL FREE RADICAL + ETHANE-d ₆ 76 KER/PAR REACTION ORDER: 2.	500-900	5.6(+11)	0	6600±250	0.7 1.3
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}_2\cdot$ METHYL-d ₃ FREE RADICAL + ETHANE 72 KON REACTION ORDER: 2.	390-800	1.0(+12)	0	6085±165	0.7 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{CD}_3 \rightarrow \text{CD}_3\text{H} + \text{CD}_3\text{CH}_2\cdot$ METHYL-d ₃ FREE RADICAL + ETHANE-1,1,1-d ₃ 76 KER/PAR REACTION ORDER: 2.	500-750	3.0(+11)	0	5900±250	0.7 1.3
$\text{CD}_3\cdot + \text{CH}_3\text{CD}_3 \rightarrow \text{CD}_4 + \text{CH}_3\text{CD}_2\cdot$ METHYL-d ₃ FREE RADICAL + ETHANE-1,1,1-d ₃ 76 KER/PAR REACTION ORDER: 2.	500-750	4.3(+11)	0	6845±250	0.7 1.3
$\text{CD}_3\cdot + \text{CD}_3\text{CD}_3 \rightarrow \text{CD}_4 + \text{CD}_3\text{CD}_2\cdot$ METHYL-d ₃ FREE RADICAL + ETHANE-d ₆ 72 KON REACTION ORDER: 2.	550-760	4.6(+11)	0	6405	
$\text{CH}_3\cdot + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + ACETALDEHYDE 76 KER/PAR REACTION ORDER: 2.	300-525	8.5(+10)	0	3000±250	0.4 1.6
$\text{CH}_3\cdot + \text{CH}_3\text{CDO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + ACETALDEHYDE-1-d 76 KER/PAR REACTION ORDER: 2.	300-500	1.0(+11)	0	3975±500	0.5 1.5
$\text{CH}_3\cdot + \text{cy-CH}_2\text{CH}_2\text{O} \rightarrow \text{CH}_4 + \text{cy-CH}_2\text{CH}(\cdot)\text{O}$ METHYL FREE RADICAL + OXIRANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	5435±750	0.5 2.0
$\text{CH}_3\cdot + \text{HCOOCH}_3 \rightarrow \text{CH}_4 + \cdot\text{COOCH}_3$ METHYL FREE RADICAL + FORMIC ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	350-550	2.0(+11)	0	4900±500	0.5 1.5
$\text{CH}_3\cdot + \text{HCOOCH}_3 \rightarrow \text{CH}_4 + \text{HCOOCH}_2\cdot$ METHYL FREE RADICAL + FORMIC ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	350-550	1.6(+11)	0	5635±500	0.5 1.5
$\text{CH}_3\cdot + \text{HCOOCH}_3 \rightarrow \text{CH}_4 + \cdot\text{COOCH}_3 + \text{HCOOCH}_2\cdot$ METHYL FREE RADICAL + FORMIC ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	350-550	3.0(+11)	0	4980±500	0.5 1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + \text{DCOOCH}_3 \rightarrow \text{CH}_3\text{D} + \cdot\text{COOCH}_3$ METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	350-550	2.5(+11)	0	5900±500	0.5 1.5
$\text{CH}_3\cdot + \text{DCOOCH}_3 \rightarrow \text{CH}_4 + \text{DCOOCH}_2\cdot$ METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-550	1.6(+11)	0	5635±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{COOD} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{COOD}$ METHYL FREE RADICAL + ACETIC ACID-d 76 KER/PAR REACTION ORDER: 2.	300-600	1.6(+11)	0	5135±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{O}\cdot$ METHYL FREE RADICAL + ETHANOL 76 KER/PAR REACTION ORDER: 2.	400-625	7.9(+10)	0	4730±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{OH}$ METHYL FREE RADICAL + ETHANOL 76 KER/PAR REACTION ORDER: 2.	400-625	4.00(+11)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{O}\cdot + \text{CH}_3\text{CH}(\cdot)\text{OH}$ + $\cdot\text{CH}_2\text{CH}_2\text{OH}$ METHYL FREE RADICAL + ETHANOL 76 KER/PAR REACTION ORDER: 2.	400-625	5.1(+11)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CD}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{O}\cdot + \cdot\text{CH}_2\text{CD}_2\text{OH}$ METHYL FREE RADICAL + ETHAN-1,1-d ₂ -OL 76 KER/PAR REACTION ORDER: 2.	400-550	7.1(+10)	0	4530±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CD}_2\text{OH} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CD}(\cdot)\text{OH}$ METHYL FREE RADICAL + ETHAN-1,1-d ₂ -OL 76 KER/PAR REACTION ORDER: 2.	400-550	4.1(+11)	0	5735±500	0.6 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_2\text{OD} \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}(\cdot)\text{OD} + \cdot\text{CH}_2\text{CH}_2\text{OD}$ METHYL-d ₃ FREE RADICAL + ETHANOL-d 76 KER/PAR REACTION ORDER: 2.	400-525	4.4(+11)	0	4900±500	0.6 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_2\text{OD} \rightarrow \text{CD}_4 + \text{CH}_3\text{CH}_2\text{O}\cdot$ METHYL-d ₃ FREE RADICAL + ETHANOL-d 76 KER/PAR REACTION ORDER: 2.	400-525	6.2(+10)	0	5135±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{OCH}_2\cdot$ METHYL FREE RADICAL + METHANE, OXYBIS- 76 KER/PAR REACTION ORDER: 2.	300-550	4.2(+11)	0	5035±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{OOCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{OOCH}_2\cdot$ METHYL FREE RADICAL + PEROXIDE, DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	4.2(+11)	0	5000±1000	0.3 3.0
$\text{CD}_3\cdot + \text{cy-CH}_2\text{CH}_2\text{S} \rightarrow \text{CD}_3\text{H} + \text{cy-CH}_2\text{CH}(\cdot)\text{S}$ METHYL-d ₃ FREE RADICAL + THIIRANE 76 KER/PAR REACTION ORDER: 2.	300-500	2.2(+11)	0	4800±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{S}\cdot + \text{CH}_3\text{CH}(\cdot)\text{SH}$ + $\cdot\text{CH}_2\text{CH}_2\text{SH}$ METHYL FREE RADICAL + ETHANETHIOL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	3.5(+ 7)	-	-	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CN} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CN}$ METHYL FREE RADICAL + ACETONITRILE 76 KER/PAR REACTION ORDER: 2.	350-600	5.4(+11)	0	5100±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{NH}\cdot + \text{CH}_3\text{CH}(\cdot)\text{NH}_2$ + $\cdot\text{CH}_2\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + ETHANAMINE 76 KER/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{NH}\cdot$ METHYL FREE RADICAL + ETHANAMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	4600±500	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + \text{CD}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{D} + \text{CD}_3\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CD}_2\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + ETHAN-2,2,2-d ₃ -AMINE 76 KER/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\cdot + \text{CD}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CD}_3\text{CH}_2\text{NH}\cdot$ METHYL FREE RADICAL + ETHAN-2,2,2-d ₃ -AMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	423	4.0(+ 5)	-	-	
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N}\cdot + \cdot\text{CH}_2\text{NHCH}_3$ METHYL FREE RADICAL + METHANAMINE, N-METHYL- 76 KER/PAR REACTION ORDER: 2.	350-650	1.6(+11)	0	3500±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N}\cdot$ METHYL FREE RADICAL + METHANAMINE, N-METHYL- 76 KER/PAR REACTION ORDER: 2.	350-650	6.5(+10)	0	3200±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{ND} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{NDCH}_3$ METHYL FREE RADICAL + METHANAMINE-d, N-METHYL- 76 KER/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4400±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{ND} \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{N}\cdot$ METHYL FREE RADICAL + METHANAMINE-d, N-METHYL- 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	4300±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}=\text{NCH}_3$ METHYL FREE RADICAL + DIAZENE, DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	300-500	1.1(+11)	0	3975±250	0.7 1.3
$\text{CH}_3\cdot + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow (\text{CH}_3)_2\text{NN}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + DIAZENE, DIMETHYL- 72 KON REACTION ORDER: 2.	300-450	5.0(+10)	0	3040±355	0.4 2.6
$\text{CD}_3\cdot + \text{CD}_3\text{N}=\text{NCD}_3 \rightarrow \text{CD}_4 + \text{CD}_2\text{N}=\text{NCD}_3$ METHYL-d ₃ FREE RADICAL + DIAZENE, DI(METHYL-d ₃)- 76 KER/PAR REACTION ORDER: 2.	300-500	6.6(+10)	0	4125±500	0.5 1.5
$\text{CH}_3\cdot + \text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \cdot\text{NHCH}_2\text{CH}_2\text{NH}_2$ $+ \text{NH}_2\text{CH}(\cdot)\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + 1,2-ETHANEDIAMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	3.8(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\cdot + \text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \cdot\text{NHCH}_2\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + 1,2-ETHANEDIAMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	4430±500	0.5 2.0
$\text{CH}_3\cdot + \text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 \rightarrow \text{CH}_4 + \text{ND}_2\text{CH}(\cdot)\text{CH}_2\text{ND}_2$ METHYL FREE RADICAL + 1,2-ETHANEDI(AMINE-d ₂) 76 KER/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	4000±500	0.5 2.0
$\text{CH}_3\cdot + \text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 \rightarrow \text{CH}_3\text{D} + \cdot\text{NDCH}_2\text{CH}_2\text{ND}_2$ METHYL FREE RADICAL + 1,2-ETHANEDI(AMINE-d ₂) 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	3.2(+11)	0	5100±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NNH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{NNH}\cdot$ METHYL FREE RADICAL + HYDRAZINE, 1,1-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-500	1.7(+11)	0	2870±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NNH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{NNH}\cdot + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{NH}_2$ METHYL FREE RADICAL + HYDRAZINE, 1,1-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-500	2.4(+11)	0	2970±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{ND}$ METHYL FREE RADICAL + HYDRAZINE-d ₂ , 1,1-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	3.2(+11)	0	4125±750	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{NND}\cdot$ METHYL FREE RADICAL + HYDRAZINE-d ₂ , 1,1-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-500	2.1(+11)	0	3400±500	0.5 1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3\cdot + \text{CH}_3\text{NHNHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}(\cdot)\text{NHCH}_3 + \cdot\text{CH}_2\text{NHNHCH}_3$ METHYL FREE RADICAL + HYDRAZINE, 1,2-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	2400±250	0.5	2.0
$\text{CH}_3\cdot + \text{CH}_3\text{NDNDCH}_3 \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{N}(\cdot)\text{NDCH}_3$ METHYL FREE RADICAL + HYDRAZINE-1,2-d ₂ , 1,2-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	2700±500	0.5	2.0
$\text{CH}_3\cdot + \text{HCONHCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CONHCH}_3 + \text{HCON}(\cdot)\text{CH}_3$ + HCONHCH ₂ . METHYL FREE RADICAL + FORMAMIDE, N-METHYL- 76 KER/PAR REACTION ORDER: 2.	400-600	7.9(+10)	0	3800±500	0.5	1.5
$\text{CH}_3\cdot + \text{CH}_3\text{CONH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CONH}\cdot + \cdot\text{CH}_2\text{CONH}_2$ METHYL FREE RADICAL + ACETAMIDE 76 KER/PAR REACTION ORDER: 2.	350-600	2.1(+11)	0	5235±500	0.5	1.5
$\text{CH}_3\cdot + \text{CH}_3\text{CONH}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CONH}_2$ METHYL FREE RADICAL + ACETAMIDE 76 KER/PAR REACTION ORDER: 2.	350-600	1.0(+11)	0	5200±500	0.5	1.5
$\text{CD}_3\cdot + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_3\text{H} + \text{CD}_3\text{CONH}\cdot$ METHYL FREE RADICAL + ACETAMIDE-2,2,2-d ₃ 76 KER/PAR REACTION ORDER: 2.	350-600	1.1(+11)	0	5235±500	0.5	1.5
$\text{CD}_3\cdot + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_4 + \cdot\text{CD}_2\text{CONH}_2$ METHYL FREE RADICAL + ACETAMIDE-2,2,2-d ₃ 76 KER/PAR REACTION ORDER: 2.	350-600	1.4(+11)	0	5800±500	0.5	1.5
$\text{CH}_3\cdot + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}\cdot + \text{CH}_3\text{C}(\cdot)=\text{CHCH}_3$ METHYL FREE RADICAL + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. CH ₃ ADDITION OCCURS PREDOMINANTLY AT TERMINAL C ATOM.	379-465	5.0(+11)	0	4400		
$\text{CH}_3\cdot + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ METHYL FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2.	373-483	2.0(+11)	0	4100		
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\cdot)=\text{CH}_2$ METHYL FREE RADICAL + 1-PROPENE 76 KER/PAR REACTION ORDER: 2.	350-600	1.4(+11)	0	4430±500	0.6	1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_4 + [\text{C}_3\text{H}_5\cdot]$ METHYL FREE RADICAL + 1-PROPENE 72 KON REACTION ORDER: 2.	350-580	3.2(+10)	0	3775±300	0.5	2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\cdot$ METHYL FREE RADICAL + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.72	353-453 453	1.7(+11) -	0 -	3700 -		
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CH}\cdot$ METHYL FREE RADICAL + PROPANE 76 KER/PAR REACTION ORDER: 2.	550-750	2.0(+11)	0	4830±250	0.7	1.3
$\text{CD}_3\cdot + \text{CH}_3\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CD}_2\text{CH}_2\cdot$ METHYL-d ₃ FREE RADICAL + PROPANE-2,2-d ₂ 76 KER/PAR REACTION ORDER: 2.	550-750	4.4(+11)	0	5735±250	0.7	1.3
$\text{CD}_3\cdot + \text{CH}_3\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_4 + (\text{CH}_3)_2\text{CD}\cdot$ METHYL-d ₃ FREE RADICAL + PROPANE-2,2-d ₂ 76 KER/PAR REACTION ORDER: 2.	550-750	2.5(+11)	0	5735±250	0.7	1.3
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + PROPANAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	2970±500	0.4	1.6

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\cdot$ METHYL FREE RADICAL + 2-PROPANONE 76 KER/PAR REACTION ORDER: 2.	350-700	3.5(+11)	0	4900±250	0.8 1.3
$\text{CD}_3\cdot + (\text{CD}_3)_2\text{CO} \rightarrow \text{CD}_4 + \text{CD}_3\text{C}(\text{O})\text{CD}_2\cdot$ METHYL- d_3 FREE RADICAL + 2-PROPANONE-1,1,1,3,3,3- d_6 76 KER/PAR REACTION ORDER: 2.	350-800	4.8(+11)	0	5735±250	0.8 1.3
$\text{CH}_3\cdot + \text{HCOOCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \cdot\text{COOCH}_2\text{CH}_3 + \text{HCOOCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + FORMIC ACID ETHYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	5100±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{COOCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{COOCH}_3 + \text{CH}_3\text{COOCH}_2\cdot$ METHYL FREE RADICAL + ACETIC ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	350-600	2.1(+11)	0	5035±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{COOCD}_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{COOCD}_3$ METHYL FREE RADICAL + ACETIC ACID METHYL- d_3 ESTER 76 KER/PAR REACTION ORDER: 2.	350-650	1.9(+11)	0	5035±500	0.4 1.6
$\text{CH}_3\cdot + \text{CD}_3\text{COOCH}_3 \rightarrow \text{CH}_4 + \text{CD}_3\text{COOCH}_2\cdot$ METHYL FREE RADICAL + ACETIC- d_3 ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	400-600	1.7(+11)	0	5990±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{OCOOCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{OCOOCH}_3$ METHYL FREE RADICAL + CARBONIC ACID DIMETHYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	3.2(+11)	0	5800±750	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CDOH} \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{C}(\cdot)\text{OH}$ METHYL FREE RADICAL + 2-PROPAN-2- d -OL 76 KER/PAR REACTION ORDER: 2.	400-525	1.9(+11)	0	4900±500	0.6 1.4
$\text{CD}_3\cdot + (\text{CH}_3)_2\text{CHOD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{C}(\cdot)\text{OD} + \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OD}$ METHYL- d_3 FREE RADICAL + 2-PROPANOL- d 76 KER/PAR REACTION ORDER: 2.	400-525	1.5(+11)	0	3975±500	0.6 1.4
$\text{CH}_3\cdot + \text{cy-CH}_2\text{CH}_2\text{CH}_2\text{S} \rightarrow \text{CH}_4 + \text{cy-CH}_2\text{CH}(\cdot)\text{CH}_2\text{S}$ METHYL FREE RADICAL + THIETANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-450	3.2(+11)	0	4630±750	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHSH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHS}\cdot + (\text{CH}_3)_2\text{C}(\cdot)\text{SH}$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{SH}$ METHYL FREE RADICAL + 2-PROPANETHIOL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	4.1(+ 7)	—	—	0.5 2.0
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}_2\text{CN}$ METHYL- d_3 FREE RADICAL + PROPANENITRILE 76 KER/PAR REACTION ORDER: 2.	400-600	3.6(+11)	0	4330±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{N} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}(\text{CH}_3)_2$ METHYL FREE RADICAL + METHANAMINE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-600	4.7(+11)	0	4600±500	0.7 1.3
$\text{CH}_3\cdot + \text{HCON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{CON}(\text{CH}_3)_2 + \text{HCO}-(\text{CH}_3)\text{NCH}_2\cdot$ METHYL FREE RADICAL + FORMAMIDE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-600	6.3(+10)	0	3600±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{C}\equiv\text{CH}$ $+ \cdot\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} + \text{CH}_3\text{CH}_2\text{C}\equiv\text{C}\cdot$ METHYL FREE RADICAL + 1-BUTYNE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	456-620	1.9(+12)	0	5135±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{C}\equiv\text{CCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}\equiv\text{CCH}_2\cdot$ METHYL FREE RADICAL + 2-BUTYNE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	486-619	1.1(+12)	0	4900±500	0.6 1.4

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3 \cdot + \text{CH}_3=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2.	353-453	8.1(+10)	0	2065		
$\text{CH}_3 \cdot + \text{CH}_2=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 12.0$ NOTE: $k_{\text{ref}}: \text{CH}_3 + \text{CH}_2=\text{CH}_2$	453	-	-	-		
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1-BUTENE 76 KER/PAR REACTION ORDER: 2.	350-650	2.5(+11)	0	4200±500	0.6	1.4
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CHCH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2 \cdot$ METHYL FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.7$ NOTE: $k_{\text{ref}}: \text{CH}_3 + \text{CH}_2=\text{CH}_2$	353-453 453	1.0(+11) -	0 -	3600 -		
$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHCH}_2 \cdot$ METHYL FREE RADICAL + cis-2-BUTENE 76 KER/PAR REACTION ORDER: 2.	350-650	1.8(+11)	0	4100±500	0.6	1.4
$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.2$ NOTE: $k_{\text{ref}}: \text{CH}_3 + \text{CH}_2=\text{CH}_2$	353-453 453	4.5(+10) -	0 -	3675 -		
$\text{CH}_3 \cdot + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHCH}_2 \cdot$ METHYL FREE RADICAL + trans-2-BUTENE 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+12)	0	4830±500	0.6	1.4
$\text{CH}_3 \cdot + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.4$ NOTE: $k_{\text{ref}}: \text{CH}_3 + \text{CH}_2=\text{CH}_2$	353-453 453	1.4(+11) -	0 -	4075 -		
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ METHYL FREE RADICAL + 1-PROPENE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2.	350-600	3.0(+11)	0	4500±500	0.6	1.4
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2 \cdot + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.1$ NOTE: $k_{\text{ref}}: \text{CH}_3 + \text{CH}_2=\text{CH}_2$	353-453 453	1.4(+11) -	0 -	3475 -		
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + BUTANE 76 KER/PAR REACTION ORDER: 2.	350-750	4.0(+11)	0	4830±250	0.7	1.3
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \cdot$ METHYL FREE RADICAL + BUTANE 72 KON REACTION ORDER: 2.	350-500	1.6(+11)	0	4540±150	0.7	1.4
$\text{CD}_3 \cdot + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_2 \cdot$ METHYL-d ₃ FREE RADICAL + BUTANE-2,2,3,3-d ₄ 76 KER/PAR REACTION ORDER: 2.	600-750	4.8(+11)	0	5735±250	0.7	1.3
$\text{CD}_3 \cdot + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_4 + \text{CH}_3\text{CD}_2\text{CD}(\cdot)\text{CH}_3$ METHYL-d ₃ FREE RADICAL + BUTANE-2,2,3,3-d ₄ 76 KER/PAR REACTION ORDER: 2.	600-750	4.5(+11)	0	5735±250	0.7	1.3
$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C} \cdot + (\text{CH}_3)_2\text{CHCH}_2 \cdot$ METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2.	300-500	8.3(+10)	0	4000±500	0.5	2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C}\cdot$ METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2.	550-750	9.6(+10)	0	3975±250	0.7 1.3
$\text{CD}_3\cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{CDCH}_2\cdot$ METHYL- d_3 FREE RADICAL + PROPANE-2-d, 2-METHYL- 76 KER/PAR REACTION ORDER: 2.	550-750	6.0(+11)	0	5735±250	0.7 1.3
$\text{CD}_3\cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_4 + (\text{CH}_3)_3\text{C}\cdot$ METHYL- d_3 FREE RADICAL + PROPANE-2-d, 2-METHYL- 76 KER/PAR REACTION ORDER: 2.	550-750	1.2(+11)	0	4800±250	0.7 1.3
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{CHCHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHC}(\text{O})\cdot$ METHYL FREE RADICAL + 2-BUTENAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3400±500	0.4 2.5
$\text{CH}_3\cdot + \text{CH}_3\text{COCOCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{COCOCH}_2\cdot$ METHYL FREE RADICAL + 2,3-BUTANEDIONE 76 KER/PAR REACTION ORDER: 2.	300-800	2.2(+11)	0	4300±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3\text{CO})_2\text{O} \rightarrow \text{CH}_4 + \text{CH}_3\text{COOCCCH}_2\cdot$ METHYL FREE RADICAL + ACETIC ACID ANHYDRIDE 76 KER/PAR REACTION ORDER: 2.	300-500	1.8(+11)	0	4830±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + BUTANAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	2970±500	0.4 1.6
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCHO} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHC}(\text{O})\cdot$ METHYL FREE RADICAL + PROPANAL, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	2970±500	0.4 1.6
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{COCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{COCH}_3 + \cdot\text{CH}_2\text{CH}_2\text{COCH}_3$ $+ \text{CH}_3\text{CH}_2\text{COCH}_2\cdot$ METHYL FREE RADICAL + 2-BUTANONE 76 KER/PAR REACTION ORDER: 2.	300-500	8.2(+10)	0	3700±500	0.5 1.5
$\text{CH}_3\cdot + \text{HCOOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \cdot\text{COOCH}_2\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + FORMIC ACID PROPYL ESTER 72 KON REACTION ORDER: 2.	347-455	1.3(+10)	0	3675	
$\text{CH}_3\cdot + \text{HCOOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \cdot\text{COOCH}_2\text{CH}_2\text{CH}_3$ $+ \text{HCOOCH}(\cdot)\text{CH}_2\text{CH}_3 + \text{HCOOCH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{HCOOCH}_2\text{CH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + FORMIC ACID PROPYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	5000±500	0.5 2.0
$\text{CH}_3\cdot + \text{HCOOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{COOCH}(\text{CH}_3)_2$ $+ \text{HCOOC}(\cdot)(\text{CH}_3)_2 + \text{HCOOCH}(\text{CH}_3)\text{CH}_2\cdot$ METHYL FREE RADICAL + FORMIC ACID 1-METHYLETHYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	4980±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{OCH}(\cdot)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + ETHANE, 1,1'-OXYBIS- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-500	2.5(+11)	0	4200±750	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CSH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CS}\cdot + \cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{SH}$ METHYL FREE RADICAL + 2-PROPANETHIOL, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	5.9(+ 7)	—	—	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{NN}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\cdot)=\text{NN}=\text{CHCH}_3$ $+ \cdot\text{CH}_2\text{CH}=\text{NN}=\text{CHCH}_3$ METHYL FREE RADICAL + ACETALDEHYDE ETHYLIDENEHYDRAZONE 76 KER/PAR REACTION ORDER: 2.	350-600	2.5(+11)	0	3975±500	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}\cdot$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + 1-BUTANAMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	426	3.2(+ 7)	-	-	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{N}\cdot$ $+ \text{CH}_3\text{CH}(\cdot)\text{NHCH}_2\text{CH}_3 + \cdot\text{CH}_2\text{CH}_2\text{NHCH}_2\text{CH}_3$ METHYL FREE RADICAL + ETHANAMINE, N-ETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.2(-11)	0	3550±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_3)_2$ $+ \text{CH}_2\text{CH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)\text{CH}_2\cdot$ METHYL FREE RADICAL + ETHANAMINE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	420	2.6(+ 7)	-	-	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CON}(\text{CH}_3)_2$ $+ \text{CH}_3\text{C}\dot{\text{O}}\text{N}(\text{CH}_3)_2$ METHYL FREE RADICAL + ACETAMIDE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-600	2.0(+11)	0	4200±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{CON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2\cdot$ METHYL FREE RADICAL + ACETAMIDE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-600	1.6(+11)	0	4125±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1-PENTENE 76 KER/PAR REACTION ORDER: 2.	450-650	4.5(+11)	0	4500±500	0.6 1.4
$\text{CH}_3\cdot + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
$\text{CH}_3\cdot + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4125	
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	-	-	3500	
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1-BUTENE, 3-METHYL- 76 KER/PAR REACTION ORDER: 2.	450-600	4.4(+11)	0	4225±7500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}=\text{CHCH}_2\cdot$ $+ \cdot\text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3$ METHYL FREE RADICAL + 2-BUTENE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-500	4.9(-11)	0	4300±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}_3$ $+ (\text{CH}_3)_2\dot{\text{C}}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.4$ NOTE: $k_{\text{ref}}: \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$ TENTATIVE k VALUE.	453 403-455	- 1.4(-10)	- 0	- 3070	
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + PENTANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	4.8(+11)	0	5800±250	0.7 1.3
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2(\cdot)\text{CH}_3$ METHYL FREE RADICAL + PENTANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	6.0(-11)	0	4830±250	0.7 1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + BUTANE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.6(+10)	0	3975±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + BUTANE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	2.0(+11)	0	4830±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ $\cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + BUTANE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_4\text{C} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\cdot$ METHYL FREE RADICAL + PROPANE, 2,2-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	400-600	8.3(+11)	0	5940±350	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + PENTANAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3000±500	0.4 1.6
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + BUTANAL, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3200±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{O})\cdot$ METHYL FREE RADICAL + BUTANAL, 3-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3070±500	0.4 1.6
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCHO} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CC}(\text{O})\cdot$ METHYL FREE RADICAL + PROPANOL, 2,2-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3170±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{COCH}_2\text{CH}_3$ $\cdot\text{CH}_2\text{CH}_2\text{CONH}_2\text{CH}_3$ METHYL FREE RADICAL + 3-PENTANONE 76 KER/PAR REACTION ORDER: 2.	300-450	1.9(+11)	0	3675±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3\text{CD}_2)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{COCDD}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d ₄ 76 KER/PAR REACTION ORDER: 2.	500-600	2.0(+11)	0	5535±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CD}_2)_2\text{CO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CD}_2\text{COCDD}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d ₄ 76 KER/PAR REACTION ORDER: 2.	500-600	1.3(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\cdot + \text{HCOO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_4 + \cdot\text{COO}(\text{CH}_2)_3\text{CH}_3$ $+ \text{HCOOCH}(\cdot)(\text{CH}_2)_2\text{CH}_3 + \text{HCOOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{HCOOCH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{HCOO}(\text{CH}_2)_3\text{CH}_2\cdot$ METHYL FREE RADICAL + FORMIC ACID BUTYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	4980±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{COOCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}(\cdot)\text{CH}_3 + \cdot\text{CH}_2\text{CH}_2\text{COOCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + PROPANOIC ACID ETHYL ESTER 76 KER/PAR REACTION ORDER: 2.	300-650	2.5(+11)	0	4125±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_2\text{NCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)\text{CH}_3 + (\text{CH}_3\text{CH}_2)_2\text{NCH}_2\cdot$ METHYL FREE RADICAL + ETHANAMINE, N-ETHYL-N-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	420	3.0(+ 7)	-	-	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NCON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{CON}(\text{CH}_3)_2$ METHYL FREE RADICAL + UREA TETRAMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-550	2.0(+11)	0	3975±500	0.5 1.5
$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + cis-2-HEXENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + cis-2-HEXENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4150	
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + 1-PENTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	-	-	3450	
$\text{CH}_3 \cdot + \text{cis-}(\text{CH}_3)_2\text{CHCH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + cis-2-PENTENE, 4-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	-	-	4390	
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}=(\text{CH}_3)\text{CCH}_2\cdot$ METHYL FREE RADICAL + 2-BUTENE, 2-3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	403-614	7.8(+11)	0	4400±500	0.6 1.4
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{CC}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + 2-BUTENE, 2-3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.	403-453	1.0(+10)	0	3400	
NOTE: TENTATIVE k VALUE.					
k/k _{ref} : 0.2	453	-	-	-	
NOTE: k _{ref} : $\text{CH}_3 \cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3 \cdot + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ METHYL FREE RADICAL + HEXANE 76 KER/PAR REACTION ORDER: 2.	350-800	4.8(+11)	0	5800±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3 \cdot + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + HEXANE 76 KER/PAR REACTION ORDER: 2.	350-800	7.9(+11)	0	4830±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-750	9.5(+11)	0	5800±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-750	1.9(+11)	0	3975±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHC}(\cdot)(\text{CH}_3)_2$ $+ \cdot\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KON REACTION ORDER: 2.	300-500	5.0(+10)	0	3445	
$\text{CD}_3 \cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ METHYL-d ₃ FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KON REACTION ORDER: 2.	439-566	4.7(+11)	0	4525	
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{OCH}(\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OCH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PROPANE, 2,2'-OXYBIS- 76 KER/PAR REACTION ORDER: 2.	400-600	2.1(+11)	0	4100±500	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHOOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{OOCH}(\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OOCH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PEROXIDE, BIS(1-METHYLETHYL)- 76 KER/PAR REACTION ORDER: 2.	300-450	2.3(+11)	0	4100±500	0.5 1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{NC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\cdot)=\text{NC}(\text{CH}_3)_3$ $+ \cdot\text{CH}_2\text{CH}=\text{NC}(\text{CH}_3)_3 + \text{CH}_3\text{CH}=\text{NC}(\text{CH}_3)_2\text{CH}_2\cdot$ METHYL FREE RADICAL + PROPANIMINE, N-ETHYLIDENE-2-METHYL- 76 KER/PAR REACTION ORDER: 2.	350-500	8.9(+10)	0	3925±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHNHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHN}(\cdot)\text{CH}(\text{CH}_3)_2$ $+ (\text{CH}_3)_2\dot{\text{C}}(\cdot)\text{NHCH}(\text{CH}_3)_2$ METHYL FREE RADICAL + 2-PROPANAMINE, N-(1-METHYLETHYL)- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	3370±750	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{N} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2$ METHYL FREE RADICAL + ETHANAMINE, N,N-DIETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-600	5.0(+11)	0	4000±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_3\dot{\text{C}}\cdot$ METHYL FREE RADICAL + PENTANE, 3-ETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + PENTANE, 3-ETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	6.0(+11)	0	4830±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{CHCH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + PENTANE, 3-ETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot$ METHYL FREE RADICAL + OCTANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	4.8(+11)	0	5800±250	0.7 1.3
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\dot{\text{C}}\text{H}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_5\dot{\text{C}}\text{H}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + OCTANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	1.2(+12)	0	4830±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	2.0(+11)	0	4830±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\dot{\text{C}}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ $+ \cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CHO})\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CHO})\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,3,4-TRIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4$ $+ (\text{CH}_3)_2\dot{\text{C}}\text{H}(\cdot)(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + (\text{CH}_3)\dot{\text{C}}(\cdot)\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,3,4-TRIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	2.9(+11)	0	3975±250	0.7 1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + [\text{C}_8\text{H}_{17}\cdot]$ METHYL FREE RADICAL + PENTANE, 2,3,4-TRIMETHYL- 72 KON REACTION ORDER: 2.	414-605	4.7(+11)	0	4575		
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3$ METHYL FREE RADICAL + BUTANE, 2,2,3,3-TETRAMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	1.4(+12)	0	5800±250	0.7	1.3
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{COOC}(\text{CH}_3)_3$ METHYL FREE RADICAL + PEROXIDE, BIS(1,1-DIMETHYLETHYL)- 76 KER/PAR REACTION ORDER: 2.	350-500	1.8(+12)	0	5900±750	0.3	3.0
$\text{CH}_4 \rightarrow \text{CH}_3\cdot + \text{H}$ METHANE 70 BEN/O'N REACTION ORDER: 1.	1200-1800	2.0(+15)	0	52340		
$\text{CH}_4 + \text{O} \rightarrow \text{CH}_3\cdot + \text{OH}$ METHANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	350-1000	2.1(+13)	0	4550	0.7	1.3
$\text{CH}_4 + \text{O} \rightarrow \text{CH}_3\cdot + \text{OH}$ METHANE + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+13)	0	4530±500	0.6	1.6
$\text{CH}_4 + \text{H} \rightarrow \text{CH}_3\cdot + \text{H}_2$ METHANE + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+13)	0	5990±150	0.5	2.0
$\text{CH}_4 + \text{D} \rightarrow \text{CH}_3\cdot + \text{HD}$ METHANE + DEUTERIUM ATOM 72 KON REACTION ORDER: 2.	523-673	8.3(+12)	0	5100		
$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\cdot + \text{H}_2\text{O}$ METHANE + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+13)	0	2500±250	0.5	2.0
$\text{CH}_4 + \text{CH} \rightarrow \text{CH}_3\cdot + \cdot\text{CH}_2$ METHANE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.5(+11)	0.7	3000±2500	0.3	3.2
$\text{CH}_4 + \text{CH}_2 \rightarrow \text{CH}_3\cdot + \text{CH}_3\cdot$ METHANE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.3(+12)	0.7	10000±2500	0.3	3.2
$\text{CH}_4 + \text{CH}_3\cdot \rightarrow \text{CH}_3\cdot + \text{CH}_4$ METHANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	450-800	4.0(+11)	0	7045±250	0.7	1.3
$\text{CH}_3\text{D} + \text{CD}_3\cdot \rightarrow \text{CH}_3\cdot + \text{CD}_4$ METHANE-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-650	5.0(+10)	0	7200±500	0.5	1.5
$\text{CHD}_3 + \text{CH}_3\cdot \rightarrow \text{CD}_3\cdot + \text{CH}_4$ METHANE-d ₃ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-650	1.1(+11)	0	6995±250	0.7	1.3
$\text{CD}_4 + \text{CH}_3\cdot \rightarrow \text{CD}_3\cdot + \text{CDH}_3$ METHANE-d ₄ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	370-550	2.5(+11)	0	7700±500	0.5	1.5
$\text{CD}_4\cdot + \text{CD}_3\cdot \rightarrow \text{CD}_3\cdot + \text{CD}_4$ METHANE-d ₄ + METHYL-d ₃ FREE RADICAL 72 KON REACTION ORDER: 2.	473-623	4.1(+12)	0	8960±250		
$\text{CH}_4 + \text{CN} \rightarrow \text{HCN} + \text{CH}_3\cdot$ METHANE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.7	2500±2500	0.3	3.2
$\text{CH}_4 + \text{M} \rightarrow \text{CH}_3\cdot + \text{H} + \text{M}$ METHANE 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+17)	0	44035±1000	0.5	2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
.CHO → CO + H METHYL, OXO-, FREE RADICAL 76 BEN/O'N REACTION ORDER: 1.	298	5.0(+13)	0	9560		
.CHO + O → CO ₂ + H METHYL, OXO-, FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0	0±1500		
NOTE: k ESTIMATED.						
.CHO + O → CO + OH METHYL, OXO-, FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	1.0	250±1500		
NOTE: k ESTIMATED.						
.CHO + O ₂ → CO + HO ₂ METHYL, OXO-, FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500-2500	1.6(+12)	0	3500±1500		
NOTE: k ESTIMATED.						
.CHO + H → CO + H ₂ METHYL, OXO-, FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.6(+12)	0.5	0±2500	0.3	3.2
.CHO + OH → CO + H ₂ O METHYL, OXO-, FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+10)	1.0	0±1500		
NOTE: k ESTIMATED.						
.CHO + HO ₂ → HCHO + O ₂ METHYL, OXO-, FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+14)	0	1500±1500		
NOTE: k ESTIMATED.						
.CHO + N → HCN + O METHYL, OXO-, FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+14)	0	0±1000		
NOTE: k ESTIMATED.						
.CHO + N → CO + NH METHYL, OXO-, FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	1000±2500	0.3	3.2
.CHO + NO → CO + HNO METHYL, OXO-, FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	1000±2500	0.3	3.2
.CHO + HNO → HCHO + NO METHYL, OXO-, FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.5	0±2500	0.3	3.2
.CHO + CH → CO + CH ₂ METHYL, OXO-, FREE RADICAL + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+10)	0.7	500±2500	0.3	3.2
.CHO + CH ₂ → CO + CH ₃ METHYL, OXO-, FREE RADICAL + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+10)	0.7	500±2500	0.3	3.2
.CHO + CH ₃ → CO + CH ₄ METHYL, OXO-, FREE RADICAL + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.5	0±2500	0.3	3.2
.CHO + .CHO → HCHO + CO METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.6(+11)	0.5	0±2500	0.3	3.2
.CHO + CN → HCN + CO METHYL, OXO-, FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	0±2500	0.3	3.2
HCHO + O → .CHO + OH FORMALDEHYDE + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	1.0	1750±1000	0.5	2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
HCHO + O → products FORMALDEHYDE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	300	9.0(+10)	-	-	0.7 1.3
HCDO + O → products FORMALDEHYDE-d + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	300	4.9(+10)	-	-	0.7 1.3
HCHO + H → .CHO + H ₂ FORMALDEHYDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.3(+10)	1.0	1600	0.3 3.2
HCHO + OH → .CHO + H ₂ O FORMALDEHYDE + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+10)	1.0	0±1500	0.5 2.0
HCHO + HO ₂ → .CHO + H ₂ O ₂ FORMALDEHYDE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: k FACTORS ARE: f = 0.1; F = 10. AT 300K.	300-800	1.0(+12)	0	4000	0.7 1.5
HCHO + CH → .CHO + CH ₂ FORMALDEHYDE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.7	2000±2500	0.3 3.2
HCHO + CH ₂ → .CHO + CH ₃ FORMALDEHYDE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	2.0(+11)	0	3270±1500	- -
HCHO + CH ₃ → .CHO + CH ₄ FORMALDEHYDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. 76 ENG	300-500 1500-2500	1.1(+11) 1.0(+10)	0 0.5	3070±500 3000±2500	0.5 1.5 0.3 3.2
DCDO + CH ₃ → .CDO + CH ₃ D FORMALDEHYDE-d + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	1.4(+11)	0	3975±500	0.5 1.5
HCHO + CN → .CHO + HCN FORMALDEHYDE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.3(+11)	0.7	1500±2500	0.3 3.2
HCHO + M → .CHO + H + M FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+17)	0	43800±2500	0.3 3.2
CH ₂ OH → HCHO + H METHYL, HYDROXY-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 2.	673-773	1.1(+13)	0	14600	
CH ₃ O. + O → HCHO + OH METHOXY FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	0±1500	
CH ₃ O. + O ₂ → HCHO + HO ₂ METHOXY FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+12)	0	3000±1500	
CH ₃ O. + H → HCHO + H ₂ METHOXY FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	0±1500	
CH ₃ O. + OH → HCHO + H ₂ O METHOXY FREE RADICAL + HYDROXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+13)	0	0±1500	
CH ₃ O. + N → HCHO + NH METHOXY FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+14)	0	0±1500	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3\text{O} \cdot + \text{M} \rightarrow \text{HCHO} + \text{H} + \text{M}$ METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	4.0(+40)	-7.5	11375±1500		
$\text{CH}_3\text{OH} + \text{CH}_3 \cdot \rightarrow \cdot\text{CH}_2\text{OH} + \text{CH}_4$ METHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.9(+11)	0	5035±500	0.6	1.4
$\text{CH}_3\text{OH} + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{O} \cdot + \text{CH}_4$ METHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.		6.2(+10)	0	4900±500	0.6	1.4
$\text{CH}_3\text{OH} + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{O} \cdot + \cdot\text{CH}_2\text{OH} + \text{CH}_4$ METHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-550	2.3(+11)	0	4930±500	0.6	1.4
$\text{CH}_3\text{OD} + \text{CD}_3 \cdot \rightarrow \cdot\text{CH}_2\text{OD} + \text{CD}_3\text{H}$ METHANOL-d - METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-500	1.9(+11)	0	5000±500	0.5	2.0
$\text{CH}_3\text{OD} + \text{CD}_3 \cdot \rightarrow \text{CH}_3\text{O} \cdot + \text{CD}_4$ METHANOL-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: GIVEN WITH CAUTION.	400-500	3.2(+10)	0	5700±1000	0.5	2.0
$\text{CD}_3\text{OH} + \text{CH}_3 \cdot \rightarrow \cdot\text{CD}_2\text{OH} + \text{CH}_3\text{D}$ METHAN-d ₃ -OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	370-550	2.0(+11)	0	5940±500		
$\text{CD}_3\text{OH} + \text{CH}_3 \cdot \rightarrow \text{CD}_3\text{O} \cdot + \text{CH}_4$ METHAN-d ₃ -OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	370-550	6.2(+10)	0	4900±500	0.6	1.4
$\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O} \cdot + \text{OH}$ HYDROPEROXIDE, METHYL 70 BEN/O'N REACTION ORDER: 1. NOTE: RATE CONSTANTS MAY BE SLIGHTLY LOW.	565-651	7.9(+14)	0	21640		
$\text{CS} + \text{O} \rightarrow \text{S} + \text{CO}$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	300	1.3(+13)	-	-	0.5	1.5
$\text{CS} + \text{O} \rightarrow \text{S} + \text{CO}$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CS} + \text{O} \rightarrow \text{SO} + \text{C}$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	28940		
$\text{CS} + \text{H} \rightarrow \text{S} + \text{CH}$ CARBON MONOSULFIDE FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+13)	0.5	50930		
$\text{CS} + \text{H} \rightarrow \text{SH} + \text{C}$ CARBON MONOSULFIDE FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	48870		
$\text{CS} + \text{S} \rightarrow \text{S} + \text{CS}$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CS} + \text{S} \rightarrow \text{C} + \text{S}_2$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	40463		
$\text{CS} + \text{S} + \text{M} \rightarrow \text{CS}_2 + \text{M}$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 3. NOTE: $k_1 = Kk_{-1}$	1800-3700	8.7(+13)	0	4370	0.5	1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
CS + N → S + CN CARBON MONOSULFIDE FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	1160	
CS + N → C + NS CARBON MONOSULFIDE FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	37200	
CS + C → S + C ₂ CARBON MONOSULFIDE FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		5.0(+11)	0.5	20435	
CS + C → C + CS CARBON MONOSULFIDE FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CS ₂ + O → CS + SO CARBON DISULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	200-1000	2.2(+13)	0	700	0.7 1.3
CS ₂ + O → COS + S CARBON DISULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	302	2.2(+11)	-	-	0.5 1.5
CS ₂ + S → CS + S ₂ CARBON DISULFIDE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2.	298	3.9(+11)	-	-	0.5 1.5
CS ₂ + M → CS + S + M CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2. M: AR	1800-3700	2.6(+15)	0	38960±9000	0.5 1.5
COS + O → CO + SO CARBON OXIDE SULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 ABOVE 300K.	190-1200	1.6(+13)	0	2250±250	0.5 1.5
COS + H → CO + HS CARBON OXIDE SULFIDE 76 BAU/DRY REACTION ORDER: 2.	298	1.3(+10)	-	-	0.8 1.3
COS + S → CO + S ₂ CARBON OXIDE SULFIDE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2.	230-2600	1.7(+12)	0	2050±230	0.3 3.0
CH ₃ S. + CH=CH → CH ₃ SCH=CH. METHYLTHIO FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2.	298-333	7.9(+ 7)	-	-	
CH ₃ S. + CH ₂ =CH ₂ → CH ₃ SCH ₂ CH ₂ . METHYLTHIO FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	298	4.8(+ 8)	-	-	
CH ₃ S. + CH ₃ CH=CHCH ₃ → CH ₃ CH(SCH ₃)CH(.)CH ₃ METHYLTHIO FREE RADICAL + 2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: cis-trans EQUILIBRIUM - WEIGHTED k.	298-333	1.6(+ 9)	-	-	
CH ₃ SH → CH ₃ . + SH METHANETHIOL 70 BEN/O'N REACTION ORDER: 1.	1005-1102	3.2(+15)	0	38550	
CH ₃ SH + CH ₃ . → CH ₃ S. + .CH ₂ SH + CH ₄ METHANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	303	1.2(+ 8)	-	-	0.5 2.0
CD ₃ SH + CH ₃ . → CD ₃ S. + CH ₄ METHANE-d ₃ -THIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-500	1.1(+11)	0	2065±500	0.5 2.0
CD ₃ SH + CH ₃ . → .CD ₂ SH + CH ₃ D METHANE-d ₃ -THIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-500	7.6(+10)	0	4200±250	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CN} + \text{O} \rightarrow \text{N} + \text{CO}$ CYANOGEN FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+12)	0	0±2500	0.3	3.2
$\text{CN} + \text{O} \rightarrow \text{NO} + \text{C}$ CYANOGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	14545		
$\text{CN} + \text{O}_2 \rightarrow \text{NO} + \text{CO}$ CYANOGEN FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+11)	0	0±5000	0.3	3.2
$\text{CN} + \text{H} \rightarrow \text{N} + \text{CH}$ CYANOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+12)	0.5	49775		
$\text{CN} + \text{H} \rightarrow \text{NH} + \text{C}$ CYANOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+13)	0.5	52745		
$\text{CN} + \text{H} + \text{M} \rightarrow \text{HCN} + \text{M}$ CYANOGEN FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 3.	1500–2500	3.2(+16)	–0.5	0±2500	0.3	3.2
$\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$ CYANOGEN FREE RADICAL + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	2500±1500		
$\text{CN} + \text{OH} \rightarrow \text{HCN} + \text{O}$ CYANOGEN FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	1500±1500		
$\text{CN} + \text{S} \rightarrow \text{N} + \text{CS}$ CYANOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CN} + \text{S} \rightarrow \text{C} + \text{NS}$ CYANOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+12)	0.5	32010		
$\text{CN} + \text{N} \rightarrow \text{C} + \text{N}_2$ CYANOGEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CN} + \text{NO} \rightarrow \text{CO} + \text{N}_2$ CYANOGEN FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+11)	0	0±2500	0.3	3.2
$\text{CN} + \text{NH} \rightarrow \text{HCN} + \text{N}$ CYANOGEN FREE RADICAL + IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	1000±2500	0.3	3.2
$\text{CN} + \text{HNO} \rightarrow \text{HCN} + \text{NO}$ CYANOGEN FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	4.0(+11)	0.5	0±2500	0.3	3.2
$\text{CN} + \text{C} \rightarrow \text{N} + \text{C}_2$ CYANOGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+11)	0.5	19300		
$\text{CN} + \text{C} \rightarrow \text{C} + \text{CN}$ CYANOGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
$\text{CN} + \text{CH}_2 \rightarrow \text{HCN} + \text{CH}$ CYANOGEN FREE RADICAL + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	2500±1500		
$\text{CN} + \text{CH}_3 \rightarrow \text{HCN} + \text{CH}_2$ CYANOGEN FREE RADICAL + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.7	1500±2500		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CN} + \text{CH}_4 \rightarrow \text{HCN} + \text{CH}_3$ CYANOGEN FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+11)	0.7	2500±2500	0.3 3.2
$\text{CN} + \text{CHO} \rightarrow \text{CO} + \text{HCN}$ CYANOGEN FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.5	0±2500	0.3 3.2
$\text{CN} + \text{HCHO} \rightarrow \text{HCN} + \text{CHO}$ CYANOGEN FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.3(+11)	0.7	1500±2500	0.3 3.2
$\text{C}(\text{NO}_2)_4 \rightarrow \text{C}(\text{NO}_2)_3 + \text{NO}_2$ METHANE, TETRANITRO- 70 BEN/O'N REACTION ORDER: 1.	443-506	3.4(+17)	0	20575	
$\text{HCN} + \text{OH} \rightarrow \text{CN} + \text{H}_2\text{O}$ HYDROCYANIC ACID + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.6	2500±2500	0.3 3.2
$\text{CH}_3\text{NH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{NH} \cdot + \text{CH}_2\text{NH}_2 + \text{CH}_4$ METHANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	2.1(+11)	0	4330±500	0.7 1.3
$\text{CH}_3\text{NH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_2\text{NH}_2 + \text{CH}_4$ METHANAMINE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	388-617	5.4(+11)	0	5020±500	0.3 3.0
$\text{CH}_3\text{ND}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{ND} \cdot + \text{CH}_3\text{D}$ METHANAMINE-d ₂ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-450	2.0(+11)	0	5135±1000	0.5 1.5
$\text{CH}_3\text{ND}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_2\text{ND}_2 + \text{CH}_4$ METHANAMINE-d ₂ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-450	1.4(+11)	0	4530±500	0.7 1.3
$\text{CD}_3\text{NH}_2 + \text{CH}_3 \cdot \rightarrow \text{CD}_2\text{NH}_2 + \text{CH}_3\text{D}$ METHAN-d ₃ -AMINE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	400-500	7.2(+10)	0	5100±500	0.5 1.5
$\text{CD}_3\text{NH}_2 + \text{CH}_3 \cdot \rightarrow \text{CD}_3\text{NH} \cdot + \text{CH}_4$ METHAN-d ₃ -AMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-500	2.0(+11)	0	4530±750	0.5 2.0
$\text{CH}_2=\text{N}=\text{N} \rightarrow \text{CH}_2 + \text{N}_2$ METHANE, DIAZO- 70 BEN/O'N REACTION ORDER: 1.	498-723	1.0(+13)	0	17600	
$\text{CH}_3\text{NHNH}_2 \rightarrow \text{CH}_3\text{NH} \cdot + \text{NH}_2$ HYDRAZINE, METHYL- 70 BEN/O'N REACTION ORDER: 1. NOTE: SUSPECT ARRHENIUS FACTORS.	746-862	5.0(+16)	-	32600	
$\text{CH}_3\text{NHNH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{N}(\cdot)\text{NH}_2 + \text{CH}_3\text{NHNH} \cdot$ $+ \text{CH}_2\text{NHNH}_2 + \text{CH}_4$ HYDRAZINE, METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	420	6.3(+ 8)	-	-	
$\text{CH}_3\text{NO} \rightarrow \text{CH}_2=\text{NOH}$ METHANE, NITROSO- 70 BEN/O'N REACTION ORDER: 1.	633-698	7.9(+12)	0	19800	
$\text{HCONH}_2 + \text{CH}_3 \cdot \rightarrow \text{HCONH} \cdot + \text{CONH}_2 + \text{CH}_4$ FORMAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.6(+10)	0	3300±5000	0.5 1.5
$\text{HCOND}_2 + \text{CH}_3 \cdot \rightarrow \text{HCOND} \cdot + \text{CH}_3\text{D}$ FORMAMIDE-N, N-d ₂ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	4900±500	0.5 2.0

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{HCOND}_2 + \text{CH}_3 \rightarrow \text{COND}_2 + \text{CH}_4$ FORMAMIDE-N,N-d ₂ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	5.5(+10)	0	3575±500	0.5 2.0
$\text{CH}_3\text{ONO} \rightarrow \text{CH}_3\text{O} + \text{NO}$ NITROUS ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	453-513	4.0(+15)	0	20700	
$\text{CH}_3\text{NO}_2 \rightarrow \text{CH}_3 + \text{NO}_2$ METHANE, NITRO- 70 BEN/O'N REACTION ORDER: 1.	660	4.0(+15)	0	29700	
$\text{CH}_3\text{NO}_2 + \text{CH}_3 \rightarrow \text{CH}_2\text{NO}_2 + \text{CH}_4$ METHANE, NITRO- + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-500	1.0(+11)	0	5100±750	0.4 2.5
$\text{CH}_3\text{ONO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_2$ NITRIC ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	483-513	3.2(+15)	0	20030	
$\text{CH}_3\text{ONH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{ONH} + \text{CH}_4$ HYDROXYLAMINE, O-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	5.0(+10)	0	2265±500	0.5 1.5
$\text{CH}_3\text{OND}_2 + \text{CH}_3 \rightarrow \text{CHO}_3\text{ND} + \text{CH}_3\text{D}$ HYDROXYLAMINE-N,N-d ₂ , O-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	3.5(+10)	0	2970±500	0.5 1.5
$\text{C}_2 + \text{O} \rightarrow \text{C} + \text{CO}$ CARBON DIMER + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{C}_2 + \text{H} \rightarrow \text{C} + \text{CH}$ CARBON DIMER + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+13)	0.5	30450	
$\text{C}_2 + \text{S} \rightarrow \text{C} + \text{CS}$ CARBON DIMER + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{C}_2 + \text{N} \rightarrow \text{C} + \text{CN}$ CARBON DIMER + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{C}_2 + \text{C} \rightarrow \text{C} + \text{C}_2$ CARBON DIMER + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{CCO} + \text{CH}\equiv\text{CH} \rightarrow \text{products}$ CARBON OXIDE(C ₂ O) + ETHYNE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.3 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	304	-	-	-	
$\text{CCO} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CO} + \text{CH}_3\text{CH}=\text{C}=\text{CH}_2$ CARBON OXIDE(C ₂ O) + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 5.7 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$\text{CCO} + \text{CH}_3\text{C}\equiv\text{CCH}_3 \rightarrow \text{products}$ CARBON OXIDE(C ₂ O) + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 8.5 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	304	-	-	-	
$\text{CCO} + \text{CH}_2=\text{CHCH}=\text{CH}_2 \rightarrow \text{CO} + \text{CH}_2=\text{C}=\text{CHCH}=\text{CH}_2$ CARBON OXIDE(C ₂ O) + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 210. NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	298	-	-	-	
$\text{CCO} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}=\text{CH}_2 + \text{CO}$ CARBON OXIDE(C ₂ O) + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 7.0 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	298	-	-	-	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CCO} + \text{cis-CH}_3\text{CH=CHCH}_3 \rightarrow \text{CO} + \text{cis-CH}_3\text{CH=C=CHCH}_3$ CARBON OXIDE(C ₂ O) + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 9.1 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$\text{CCO} + \text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow \text{CO} + \text{trans-CH}_3\text{CH=C=CHCH}_3$ CARBON OXIDE(C ₂ O) + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 10.6 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$\text{CCO} + (\text{CH}_3)_2\text{C=CH}_2 \rightarrow \text{CO} + (\text{CH}_3)_2\text{C=C=CH}_2$ CARBON OXIDE(C ₂ O) + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 50.0 NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$\text{CCO} + (\text{CH}_3)_2\text{C=CHCH}_3 \rightarrow \text{CO} + (\text{CH}_3)_2\text{C=C=CHCH}_3$ CARBON OXIDE(C ₂ O) + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 100. NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	298	-	-	-	
$\text{CCO} + (\text{CH}_3)_2\text{C=C(CH}_3)_2 \rightarrow \text{CO} + (\text{CH}_3)_2\text{C=C=C(CH}_3)_2$ CARBON OXIDE(C ₂ O) + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 250. NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	298	-	-	-	
$\text{CCO} + (\text{CH}_3)_2\text{C=C=C(CH}_3)_2 \rightarrow \text{CO} + (\text{CH}_3)_2\text{C=C=C(CH}_3)_2$ CARBON OXIDE(C ₂ O) + 2,3-PENTADIENE, 2,4-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 113. NOTE: k _{ref} : $\text{CCO} + \text{CH}_2=\text{CH}_2$	304	-	-	-	
$\text{CH=CH} + \text{O} \rightarrow \text{products}$ ETHYNE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	200-700	1.4(+13)	0	1500	0.8 1.2
$\text{CH=CH} + \text{OH} \rightarrow \text{CH=C.} + \text{H}_2\text{O}$ ETHYNE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-2000	7.6(+12)	0	2335+400	0.5 2.1
$\text{CH=CH} + \text{S} \rightarrow \text{cy-CH=CHS}$ ETHYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	1.7(+11)	-	-	
$\text{CH=CH} + \text{N} \rightarrow \text{C}_2\text{H}_2\text{N}$ ETHYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: UPPER LIMIT.	440	2.0(+ 9)	-	-	
$\text{CH=CH} + \text{CH}_3. \rightarrow \text{CH=C.} + \text{CH}_4$ ETHYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: GIVEN WITH CAUTION.	473-773	-	-	7100	
$\text{CH=CH} + \text{CH}_3. \rightarrow \text{CH}_3\text{CH=CH.}$ ETHYNE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	371-479	2.5(+11)	0	3900	
$\text{CH=CH} + \text{CH}_3\text{S.} \rightarrow \text{CH}_3\text{SCH=CH.}$ ETHYNE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298-333	7.9(+ 7)	-	-	
$\text{CH=CH} + \text{CCO} \rightarrow \text{products}$ ETHYNE + CARBON OXIDE(C ₂ O) 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.3 NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	304	-	-	-	
$\text{CH=CH} + \text{CH}_3\text{CH}_2. \rightarrow \text{CH}_3\text{CH}_2\text{CH=CH.}$ ETHYNE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	373-473	5.0(+10)	0	3500	
$\text{CH=CH} + (\text{CH}_3)_2\text{CH.} \rightarrow (\text{CH}_3)_2\text{CHCH=CH.}$ ETHYNE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.		5.0(+10)	0	3475	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}=\text{CH} + (\text{CH}_3)_3\text{C} \cdot \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH} \cdot$ ETHYNE + ETHYL, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	363-577	1.0(+11)	0	3875		
$\text{cis-CDH}=\text{CDH} \rightarrow \text{trans-CDH}=\text{CHD}$ $\text{cis-ETHENE-1,2-d}_2$ 70 BEN/O'N REACTION ORDER: 1.	723-823	1.0(+13)	0	32700		
$\text{CH}_2=\text{CH}_2 + \text{O} \rightarrow \text{cy-CH}_2\text{CH}_2\text{O}$ ETHENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	200-500	3.3(+12)	0	565	0.8	1.2
$\text{CH}_2=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2 \cdot$ ETHENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	9.3(+13)	0	1410		
$\text{CH}_2=\text{CH}_2 + \text{H} + \text{M} \rightarrow \text{CH}_3\text{CH}_2 \cdot + \text{M}$ ETHENE + HYDROGEN ATOM 72 KON REACTION ORDER: 3. M: H_2	298-813	5.6(+17)	0.5	495		
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_2=\text{CH} \cdot + \text{H}_2\text{O}$ ETHENE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.	3500-1400	1.6(+14)	0	2831+445	0.4	2.4
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \cdot\text{CH}_2\text{CH}_2\text{OH}$ ETHENE + HYDROXYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.		1.1(+12)	-	-	0.8	1.3
$\text{CH}_2=\text{CH}_2 + \text{HO}_2 \rightarrow \text{products}$ ETHENE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: RATIO DATA VERSUS k _{ref} . FOR $\text{HO}_2 + \text{CO} \rightarrow \text{CO}_2 + \text{OH}$ k FACTORS MIGHT BE HIGH.	300	1.0(+ 7)	-	-	0.1	10.
$\text{CH}_2=\text{CH}_2 + \text{S} \rightarrow \text{cy-CH}_2\text{CH}_2\text{S}$ ETHENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	8.1(+11)	-	-		
$\text{CH}_2=\text{CH}_2 + \text{N} \rightarrow \text{products}$ ETHENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	320-550	2.0(+10)	0	353		
$\text{CH}_2=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_2=\text{CH} \cdot + \text{CH}_4$ ETHENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	4.2(+11)	0	5600±500	0.5	1.5
$\text{CH}_2=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 \cdot$ ETHENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	353-453	3.3(+11)	0	3900		
$\text{CH}_2=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 \cdot + (\text{CH}_3)_2\text{CH} \cdot$ ETHENE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	350-705	2.0(+11)	0	3575±105	0.8	1.3
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{S} \cdot \rightarrow \text{CH}_3\text{SCH}_2\text{CH}_2 \cdot$ ETHENE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	4.8(+ 8)	-	-		
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \cdot$ ETHENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	348-482	1.6(+11)	0	3675		
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \cdot$ ETHENE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	375-503	1.9(+10)	0	3070		
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{CH} \cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2 \cdot$ ETHENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	340-457	6.9(+10)	0	3475		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ ETHENE + BUTYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	352-405	2.3(+10)	0	3370	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_3\text{C}\cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2\cdot$ ETHENE + ETHYL, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	300-650	2.8(+10)	0	3575	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot \rightarrow (\text{CH}_3)_2\text{CH}(\text{CH}_2)_3\text{CH}_2\cdot$ ETHENE + BUTYL, 3-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	340-413	1.2(+10)	0	3235	
$\text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_2=\text{CH}_2 + \text{H}$ ETHYL FREE RADICAL 72 KON REACTION ORDER: 1.	673-893	2.3(+14)	0	19990±355	0.6 1.6
$\text{CH}_3\text{CH}_2\cdot + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_3 + \text{H}$ ETHYL FREE RADICAL + HYDROGEN MOLECULE 72 KON REACTION ORDER: 2.	473-823	3.0(+11)	0	5435	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}=\text{CH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}\cdot$ ETHYL FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2.	373-473	5.0(+10)	0	3500	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}\cdot$ ETHYL FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	348-482	1.6(+11)	0	3675	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ ETHYL FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2.	379-465	3.2(+11)	0	4630	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHCH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{OH}$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{OH}$ ETHYL FREE RADICAL + 2-PROPEN-1-OL 72 KER/PAR REACTION ORDER: 2.	323-415	1.9(+11)	0	3901	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHCN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + 2-PROPENENITRILE 72 KER/PAR REACTION ORDER: 2.	323-454	6.2(+10)	0	1700	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ ETHYL FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	3675	
$\text{CH}_3\text{CH}_2\cdot + \text{cis-CH}_3\text{CH}=\text{CHCH}_2\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4265	
$\text{CH}_3\text{CH}_2\cdot + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4350	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{COOCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + ACETIC ACID ETHENYL ESTER 72 KER/PAR REACTION ORDER: 2.	303-417	7.8(+10)	0	3475	
$\text{CH}_3\text{CH}_2\cdot + \text{cis-CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ $+ \text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + cis-2-BUTENENITRILE 72 KER/PAR REACTION ORDER: 2.	323-454	1.5(+10)	0	2500	
$\text{CH}_3\text{CH}_2\cdot + \text{trans-CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ $+ \text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + trans-2-BUTENENITRILE 72 KER/PAR REACTION ORDER: 2.	323754	3.1(+10)	0	2600	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{C}(\text{CH}_3)\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CN}$ $+ \text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + 2-PROPENENITRILE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	312-400	2.5(+11)	0	2300	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}_2\cdot + \text{cis-CH}_3\text{CH}_2\text{CH=CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	—	—	4300	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_2\text{CHCH=CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ ETHYL FREE RADICAL + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	—	—	3620	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{COOCH}_2\text{CH=CH}_2 \rightarrow \text{CH}_3\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + ACETIC ACID 2-PROPENYL ESTER 72 KER/PAR REACTION ORDER: 2.	308-448	2.5(+11)	0	3900	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{COCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \cdot\text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3$ ETHYL FREE RADICAL + 3-PENTANONE 72 KON REACTION ORDER: 2.	300-520	2.8(+11)	0	3986+100	0.4 2.2
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ $+ \cdot\text{CH}_2\text{C}(\text{CH}_2)(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ ETHYL FREE RADICAL + 1,3-BUTADIENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.	318-414	1.6(+11)	0	2265	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_3\text{CH=CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-HEXENE 72 KER/PAR REACTION ORDER: 2.	338-435	3.9(+10)	0	3400	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH=CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + PROPANOIC ACID 2-PROPENYL ESTER 72 KER/PAR REACTION ORDER: 2.	352-435	2.5(+11)	0	3875	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{O}(\text{CH}_2)_3\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{O}(\text{CH}_2)_3\text{CH}_3$ ETHYL FREE RADICAL + BUTANE, 1-ETHENYLOXY- 72 KER/PAR REACTION ORDER: 2.	303-435	2.5(+10)	0	3070	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_4\text{C}\equiv\text{CH} \rightarrow \text{CH}_3((\text{CH}_2)_4\text{C}(\cdot)=\text{CHCH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH}\cdot$ ETHYL FREE RADICAL + 1-HEPTYNE 72 KER/PAR REACTION ORDER: 2.	300-455	3.9(+11)	0	4430	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_4\text{CH=CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-HEPTENE 72 KER/PAR REACTION ORDER: 2.	359-439	6.2(+10)	0	3500	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 \rightarrow$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-BUTENE, 2,3,3-TRIMETHYL- 72 KER/PAR REACTION ORDER: 2.	322-364	7.8(+ 9)	0	2800	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_2\text{C=CHCH=C}(\text{CH}_3)_2 \rightarrow$ $(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH=C}(\text{CH}_3)_2$ $+ (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CH=C}(\text{CH}_3)_2$ ETHYL FREE RADICAL + 2,4-HEXADIENE, 2,5-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.	328-420	6.2(+10)	0	3300	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_5\text{CH=CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-OCTENE 72 KER/PAR REACTION ORDER: 2.	339-425	1.2(+11)	0	3825	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow$ $(\text{CH}_3)_3\text{CCH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ (\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-PENTENE, 2,4,4-TRIMETHYL- 72 KER/PAR REACTION ORDER: 2.	309-364	1.9(+10)	0	2870	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\cdot + \text{CH}_3\cdot$ ETHANE 70 BEN/O'N REACTION ORDER: 1.	298-858	5.6(+16)	0	45045	
$\text{CH}_3\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{OH}$ ETHANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.		2.5(+13)	0	3200	0.7 1.3
$\text{CH}_3\text{CH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{H}_2$ ETHANE + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	285-1440	1.0(+14)	0	4815±70	0.8 1.2
$\text{CH}_3\text{CH}_3 + \text{OH} \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{H}_2\text{O}$ ETHANE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.		1.3(+14)	0	1998	
$\text{CH}_3\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{H}_2\text{O}_2$ ETHANE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} FOR $\text{HO}_2 + \text{CO} \rightarrow \text{HO} + \text{CO}_2$	300-1000	1.0(+12)	0	7000	0.1 10.
$\text{CH}_3\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{CH}_4$ ETHANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.		5.6(+11)	0	5840±250	0.7 1.3
$\text{CH}_3\text{CH}_3 + \text{CD}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{CD}_3\text{H}$ ETHANE + METHYL-d ₃ FREE RADICAL 72 KON REACTION ORDER: 2.	390-800	1.0(+12)	0	6085±165	0.7 1.4
$\text{CH}_3\text{CD}_3 + \text{CD}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\cdot + \text{CD}_4$ ETHANE-1,1,1-d ₃ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	500-750	4.3(+11)	0	6845±250	0.7 1.3
$\text{CD}_3\text{CH}_3 + \text{CD}_3\cdot \rightarrow \text{CD}_3\text{CH}_2\cdot + \text{CD}_3\text{H}$ ETHANE-1,1,1-d ₃ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.		3.0(+11)	0	5900±250	0.7 1.3
$\text{CD}_3\text{CD}_3 + \text{CH}_3\cdot \rightarrow \text{CD}_3\text{CD}_2\cdot + \text{CH}_3\text{D}$ ETHANE-d ₆ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	500-900	5.6(+11)	0	6600±250	0.7 1.3
$\text{CD}_3\text{CD}_3 + \text{CD}_3\cdot \rightarrow \text{CD}_3\text{CD}_2\cdot + \text{CD}_4$ ETHANE-d ₆ + METHYL-d ₃ FREE RADICAL 72 KON REACTION ORDER: 2.		4.6(+11)	0	6405	
$\text{CH}_2=\text{C}=\text{O} + \text{O} \rightarrow \text{products}$ ETHENONE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	5.3(+11)	-	-	0.7 1.3
$\text{HOOC}-\text{COOH} \rightarrow \text{HCOOH} + \text{CO}_2$ ETHANEDIOIC ACID 70 BEN/O'N REACTION ORDER: 1.	390-420	7.9(+11)	0	15100	
$\text{CH}_3\text{C}(\text{O})\cdot \rightarrow \text{CH}_3\cdot + \text{CO}$ ETHYL, 1-OXO-, FREE RADICAL 72 KON REACTION ORDER: 1.	273-413	1.5(+10)	0	6790±115	0.7 1.4
$\text{CH}_3\text{C}(\text{O})\cdot \rightarrow \text{CH}_3\cdot + \text{CO}$ ETHYL, 1-OXO-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.		2.0(+10)	0	7550	
$\text{CH}_3\text{CHO} + \text{O} \rightarrow \text{products}$ ACETALDEHYDE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-500	1.4(+13)	0	1140	0.5 2.0
$\text{CH}_3\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\text{O})\cdot + \text{CH}_4$ ACETALDEHYDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-525	8.5(+10)	0	3000±250	0.4 1.6
$\text{CH}_3\text{CDO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\text{O})\cdot + \text{CH}_3\text{D}$ ACETALDEHYDE-1-d + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	1.0(+11)	0	3975±500	0.5 1.5

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{cy-CH}_2\text{CH}_2\text{O} + \text{O} \rightarrow \text{products}$ OXIRANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	7.0(+ 8)	-	-	0.6	1.5
$\text{cy-CH}_2\text{CH}_2\text{O} + \text{CH}_3 \rightarrow \text{cy-CH}_2\text{CH}(\cdot)\text{O} + \text{CH}_4$ OXIRANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.5(+11)	0	5435±750	0.5	2.0
$\text{HCOOCH}_3 + \text{CH}_3 \rightarrow \cdot\text{COOCH}_3 + \text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-550	2.0(+11)	0	4900±500	0.5	1.5
$\text{HCOOCH}_3 + \text{CH}_3 \rightarrow \text{HCOOCH}_2 \cdot + \text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-550	1.6(+11)	0	5635±500	0.5	1.5
$\text{HCOOCH}_3 + \text{CH}_3 \rightarrow \cdot\text{COOCH}_3 + \text{HCOOCH}_2 \cdot + \text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-550	3.0(+11)	0	4980±500	0.5	1.5
$\text{DCOOCH}_3 + \text{CH}_3 \rightarrow \cdot\text{COOCH}_3 + \text{CH}_3\text{D}$ FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-550	2.5(+11)	0	5900±500	0.5	1.5
$\text{DCOOCH}_3 + \text{CH}_3 \rightarrow \text{DCOOCH}_2 \cdot + \text{CH}_4$ FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.		1.6(+11)	0	5635±500	0.5	1.5
$\text{CH}_3\text{COOH} \rightarrow \text{CH}_2=\text{C}=\text{O} + \text{H}_2\text{O}$ ACETIC ACID 70 BEN/O'N REACTION ORDER: 1. NOTE: SUSPECT VALUE.	773-973	8.9(+12)	0	33970		
$\text{CH}_3\text{COOD} + \text{CH}_3 \rightarrow \cdot\text{CH}_2\text{COOD} + \text{CH}_4$ ACETIC ACID-d + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-600	1.6(+11)	0	5135±500	0.6	1.4
$\text{CH}_3\text{CH}_2\text{O} \cdot \rightarrow \text{CH}_3 \cdot + \text{HCHO}$ ETHOXY FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	488-468	2.5(+13)	0	8805		
$\text{CH}_3\text{CH}_2\text{OH} + \text{O} \rightarrow \text{products}$ ETHANOL + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	8.7(+10)	-	-	0.6	1.5
$\text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{CH}_4$ ETHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-625	7.9(+10)	0	4730±500	0.6	1.4
$\text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{OH} + \text{CH}_4$ ETHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-625	4.0(+11)	0	4900±500	0.6	1.4
$\text{CH}_3\text{CH}_2\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{CH}_3\text{CH}(\cdot)\text{OH} + \cdot\text{CH}_2\text{CH}_2\text{OH} + \text{CH}_4$ ETHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-625	5.1(+11)	0	4900±500	0.6	1.4
$\text{CH}_3\text{CD}_2\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CD}(\cdot)\text{OH} + \text{CH}_3\text{D}$ ETHAN-1,1-d ₂ -OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-550	4.1(+11)	0	5735±500	0.6	1.4
$\text{CH}_3\text{CD}_2\text{OH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CD}_2\text{O} \cdot + \cdot\text{CH}_2\text{CD}_2\text{OH} + \text{CH}_4$ ETHAN-1,1-d ₂ -OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-550	7.1(+10)	0	4530±500	0.6	1.4
$\text{CH}_3\text{CH}_2\text{OD} + \text{CD}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{CD}_4$ ETHANOL-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-525	6.2(+10)	0	5135±500	0.5	2.0
$\text{CH}_3\text{CH}_2\text{OD} + \text{CD}_3 \cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{OD} + \cdot\text{CH}_2\text{CH}_2\text{OD} + \text{CD}_3\text{H}$ ETHANOL-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-525	4.4(+11)	0	4900±500	0.6	1.4

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_3\text{O} + \text{CH}_3$ METHANE, OXYBIS- 70 BEN/O'N REACTION ORDER: 1.	750-820	1.0(+16)	0	40765	
$\text{CH}_3\text{OCH}_3 + \text{O} \rightarrow \text{products}$ METHANE, OXYBIS-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	200-500	5.9(+12)	0	1520	0.7 1.3
$\text{CH}_3\text{OCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{OCH}_2 + \text{CH}_4$ METHANE, OXYBIS-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-550	4.2(+11)	0	5035±500	0.5 1.5
$\text{CH}_3\text{OOCH}_3 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{O}$ PEROXIDE, DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	393-452	4.0(+15)	0	18570	
$\text{CH}_3\text{OOCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{OOCH}_2 + \text{CH}_4$ PEROXIDE, DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	4.2(+11)	0	5000±1000	0.3 3.0
$\text{CH}_3\text{CH}_2\text{OOH} \rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{OH}$ HYDROPEROXYDE, ETHYL- 70 BEN/O'N REACTION ORDER: 1. NOTE: k PROBABLY RELIABLE.	553-653	2.2(+15)	0	21640	
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CD}_3 \rightarrow \text{cy-CH}_3\text{CH}(\cdot)\text{S} + \text{CD}_3\text{H}$ THYRANE + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	2.2(+11)	0	4800±500	0.5 2.0
$\text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_2=\text{CH}_2 + \text{H}_2\text{S}$ ETHANETHIOL 70 BEN/O'N REACTION ORDER: 1.	785-938	1.0(+13)	0	25900	
$\text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_3\text{CH}_2 + \cdot\text{SH}$ ETHANETHIOL 70 BEN/O'N REACTION ORDER: 1.	785-938	6.3(+15)	0	36336	
$\text{CH}_3\text{CH}_2\text{SH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{S} + \text{CH}_3\text{CH}(\cdot)\text{SH}$ $+ \cdot\text{CH}_2\text{CH}_2\text{SH} + \text{CH}_4$ ETHANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	3.5(+ 7)	-	-	0.5 2.0
$\text{CH}_3\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{CH}_3$ METHANE, SULFONYLBIS- 70 BEN/O'N REACTION ORDER: 1.	783-913	2.0(+14)	0	30500	
$\text{CH}_3\text{NC} \rightarrow \text{CH}_3\text{CN}$ METHANE, ISOCYANO- 70 BEN/O'N REACTION ORDER: 1.	472-533	4.0(+13)	0	19325	
$\text{CH}_3\text{CN} + \text{CH}_3 \rightarrow \cdot\text{CH}_2\text{CH} + \text{CH}_4$ ACETONITRILE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	5.4(+11)	0	5100±500	0.7 1.5
$\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{NH} + \text{CH}_3\text{CH}(\cdot)\text{NH}_2$ $+ \cdot\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{NH} + \text{CH}_4$ ETHANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	4600±500	0.5 2.0
$\text{CD}_3\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{D} + \text{CD}_3\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CD}_2\text{CH}_2\text{NH}_2$ ETHAN-2,2,2-d ₃ -AMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CD}_3\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{CD}_3\text{CH}_2\text{NH} + \text{CH}_4$ ETHAN-2,2,2-d ₃ -AMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	423	4.0(+ 5)	-	-	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3)_2\text{NH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} + \text{CH}_2\text{NH}(\text{CH}_3) + \text{CH}_4$ METHANAMINE, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	1.6(+11)	0	3500±500	0.5 2.0
$(\text{CH}_3)_2\text{NH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} + \text{CH}_4$ METHANAMINE, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	6.5(+10)	0	3200±500	0.5 2.0
$(\text{CH}_3)_2\text{ND} + \text{CH}_3 \rightarrow \text{CH}_2\text{NDCH}_3 + \text{CH}_4$ METHANAMINE-d, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4400±500	0.5 1.5
$(\text{CH}_3)_2\text{ND} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} + \text{CH}_3\text{D}$ METHANAMINE-d, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	4300±500	0.5 1.5
$\text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{N}=\text{N}$ DIAZENE, DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	552-600	3.2(+16)	0	26400	
$\text{CH}_3\text{N}=\text{NCH}_3 + \text{CH}_3 \rightarrow \text{CH}_2\text{N}=\text{NCH}_3 + \text{CH}_4$ DIAZENE, DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	1.1(+11)	0	3975±250	
$\text{CH}_3\text{N}=\text{NCH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NN}(\cdot)\text{CH}_3$ DIAZENE, DIMETHYL-, + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-450	5.0(+10)	0	3040±355	
$\text{CD}_3\text{N}=\text{NCD}_3 + \text{CD}_3 \rightarrow \cdot\text{CD}_2\text{N}=\text{NCD}_3 + \text{CD}_4$ DIAZENE, DI(METHYL-d ₃)-, + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	6.6(+10)	0	4125±500	
$\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \cdot\text{NHCH}_2\text{CH}_2\text{NH}_2$ $+ \text{NH}_2\text{CH}(\cdot)\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANEDIAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.8(+11)	0	4200±500	
$\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \cdot\text{NHCH}_2\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANEDIAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	4430±500	
$\text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3 \rightarrow \cdot\text{NDCH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3\text{D}$ ETHANDI(AMINE-d ₂) + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	3.2(+11)	0	5100±500	
$\text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3 \rightarrow \text{ND}_2\text{CH}(\cdot)\text{CH}_2\text{ND}_2 + \text{CH}_4$ ETHANEDI(AMINE-d ₂) + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	4025±500	
$(\text{CH}_3)_2\text{NNH}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NNH} + \text{CH}_4$ HYDRAZINE, 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.7(+11)	0	2870±500	
$(\text{CH}_3)_2\text{NNH}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NNH} + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{NH}_2 + \text{CH}_4$ HYDRAZINE, 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.4(+11)	0	2970±500	
$(\text{CH}_3)_2\text{NND}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NND} + \text{CH}_3\text{D}$ HYDRAZINE-d ₂ , 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.1(+11)	0	3400±500	
$(\text{CH}_3)_2\text{NND}_2 + \text{CH}_3 \rightarrow \text{CH}_2\text{N}(\text{CH}_3)\text{ND}_2 + \text{CH}_4$ HYDRAZINE-d ₂ , 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	3.2(+11)	0	4125±750	
$\text{CH}_3\text{NHNHCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{N}(\cdot)\text{NHCH}_3 + \cdot\text{CH}_2\text{NHNHCH}_3 + \text{CH}_4$ HYDRAZINE, 1,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	2400±250	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{NDNDCH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{N}(\cdot)\text{NDCH}_3 + \text{CH}_3\text{D}$ HYDRAZINE- d_2 , 1,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	2700±500	
$\text{CH}_3\text{CH=NOH} \rightarrow \text{CH}_3\text{CH=N} \cdot + \text{OH}$ ACETALDEHYDE, OXIME 70 BEN/O'N REACTION ORDER: 1.	603-713	6.8(+12)	0	23655	
$\text{HCONHCH}_3 + \text{CH}_3 \cdot \rightarrow \cdot\text{CONHCH}_3 + \text{HCON}(\cdot)\text{CH}_3$ $+ \text{HCONHCH}_2 \cdot + \text{CH}_4$ FORMAMIDE, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	7.9(+10)	0	3800±500	
$\text{CH}_3\text{CONH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CONH} \cdot + \cdot\text{CH}_2\text{CONH}_2 + \text{CH}_4$ ACETAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	2.1(+11)	0	5235±500	
$\text{CH}_3\text{CONH}_2 + \text{CH}_3 \cdot \rightarrow \cdot\text{CH}_2\text{CONH}_2 + \text{CH}_4$ ACETAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	1.0(+11)	0	5200±500	
$\text{CD}_3\text{CONH}_2 + \text{CD}_3 \cdot \rightarrow \cdot\text{CD}_2\text{CONH}_2 + \text{CD}_4$ ACETAMIDE-2,2,2- d_3 + METHYL- d_3 FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	1.4(+11)	0	5800±500	
$\text{CD}_3\text{CONH}_2 + \text{CD}_3 \cdot \rightarrow \text{CD}_3\text{CONH} \cdot + \text{CD}_3\text{H}$ ACETAMIDE-2,2,2- d_3 + METHYL- d_3 FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	1.1(+11)	0	5235±500	
$\text{CH}_3\text{CH}_2\text{NO}_2 \rightarrow \text{CH}_2=\text{CH}_2 + \text{HONO}$ ETHANE, NITRO- 70 BEN/O'N REACTION ORDER: 1.	583-715	2.5(+12)	0	22645	
$\text{CH}_3\text{CH}_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{NO}$ NITROUS ACID ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	484-505	1.2(+16)	0	20400	
$\text{CH}_3\text{CH}_2\text{ONO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{NO}_2$ NITRIC ACID ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	434-474	3.2(+16)	0	19830	
$\text{O}_2\text{NOCH}_2\text{CH}_2\text{ONO}_2 \rightarrow \text{products}$ 1,2-ETHANEDIOL, DINITRATE 70 BEN/O'N REACTION ORDER: 1.	358-378	7.9(+15)	0	19630	
$\text{CH}_3\text{N}(\text{O})\text{N}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{NO} + \text{CH}_3\text{NO}$ DIAZENE, DIMETHYL-1,2-DIOXIDE- 70 BEN/O'N REACTION ORDER: 1.	374-404	2.5(+13)	0	11600	
$\text{CH}_3\text{C}\equiv\text{CH} + \text{O} \rightarrow \text{products}$ 1-PROPYNE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	4.0(+11)	-	-	0.5 2.0
$\text{CH}_3\text{C}\equiv\text{CH} + \text{H} \rightarrow \text{CH}_3\text{CH=CH} \cdot + \text{CH}_3\text{C}(\cdot)=\text{CH}_2$ 1-PROPYNE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: k TAKEN AS LOWER LIMIT.	298	2.5(+11)	-	-	
$\text{CH}_3\text{C}\equiv\text{CH} + \text{S} \rightarrow \text{cy-CH}_3\text{C=CHS}$ 1-PROPYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	1.1(+12)	-	-	
$\text{CH}_3\text{C}\equiv\text{CH} + \text{N} \rightarrow \text{products}$ 1-PROPYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	320-550	6.9(+10)	0	745	
$\text{CH}_3\text{C}\equiv\text{CH} + \text{N} \rightarrow \text{products}$ 1-PROPYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: k_{ref} : $\text{CHCH} + \text{N}$	435	-	-	-	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{C}\equiv\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}\cdot + \text{CH}_3\text{C}(\cdot)=\text{CHCH}_3$ 1-PROPYNE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. CH_3 ADDITION OCCURS PREDOMINANTLY AT TERMINAL C ATOM.	379-465	5.0(+11)	0	4400	
$\text{CH}_3\text{C}\equiv\text{CH} + (\text{CH}_3)_2\text{CH}\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\cdot)\text{CH}_3$ 1-PROPYNE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.	360-439	1.9(+ 9)	0	2870	
$\text{CH}_3\text{C}\equiv\text{CH} + (\text{CH}_3)_3\text{C}\cdot \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}\cdot$ $+ (\text{CH}_3)_3\text{CCH}=\text{C}(\cdot)\text{CH}_3$ 1-PROPYNE + ETHYL-, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.	360-439	5.0(+ 8)	0	2770	
$\text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	373-483	2.0(+11)	0	4100	
$\text{CH}_3=\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)\text{CH}_2$ 1,2-PROPADIENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	379-465	3.2(+11)	0	4630	
$\text{CH}_2=\text{C}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	366-473	3.6(+10)	0	3660	
$\text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\cdot + \text{H}$ 1-PROPENE 70 BEN/O'N REACTION ORDER: 1.	953-1143	2.0(+15)	0	44900	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{O} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{O}$ 1-PROPENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	200-500	2.5(+12)	0	38	0.8 1.2
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ 1-PROPENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	298	11.2(+12)	0	1460	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_3$ 1-PROPENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: ARRHENIUS PARAMETERS ARE MINIMUM VALUES OF THEIR HIGH PRESSURE LIMITS.	298	7.2(+12)	0	600	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{OH} + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\cdot$ 1-PROPENE + HYDROXYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: ADDITION TO TERMINAL CARBON OF DOUBLE BOND IS PROBABLY 95%.	300	6.6(+12)	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	5.8(+12)	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 6.9$ NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S}$	298	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{S}^*(^1\text{D}) \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM(^1D) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.7$ NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S}^*(^1\text{D})$	300	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-PROPENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	320-550	1.2(+11)	0	655	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-PROPENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.8 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{N}$	435	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + {}^1\text{CH}_2 \rightarrow \text{products}$ 1-PROPENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.27 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$	297	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + {}^3\text{CH}_2 \rightarrow \text{products}$ 1-PROPENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.0 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$	297	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{C}(\cdot)=\text{CH}_2 + \text{CH}_4$ 1-PROPENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. 	350-600	1.4(+11)	0	4430±500	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow [\text{C}_3\text{H}_5\cdot] + \text{CH}_4$ 1-PROPENE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2. 	350-580	3.2(+10)	0	3775+300	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\cdot$ 1-PROPENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. 	353-453	1.7(+11)	0	3770	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\cdot$ 1-PROPENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 0.72 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$	453	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CCO} \rightarrow \text{CH}_3\text{CH}=\text{C}=\text{CH}_2 + \text{CO}$ 1-PROPENE + CARBON OXIDE(C_2O) 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 5.7 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	297	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ 1-PROPENE + PROPYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	381-412	6.3(+10)	0	3725	
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$ 1-PROPYL FREE RADICAL 72 KON REACTION ORDER: 1. 	300-750	5.8(+14)	0	16880±350	
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$ 1-PROPYL FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. 	297-564	4.0(+13)	0	16660	
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$ 1-PROPYL FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. 	298-723	6.3(+13)	0	1	9100
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ 1-PROPYL FREE RADICAL + ETHENE 72 KON REACTION ORDER: 2. NOTE: TENTATIVE k VALUE	375-503	1.9(+10)	0	3070	
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ 1-PROPYL FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. 	298	-	-	3630	
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ 1-PROPYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. 	298	-	-	4370	
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow$ $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ 1-PROPYL FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. 	298	-	-	4515	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ 1-PROPYL FREE RADICAL + 1-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	3410	
$(\text{CH}_3)_2\text{CH}\cdot \rightarrow \text{CH}_3 + \text{CH}_2=\text{CH}_2$ ETHYL, 1-METHYL-, FREE RADICAL 72 KON REACTION ORDER: 1.	690-814	1.9(+11)	0	16045±1150	
$(\text{CH}_3)_2\text{CD}\cdot \rightarrow \text{CH}_3\text{CD}=\text{CH}_2 + \text{H}\cdot$ ETHYL-1-d, 1-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	673-777	2.00(+14)	0	20800	
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}=\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{CH}\cdot$ ETHYL, 1-METHYL, FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	363-577	5.0(+10)	0	3475	
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ ETHYL, 1-METHYL-, FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	340-457	6.9(+10)	0	3475	
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\cdot)\text{CH}_3$ ETHYL, 1-METHYL-, FREE RADICAL + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.	360-439	1.90(+ 9)	0	2870	
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)=\text{CH}_2$ ETHYL, 1-METHYL-, FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	366-473	3.6(+10)	0	3600	
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ ETHYL, 1-METHYL-, FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	3480	
$(\text{CH}_3)_2\text{CH}\cdot + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}[\text{CH}(\text{CH}_3)_2]\text{CH}(\cdot)\text{CH}_3$ ETHYL, 1-METHYL-, FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	3950	
$(\text{CH}_3)_2\text{CH}\cdot + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}[\text{CH}(\text{CH}_3)_2]\text{CH}(\cdot)\text{CH}_3$ ETHYL, 1-METHYL-, FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4065	
$\text{CH}_3\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{products}$ PROPANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	9.0(+ 9)	-	-	0.7 2.0
$\text{CH}_3\text{CH}_2\text{CH}_3 + \text{H} \rightarrow (\text{CH}_3)_2\text{CH}\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{H}_2$ PROPANE + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	333-933	1.0(+13)	0	3130±180	
$\text{CH}_3\text{CH}_2\text{CH}_3 + \text{HO}_2 \rightarrow (\text{CH}_3)_2\text{CH}\cdot + \text{H}_2\text{O}_2$ PROPANE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} FOR $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300-1000	2.0(+11)	0	5300	
$\text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CH}\cdot + \text{CH}_4$ PROPANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	2.0(+11)	0	4820±250	
$\text{CH}_3\text{CD}_2\text{CH}_3 + \text{CD}_3\cdot \rightarrow (\text{CH}_3)_2\text{CD}\cdot + \text{CD}_4$ PROPANE-2,2-d ₂ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	2.5(+11)	0	5735±250	
$\text{CH}_3\text{CD}_2\text{CH}_3 + \text{CD}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{CH}_2\cdot + \text{CD}_3\text{H}$ PROPANE-2,2-d ₂ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	4.4(+11)	0	5735±250	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{COCH}_2\cdot \rightarrow \text{CH}_3\cdot + \text{CH}_2=\text{C}=\text{O}$ PROPYL, 2-OXO-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	365-435	3.2(+12)	0	20130	
$\text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\cdot + \text{CH}_4$ PROPANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	2970±500	
$(\text{CH}_3)_2\text{CO} \rightarrow \text{CH}_3\text{C}(\text{O})\cdot + \text{CH}_3\cdot$ 1-PROPANONE 70 BEN/O'N REACTION ORDER: 1.	990-1101	1.8(+16)	0	40765	
$(\text{CH}_3)_2\text{CO} + \text{H} \rightarrow \text{CH}_3\text{COCH}_2\cdot + \text{H}_2$ 2-PROPANONE + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	298-873	4.6(+13)	0	4220±20	
$(\text{CH}_3)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{COCH}_2\cdot + \text{CH}_4$ 2-PROPANONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-700	3.5(+11)	0	4900±250	
$(\text{CD}_3)_2\text{CO} + \text{CD}_3\cdot \rightarrow \text{CD}_3\text{C}(\text{O})\text{CD}_2\cdot + \text{CD}_4$ 2-PROPANONE-1,1,1,3,3,3-d ₆ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-800	4.8(+11)	0	5735±250	
$\text{CH}_2=\text{CHCH}_2\text{OH} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{OH}$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{OH}$ 2-PROPEN-1-OL + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	323-415	1.9(+11)	0	3901	
$\text{HCOOCH}_2\text{CH}_3 \rightarrow \text{HCOOH} + \text{CH}_2=\text{CH}_2$ FORMIC ACID ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	648-920	2.5(+12)	0	24300	
$\text{HCOOCH}_2\text{CH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{COOCH}_2\text{CH}_2 + \text{HCOOCH}(\cdot)\text{CH}_3 + \text{CH}_4$ FORMIC ACID ETHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	5100±500	
$\text{CH}_3\text{COOCH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{COOCH}_3 + \text{CH}_3\text{COOCH}_2\cdot + \text{CH}_4$ ACETIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	2.1(+11)	0	5035±500	
$\text{CH}_3\text{COOCD}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{COOCD}_3 + \text{CH}_4$ ACETIC ACID METHYL-d ₃ ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	1.9(+11)	0	5035±500	
$\text{CD}_3\text{COOCH}_3 + \text{CH}_3\cdot \rightarrow \text{CD}_3\text{COOCH}_2\cdot + \text{CH}_4$ ACETIC-d ₃ ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	1.7(+11)	0	5990±500	
$\text{CH}_3\text{OCOOCCH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{OCOOCCH}_3 + \text{CH}_4$ CARBONIC ACID DIMETHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.2(+11)	0	5800±750	
$(\text{CH}_3)_2\text{CHOH} + \text{O} \rightarrow \text{products}$ 2-PROPANOL + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	1.3(+11)	-	-	0.6 1.5
$(\text{CH}_3)_2\text{CDOH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OH} + \text{CH}_3\text{D}$ 2-PROPAN-2-d-OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-525	1.9(+11)	0	4990±500	
$(\text{CH}_3)_2\text{CHOD} + \text{CD}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OD} + \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OD} + \text{CD}_3\text{H}$ 2-PROPANOL-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-525	1.5(+11)	0	3975±500	
$(\text{CH}_3)_2\text{CHOOH} \rightarrow (\text{CH}_3)_2\text{CHO}\cdot + \text{OH}$ HYDROPEROXIDE, 1-METHYLETHYL 70 BEN/O'N REACTION ORDER: 1.	553-653	3.2(+15)	0	21640	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{CH}_3 \rightarrow \text{cy-CH}_2\text{CH}(\cdot)\text{CH}_2\text{S} + \text{CH}_4$ THIETANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-450	3.2(+11)	0	4630±750	
$(\text{CH}_3)_2\text{CHSH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHS} + (\text{CH}_3)_2\text{C}(\cdot)\text{SH}$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{SH} + \text{CH}_4$ 2-PROPANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	4.1(+ 7)	-	-	
$\text{CH}_2=\text{CHCN} + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ 2-PROPENENITRILE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	323-454	6.2(+10)	0	1700	
$\text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CH}_3 \cdot + \cdot\text{CH}_2\text{CN}$ PROPANENITRILE 70 BEN/O'N REACTION ORDER: 1.	958-1038	1.3(+14)	0	36600	
$\text{CH}_3\text{CH}_2\text{CN} + \text{CD}_3 \cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}_2\text{CN} + \text{CD}_3\text{H}$ PROPANENITRILE + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	3.6(+11)-	0	4330±500	
$(\text{CH}_3)_3\text{N} + \text{CH}_3 \cdot \rightarrow \cdot\text{CH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_4$ METHANAMINE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	4.7(+11)	0	4600±500	
$\text{O}_2\text{NOCH}_2\text{CH}(\text{ONO}_2)\text{CH}_2\text{ONO}_2 \rightarrow \text{products}$ 1,2,3-PROPANETRIOL, TRINITRATE 70 BEN/O'N REACTION ORDER: 1.	348-378	1.3(+17)	0	20300	
$\text{O}_2\text{NOCH}_2\text{CH}(\text{ONO}_2)\text{CH}_3 \rightarrow \text{products}$ 1,2-PROPANEDIOL, DINITRATE 70 BEN/O'N REACTION ORDER: 1.	353-373	1.6(+15)	0	18800	
$\text{O}_2\text{NOCH}_2\text{CH}_2\text{CH}_2\text{ONO}_2 \rightarrow \text{products}$ 1,3-PROPANEDIOL, DINITRATE 70 BEN/O'N REACTION ORDER: 1.	358-383	1.6(+15)	0	19175	
$\text{HCON}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow \text{CON}(\text{CH}_3)_2 + \text{HCO}-(\text{CH}_3)\text{NCH}_2 \cdot + \text{CH}_4$ FORMAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-600	6.3(+10)	0	3600±500	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{NO}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HONO}$ PROPANE, 1-NITRO- 70 BEN/O'N REACTION ORDER: 1.	687-733	2.50(+13)	0	24005	
$\text{CH}_3\text{CH}(\text{NO}_2)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HONO}$ PROPANE, 2-NITRO- 70 BEN/O'N REACTION ORDER: 1.	800-1000	2.0(+11)	0	20130	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{O} \cdot + \text{NO}$ NITROUS ACID PROPYL ESTER 70 BEN/O'N REACTION ORDER: 1.	443-483	1.6(+16)	0	20230	
$(\text{CH}_3)_2\text{CHONO} \rightarrow (\text{CH}_3)_2\text{CHO} \cdot + \text{NO}$ NITROUS ACID 1-METHYL ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	443-483	3.2(+16)	0	18600	
$\text{CH}\equiv\text{CC}\equiv\text{CH} + \text{O} \rightarrow \text{products}$ 1,3-BUTADIYNE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	300	9.0(+11)	-	-	0.7 1.4
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} + \text{N} \rightarrow \text{products}$ 1-BUTYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 13.0	320-550 435	3.5(+11) -	0 -	1125 -	
NOTE: k _{ref} : CH≡CH + N					

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{C}\equiv\text{CH} + \cdot\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH}$ $+ \text{CH}_3\text{CH}_2\text{C}\equiv\text{C}\cdot + \text{CH}_4$ 1-BUTYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	456-620	1.9(+12)	0	5135±500		
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{C}=\text{C}(\text{CH}_3)\text{S}$ 2-BUTYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	1.9(+13)	-	-		
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{N} \rightarrow \text{products}$ 2-BUTYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 12.0	320-550 435	1.9(+11) -	0 -	926 -		
NOTE: k _{ref} : $\text{CH}=\text{CH} + \text{N}$						
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}=\text{CH}_2\cdot + \text{CH}_4$ 2-BUTYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	486-619	1.1(+12)	0	4900±500		
NOTE: TENTATIVE k VALUE.						
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{CCO} \rightarrow \text{products}$ 2-BUTYNE + CARBON OXIDE(C ₂ O) 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 8.5	304	-	-	-		
NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$						
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{O} \rightarrow \text{products}$ 1,3-BUTADIENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-400	3.4(+12)	0	- 380	0.7	1.3
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_2=\text{CHCH}(\cdot)\text{CH}_3 + \text{CH}_2=\text{CHCH}_2\text{CH}_2\cdot$ 1,3-BUTADIENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	4.10(+13)	0	655		
NOTE: AVERAGED k.						
NOTE: k _{ref} : $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$	300	-	-	-		
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_2=\text{CH})\text{CHCH}_2\text{S}$ 1,3-BUTADIENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	6.0(+13)	-	-		
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1,3-BUTADIENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	340	3.5(+10)	-	-		
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + {}^1\text{CH}_2 \rightarrow \text{products}$ 1,3-BUTADIENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 3.2	297	-	-	-		
NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$ ASSUMING 10% ${}^3\text{CH}_2$						
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$ 1,3-BUTADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	353-453	8.1(+10)	0	2065		
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ 1,3-BUTADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 12.0	435	-	-	-		
NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot$						
$\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CCO} \rightarrow \text{CH}_2=\text{C}=\text{CHCH}=\text{CH}_2 + \text{CO}$ 1,3-BUTADIENE + CARBON OXIDE(C ₂ O) 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 210.	298	-	-	-		
NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$						
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{O} \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2)\text{CHCH}_2\text{O}$ 1-BUTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	2.3(+12)	-	-	0.8	1.2
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ 1-BUTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 1.03	298 300	8.7(+11) -	- -	- -		
NOTE: k _{ref} : $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$						

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ 1-BUTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	5.0(+10)	-	-	
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ 1-BUTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	8.1(+11)	-	-	
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2)\text{CHCH}_2\text{S}$ 1-BUTENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 10.0$	298 298	9.3(+12) -	- -	- -	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S}$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-BUTENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 3.4$	320-550 435	1.6(+11) -	0 -	660 -	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{N}$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + {}^1\text{CH}_2\cdot \rightarrow \text{products}$ 1-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.63$	297	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2\cdot$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + {}^3\text{CH}_2\cdot \rightarrow \text{products}$ 1-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.6$	297	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2\cdot$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}=\text{CH}_2 + \text{CH}_4$ 1-BUTENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	2.5(+11)	0	4200±500	0.6 1.4
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ 1-BUTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 12.0$	353-453 453	1.0(+11) -	0 -	3600 -	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CCO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}=\text{CH}_2 + \text{CO}$ 1-BUTENE + CARBON OXIDE (C_2O) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 7.0$	298	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CCO}$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ 1-BUTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3675	
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ 1-BUTENE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3630	
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ 1-BUTENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3480	
$\text{CH}_2=\text{CHCH}_2\text{CH}_3(+\text{M}) \rightarrow \text{CH}_2=\text{CHCH}_2\cdot + \text{CH}_3\cdot(+\text{M})$ 1-BUTENE 70 BEN/O'N REACTION ORDER: 1. NOTE: k ESTIMATED.	900-1051	1.00(+16)	0	36900	
$\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{S}\cdot \rightarrow \text{CH}_3\text{CH}(\text{SCH}_3)\text{CH}(\cdot)\text{CH}_3$ 2-BUTENE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: cis-trans EQUILIBRIUM - WEIGHTED k.	298-333	1.6(+ 9)	-	-	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{cis-CH}_3\text{CH=CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH=CHCH}_3$ cis-2-BUTENE 70 BEN/O'N REACTION ORDER: 1.	686-742	6.00(+13)	0	31600		
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{O} \rightarrow \text{products}$ $\text{cis-2-BUTENE} + \text{OXYGEN ATOM}$ 73 HER/HUI REACTION ORDER: 2.	250-500	5.9(+12)	0	- 165	0.8	1.2
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-BUTENE} + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2.	208	4.6(+11)	-	-		
NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION. $k/k_{\text{ref}}: 0.47$	300	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_3\text{CH=CH}_2 + \text{H}$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{S} \rightarrow \text{cy-(CH}_3\text{CH)CH(CH}_3\text{)S}$ $\text{cis-2-BUTENE} + \text{SULFUR ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	1.4(+13)	-	-		
$k/k_{\text{ref}}: 16.0$	298	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S}$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{N} \rightarrow \text{products}$ $\text{cis-2-BUTENE} + \text{NITROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2.	320-550	2.3(+11)	0	995		
$k/k_{\text{ref}}: 2.4$	435	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{N}$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + {}^1\text{CH}_2 \rightarrow \text{products}$ $\text{cis-2-BUTENE} + \text{METHYLENE FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.37$	297	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + {}^3\text{CH}_2 \rightarrow \text{products}$ $\text{cis-2-BUTENE} + \text{METHYLENE FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.94$	297	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH=CHCH}_2 + \text{CH}_4$ $\text{cis-2-BUTENE} + \text{METHYL FREE RADICAL}$ 76 KER/PAR REACTION ORDER: 2.	350-650	1.8(+11)	0	4100±500		
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ $\text{cis-2-BUTENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	353-453	4.5(+10)	0	3675		
$k/k_{\text{ref}}: 0.2$	453	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CH}_3$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{CCO} \rightarrow \text{cis-CH}_3\text{CH=C=CHCH}_3 + \text{CO}$ $\text{cis-2-BUTENE} + \text{CARBON OXIDE}(\text{C}_2\text{O})$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 9.1$	297	-	-	-		
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CCO}$						
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-BUTENE} + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4265		
$\text{cis-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-BUTENE} + \text{PROPYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4370		
$\text{cis-CH}_3\text{CH=CHCH}_3 + (\text{CH}_3)_2\text{CH} \rightarrow \text{CH}_3\text{CH}[\text{CH}(\text{CH}_3)_2]\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-BUTENE} + \text{ETHYL, 1-METHYL-, FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	3950		
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{O} \rightarrow \text{products}$ $\text{trans-2-BUTENE} + \text{OXYGEN ATOM}$ 73 HER/HUI REACTION ORDER: 2.	298	1.4(+13)	-	-	0.7	1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
trans-CH ₃ CH=CHCH ₃ + H → CH ₃ CH ₂ CH(.)CH ₃ trans-2-BUTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGE k.	298	5.6(+11)	-	-	
k/k _{ref} : 0.59	300	-	-	-	
NOTE: k _{ref} : CH ₃ CH=CH ₂ + H					
trans-CH ₃ CH=CHCH ₃ + S → cy-(CH ₃ CH)CH(CH ₃)S trans-2-BUTENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 20.0	298	1.4(+13)	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + S	298	-	-	-	
trans-CH ₃ CH=CHCH ₃ + N → products trans-2-BUTENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 3.0	320-550	3.4(+11)	0	1055	
NOTE: k _{ref} : CH ₂ =CH ₂ + N	435	-	-	-	
trans-CH ₃ CH=CHCH ₃ + ¹ CH ₂ → products trans-2-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 1.39	297	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + ¹ CH ₂					
trans-CH ₃ CH=CHCH ₃ + ³ CH ₂ → products trans-2-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.89	297	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + ³ CH ₂					
trans-CH ₃ CH=CHCH ₃ + CH ₃ → CH ₃ CH=CHCH ₂ + CH ₄ trans-2-BUTENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+12)	0	4830±500	
trans-CH ₃ CH=CHCH ₃ + CH ₃ → (CH ₃) ₂ CHCH(.)CH ₃ trans-2-BUTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	353-453	1.4(+11)	0	4075	
trans-CH ₃ CH=CHCH ₃ + CH ₃ → (CH ₃) ₂ CHCH(.)CH ₃ trans-2-BUTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.4	453	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + CH ₃					
trans-CH ₃ CH=CHCH ₃ + CCO → CH ₃ CH=C=CHCH ₃ + CO trans-2-BUTENE + CARBON OXIDE(C ₂ O) 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 10.6	297	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + CCO					
trans-CH ₃ CH=CHCH ₃ + CH ₃ CH ₂ → CH ₃ CH(CH ₂ CH ₃)CH(.)CH ₃ trans-2-BUTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4350	
trans-CH ₃ CH=CHCH ₃ + CH ₃ CH ₂ CH ₂ → CH ₃ CH(CH ₂ CH ₂ CH ₃)CH(.)CH ₃ trans-2-BUTENE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4515	
trans-CH ₃ CH=CHCH ₃ + (CH ₃) ₂ CH → CH ₃ CH[CH(CH ₃) ₂]CH(.)CH ₃ trans-2-BUTENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4065	
(CH ₃) ₂ C=CH ₂ → .CH ₂ C(CH ₃)=CH ₂ + H 1-PROPENE, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	930-1082	1.0(+17)	0	44400	
(CH ₃) ₂ C=CH ₂ + O → cy-[(CH ₃) ₂]CCH ₂ O 1-PROPENE, 2-METHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	1.2(+13)	-	-	0.7 1.3
(CH ₃) ₂ C=CH ₂ + H → (CH ₃) ₃ C. 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	3.1(+13)	0	755	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\cdot$ 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 0.5% NON-TERMINAL ADDITION OF H TO $(\text{CH}_3)_2\text{C}=\text{CH}_2$.	298	1.3(+11)	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_3\text{C}\cdot + (\text{CH}_3)_2\text{CHCH}_2\cdot$ 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.52 NOTE: k_{ref} : $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$	300	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HO}_2 \rightarrow \text{products}$ 1-PROPENE, 2-METHYL-, + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: SUGGESTED k VALUE.	300	1.0(+ 8)	-	-	0.1 10.
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)_2\text{CCH}_2\text{S}$ 1-PROPENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 50.0 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{S}$	298 298	4.0(+13) -	- -	- -	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{S}^*(^1\text{D}) \rightarrow \text{cy}-(\text{CH}_3)_2\text{CCH}_2\text{S}$ 1-PROPENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 3.5 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{S}^*(^1\text{D})$	300	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-PROPENE, 2-METHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	320-550	7.8(+10)	0	277	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-PROPENE, 2-METHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 4.1 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{N}$	435	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + ^1\text{CH}_2 \rightarrow \text{products}$ 1-PROPENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.96 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + ^1\text{CH}_2$	297	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + ^3\text{CH}_2 \rightarrow \text{products}$ 1-PROPENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.86 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + ^3\text{CH}_2$	297	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_4$ 1-PROPENE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	3.0(+11)	0	4500±500	0.6 1.4
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\cdot + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ 1-PROPENE, 2-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.1 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$	353-453 453	1.4(+11) -	0 -	3475 -	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CCO} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CO}$ 1-PROPENE, 2-METHYL-, + CARBON OXIDE(C_2O) 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 50.0 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	297	-	-	-	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CH}_2$ BUTYL FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	334-689	4.0(+13)	0	14600	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ BUTYL FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	352-405	2.3(+10)	0	3370	
$\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3$ PROPYL, 1-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	523-622	1.4(+14)	0	17060	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ PROPYL, 1-METHYL-, FREE RADICAL + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	381-412	6.3(+10)	0	3725	
$(\text{CH}_3)_2\text{CHCH}_2\cdot \rightarrow \text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{CH}_2$ PROPYL, 2-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	299-691	1.6(+14)	0	16455	
$(\text{CH}_3)_2\text{CHCH}_2\cdot \rightarrow (\text{CH}_3)_3\text{C}=\text{CH}_2 + \text{H}$ PROPYL, 2-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	299-691	5.0(+13)	0	18420	
$(\text{CH}_3)_3\text{C}\cdot \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	300-897	4.0(+14)	0	21700	0.2 5.0
$(\text{CH}_3)_3\text{C}\cdot + \text{CH}=\text{CH}\cdot \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}\cdot$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	363-577	1.0(+11)	0	3875	
$(\text{CH}_3)_3\text{C}\cdot + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2\cdot$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	300-650	2.8(+10)	0	3575	
$(\text{CH}_3)_3\text{C}\cdot + \text{CH}_3\text{C}=\text{CH} \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}\cdot + (\text{CH}_3)_3\text{CCH}=\text{C}(\cdot)\text{CH}_3$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + 1-PROPYLENE 72 KER/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.	360-439	5.0(+ 8)	0	2770	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ BUTANE 70 BEN/O'N REACTION ORDER: 1. NOTE: k ESTIMATED.	693-803	4.0(+17)	0	43230	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\cdot$ BUTANE 70 BEN/O'N REACTION ORDER: 1.	693-803	1.9(+17)	0	41170	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{OH}$ BUTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	3.0(+13)	0	2920	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{OH}$ BUTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	4.6(+13)	0	2410	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{H}_2$ BUTANE + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	320-930	4.1(+12)	0	2637±320	0.5 2.0
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{H}_2\text{O}_2$ BUTANE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} for $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300-1000	5.0(+11)	0	5285	0.1 10.
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{CH}_4$ BUTANE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	350-00	1.6(+11)	0	4540±150	0.7 1.4
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4$ BUTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-750	4.0(+11)	0	4830±250	0.7 1.3
$\text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 + \text{CD}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{CD}(\cdot)\text{CH}_3 + \text{CD}_4$ BUTANE-2,2,3,3-d ₄ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	600-750	4.5(+11)	0	5735±250	0.7 1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 + \text{CD}_3 \rightarrow \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_2 + \text{CD}_3\text{H}$ BUTANE-2,2,3,3-d ₄ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	600-750	4.8(+11)	0	5735±250	0.7 1.3
$(\text{CH}_3)_3\text{CH} + \text{H} \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_2\text{CHCH}_2 + \text{H}_2$ PROPANE, 2-METHYL-, + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	300-800	1.9(+13)	0	2680±85	0.8 1.2
$(\text{CH}_3)_3\text{CH} + \text{HO}_2 \rightarrow (\text{CH}_3)_3\text{C} + \text{H}_2\text{O}_2$ PROPANE, 2-METHYL-, + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} for $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	300-1000	1.0(+11)	0	3500	0.1 10.
$(\text{CH}_3)_3\text{CH} + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_4$ PROPANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	9.6(+10)	0	3975±250	0.7 1.3
$(\text{CH}_3)_3\text{CH} + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_2\text{CHCH}_2 + \text{CH}_4$ PROPANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	8.3(+10)	0	4000±500	0.5 2.0
$(\text{CH}_3)_3\text{CD} + \text{CD}_3 \rightarrow (\text{CH}_3)_3\text{C} + \text{CD}_4$ PROPANE-2-d, 2-METHYL-, + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	1.2(+11)	0	4800±250	0.7 1.3
$(\text{CH}_3)_3\text{CD} + \text{CD}_3 \rightarrow (\text{CH}_3)_2\text{CDCH}_2 + \text{CD}_3\text{H}$ PROPANE-2-d, 2-METHYL-, + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	6.0(+11)	0	5735±250	0.7 1.3
$\text{CH}_3\text{CH}=\text{CHCHO} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHC}(\text{O}) + \text{CH}_4$ 2-BUTENAL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3400±500	0.4 2.5
$\text{CH}_2=\text{CHCH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2$ 3-BUTENOIC ACID 70 BEN/O'N REACTION ORDER: 1.	587-651	2.2(+11)	0	20435	
$\text{CH}_3\text{COOCH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{COOCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ACETIC ACID ETHENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	303-417	7.8(+10)	0	3475	
$\text{CH}_3\text{COCOCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{COCOCH}_2 + \text{CH}_4$ 2,3-BUTANEDIONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-800	2.2(+11)	0	4300±500	0.5 1.5
$\text{CH}_3\text{COCOCH}_3 \rightarrow \text{CH}_3\text{C}(\text{O}) + \text{CH}_3\text{C}(\text{O})$ 2,3-BUTANEDIONE 70 BEN/O'N REACTION ORDER: 1.	626-698	1.6(+16)	0	33970	
$(\text{CH}_3\text{CO})_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}=\text{O}$ ACETIC ACID ANHYDRIDE 70 BEN/O'N REACTION ORDER: 1.	553-646	1.0(+12)	0	17365	
$(\text{CH}_3\text{CO})_2\text{O} + \text{CH}_3 \rightarrow \text{CH}_3\text{COCOCH}_2 + \text{CH}_4$ ACETIC ACID ANHYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	1.8(+11)	0	4830±500	0.6 1.4
$\text{CH}_3\text{C}(\text{O})\text{OOC}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{O} + \text{CH}_3\text{C}(\text{O})\text{O}$ PEROXIDE, DIACETYL 70 BEN/O'N REACTION ORDER: 1.	363-463	1.8(+14)	0	14845	
$\text{CH}_3\text{CH}_2\text{COCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{COCH}_3 + \cdot\text{CH}_2\text{CH}_2\text{COCH}_3$ $+ \text{CH}_3\text{CH}_2\text{COCH}_2\cdot + \text{CH}_4$ 2-BUTANONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	8.2(+10)	0	3700±500	0.5 1.5
$\text{HCOOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{HCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$ FORMIC ACID PROPYL ESTER 70 BEN/O'N REACTION ORDER: 1.	613-673	1.3(+12)	0	24006	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{HCOOCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{COOCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_4$ FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	347-455	1.3(+10)	0	3675	
$\text{HCOOCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{COOCH}_2\text{CH}_2\text{CH}_3 + \text{HCOOCH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{HCOOCH}_2\text{CH}(\cdot)\text{CH}_3 + \text{HCOOCH}_2\text{CH}_2\text{CH}_2 \cdot + \text{CH}_4$ FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	5000±500	0.5 2.0
$\text{HCOOCH}(\text{CH}_3)_2 \rightarrow \text{HCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$ FORMIC ACID 1-METHYLETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	721-811	4.0(+12)	0	22145	
$\text{HCOOCH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow \text{COOCH}(\text{CH}_3)_2 + \text{HCOOC}(\cdot)(\text{CH}_3)_2$ $+ \text{HCOOCH}(\text{CH}_3)\text{CH}_2 \cdot + \text{CH}_4$ FORMIC ACID 1-METHYLETHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	4980±500	0.5 2.0
$\text{CH}_3\text{COOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CH}_2$ ACETIC ACID ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-883	3.9(+12)	0	24155	
$\text{CH}_3\text{OCOOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ CARBONIC ACID ETHYL METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	573-648	4.0(+12)	0	21640	
$\text{CH}_3\text{CH}(\cdot)\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_3\text{CH}_2 \cdot$ ETHYL, 1-ETHOXY-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. NOTE: logA PROBABLY LOW.	418-453	8.1(+10)	0	11825	
$\text{CH}_3\text{CH}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_3\text{CH}_2 \cdot$ ETHOXY, 1-ETHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. NOTE: ESTIMATED ARRHENIUS PARAMETERS (VERY LIKELY LOWER LIMITS).	423-463	1.0(+14)	0	8800	
$(\text{CH}_3)_3\text{CO} \cdot \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3 \cdot$ ETHOXY, 1,1-DIMETHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. NOTE: TENTATIVE k.	393-453	3.2(+13)	0	8300	
$(\text{CH}_3)_3\text{COH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{O}$ 2-PROPANOL, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	1050-1300	2.5(+13)	0	31001	
$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{CH}_2\text{O} \cdot$ ETHANE, 1,1'-OXYBIS- 70 BEN/O'N REACTION ORDER: 1. NOTE: k PROBABLY RELIABLE.	833-913	1.0(+18)	0	42275	
$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{OCH}(\cdot)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2 \cdot + \text{CH}_4$ ETHANE, 1,1'-OXYBIS-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-500	2.5(+11)	0	4200±750	0.5 2.0
$\text{CH}_3\text{CH}_2\text{OOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{CH}_3\text{CH}_2\text{O} \cdot$ PEROXIDE, DIETHYL 70 BEN/O'N REACTION ORDER: 1.	413-518	4.0(+15)	0	18770	
$(\text{CH}_3)_3\text{COOH} \rightarrow (\text{CH}_3)_3\text{CO} \cdot + \text{OH} \cdot$ HYDROPEROXIDE, 1,1-DIMETHYLETHYL 70 BEN/O'N REACTION ORDER: 1.	553-653	4.0(+15)	0	21640	
$(\text{CH}_3)_3\text{CSH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{S}$ 2-PROPANETHIOL, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	950-1230	2.5(+13)	0	27830	
$(\text{CH}_3)_3\text{CSH} + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_3\text{CS} \cdot + \cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{SH} + \text{CH}_4$ 2-PROPANETHIOL, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	5.9(+ 7)	-	-	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_2=\text{CHCH}_2\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\cdot + \text{CH}_3\text{SO}_2\cdot$ 1-PROPENE, 3-METHYLSULFONYL- 70 BEN/O'N REACTION ORDER: 1.	633-733	1.3(+14)	0	24006		
$\text{cis-CH}_3\text{CH=CHCN} \rightarrow \text{trans-CH}_3\text{CH=CHCN}$ cis-2-BUTENENITRILE 70 BEN/O'N REACTION ORDER: 1.	573-633	5.0(+12)	0	28030		
$\text{cis-CH}_3\text{CH=CHCN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ + $\text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ cis-2-BUTENENITRILE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	323-454	1.5(+10)	0	2500		
$\text{trans-CH}_3\text{CH=CHCN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ + $\text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ trans-2-BUTENENITRILE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	323-754	3.1(+10)	0	2600		
$\text{CH}_2=\text{C}(\text{CH}_3)\text{CN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CN}$ + $\cdot\text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CN}$ 2-PROPENENITRILE, 2-METHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	312-400	2.5(+11)	0	2300		
$\text{CH}_3\text{CH=NN=CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\cdot)=\text{NN=CHCH}_3$ + $\cdot\text{CH}_2\text{CH=NN=CHCH}_3 + \text{CH}_4$ ACETALDEHYDE ETHYLIDENEHYDRAZONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	2.5(+11)	0	3975±500	0.5	2.0
$\text{CH}_3\text{CH}_2\text{N=NCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{N=N}\cdot + \text{CH}_3\text{CH}_2\cdot$ DIAZENE, DIETHYL- 70 BEN/O'N REACTION ORDER 1.		2.0(+16)	0	25165		
$\text{CH}_3\text{N=NCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{N=N}\cdot + (\text{CH}_3)_2\text{CH}\cdot$ DIAZENE, METHYL(1-METHYLETHYL)- 70 BEN/O'N REACTION ORDER 1.	543-605	2.5(+16)	0	23900		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}\cdot$ + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$ 1-BUTANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	426	3.2(+7)	-	-	0.5	2.0
NOTE: TENTATIVE k VALUE.						
$(\text{CH}_3\text{CH}_2)_2\text{NH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3\text{CH}_2)_2\text{N}\cdot + \text{CH}_3\text{CH}(\cdot)\text{NHCH}_2\text{CH}_3$ + $\cdot\text{CH}_2\text{CH}_2\text{NHCH}_2\text{CH}_3 + \text{CH}_4$ ETHANAMINE, N-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.2(+11)	0	3550±500	0.5	2.0
NOTE: TENTATIVE k VALUE.						
$\text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_3)_2 + \cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_3)_2$ + $\text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)\text{CH}_2\cdot + \text{CH}_4$ ETHANAMINE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	420	2.6(+7)	-	-	0.5	2.0
NOTE: TENTATIVE k VALUE.						
$(\text{CH}_3)_2\text{NN=NN}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{NN=N}\cdot + (\text{CH}_3)_2\text{N}\cdot$ 2-TETRAZENE, 1,1,4,4-TETRAMETHYL- 70 BEN/O'N REACTION ORDER: 1.	466-539	2.5(+14)	0	18170		
$\text{CH}_3\text{CH}_2\text{OCH=CH}_2 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2=\text{CH}_2$ ETHENE, ETHOXY- 70 BEN/O'N REACTION ORDER: 1.	640-859	4.0(+11)	0	22345		
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH=CH}_2 + \text{HCHO}$ 3-BUTEN-1-OL 70 BEN/O'N REACTION ORDER: 1.	643-685	4.5(+11)	0	20635		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\cdot + \text{CH}_4$ BUTANAL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	2970±500	0.4	1.6
NOTE: TENTATIVE k VALUE.						

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3)_2\text{CHCHO} + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{CHC}(\text{O}) \cdot + \text{CH}_4$ PROPANAL, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	2970±500	0.4 1.6
$\text{CH}_3\text{CON}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2 \cdot + \text{CH}_4$ ACETAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-600	1.6(+11)	0	4125±500	0.5 1.5
$\text{CH}_3\text{CON}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow \cdot\text{CH}_2\text{CON}(\text{CH}_3)_2$ + $\text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2 \cdot + \text{CH}_4$ ACETAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	2.0(+11)	0	4200±500	0.5 1.5
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} \cdot + \text{NO}$ NITROUS ACID BUTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	443-485	2.0(+16)	0	20400	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} + \text{N} \rightarrow \text{products}$ 1-PENTYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 14.0 NOTE: k _{ref} : CHCH + N	320-550 435	3.0(+11) -	0 -	1047 -	
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{O} \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2)\text{CHCH}_2\text{O}$ 1-PENTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	2.8(+12)	-	-	0.7 1.3
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_2 \cdot$ 1-PENTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.89 NOTE: k _{ref} : CH ₃ CH=CH ₂ + H	298 300	8.3(+11) -	- -	- -	
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3(\text{CH}_2)_2)\text{CHCH}_2\text{S}$ 1-PENTENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	8.1(+12)	-	-	
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2 + \text{CH}_4$ 1-PENTENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	450-650	4.5(+11)	0	4500±500	0.6 1.4
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{CHCH}_2\text{CH}_2 \cdot \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)\text{CH}_2(\text{CH}_2)_2\text{CH}_3$ 1-PENTENE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3410	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{O} \rightarrow \text{products}$ cis-2-PENTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	1.1(+13)	-	-	0.7 1.3
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ cis-2-PENTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.39 NOTE: k _{ref} : CH ₃ CH=CH ₂ + H	298 300	3.8(+11) -	- -	- -	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ cis-2-PENTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ cis-2-PENTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4125	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ cis-2-PENTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4300	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$\text{trans-CH}_3\text{CH}_2\text{CH=CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ trans-2-PENTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 0.44 NOTE: k_{ref} : $\text{CH}_3\text{CH=CH}_2 + \text{H}$	300 298	- 4.1(+11)	- -	- -		
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ 1-BUTENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	9.1(+11)	-	-		
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{D} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{D}$ $+ \text{CH}_3\text{CH}_2\text{CD}(\text{CH}_3)\text{CH}_2\cdot$ 1-BUTENE, 2-METHYL-, + DEUTERIUM ATOM 72 KER/PAR REACTION ORDER: 2.	298	2.0(+12)	-	-		
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2)\text{C}(\text{CH}_3)\text{CH}_2\text{S}$ 1-BUTENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	7.4(+13)	-	-		
$(\text{CH}_3)_2\text{CHCH=CH}_2 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ 1-BUTENE, 3-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	7.4(+11)	-	-		
$(\text{CH}_3)_2\text{CHCH=CH}_2 + \text{D} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{D} + (\text{CH}_3)_2\text{CHCHDCH}_2\cdot$ 1-BUTENE, 3-METHYL-, + DEUTERIUM ATOM 72 KER/PAR REACTION ORDER: 2.	298	7.6(+11)	-	-		
$(\text{CH}_3)_2\text{CHCH=CH}_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_3$ 1-BUTENE, 3-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3500		
$(\text{CH}_3)_2\text{CHCH=CH}_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH=CH}_2 + \text{CH}_4$ 1-BUTENE, 3-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	450-600	4.4(+11)	0	4225±750	0.5	1.5
$(\text{CH}_3)_2\text{CHCH=CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ 1-BUTENE, 3-METHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3620		
$(\text{CH}_3)_2\text{C=CHCH}_3 + \text{O} \rightarrow \text{products}$ 2-BUTENE, 2-METHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-400	3.9(+12)	0	- 680	0.8	1.2
$(\text{CH}_3)_2\text{C=CHCH}_3 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHC}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ 2-BUTENE, 2-METHYL-, + HYDROGEN ATOM 73 HER/HUI REACTION ORDER: 2. k/k_{ref} : 1.03	298 300	9.1(+11) -	- -	- -		
NOTE: k_{ref} : $\text{CH}_3\text{CH=CH}_2 + \text{H}$						
$(\text{CH}_3)_2\text{C=CHCH}_3 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)_2\text{CCH}(\text{CH}_3)\text{S}$ 2-BUTENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 56.0	298 298	6.5(+13) -	- -	- -		
NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{S}$						
$(\text{CH}_3)_2\text{C=CHCH}_3 + \text{N} \rightarrow \text{products}$ 2-BUTENE, 2-METHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 3.5	320-550 435	9.3(+10) -	0 -	433 -		
NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{N}$						
$(\text{CH}_3)_2\text{C=CHCH}_3 + {}^1\text{CH}_2 \rightarrow \text{products}$ 2-BUTENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.12	297	-	-	-		
NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$						
$(\text{CH}_3)_2\text{C=CHCH}_3 + {}^3\text{CH}_2 \rightarrow \text{products}$ 2-BUTENE, 2-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.83		-	-	-		
NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$						

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_2 \cdot$ $+ \cdot\text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3 + \text{CH}_4$ 2-BUTENE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-500	4.9(+11)	0	4300±500	0.5	1.5
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}_3$ $+ (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ 2-BUTENE, 2-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	403-455	1.4(+10)	0	3070		
	453	-	-	-		
					k/k _{ref} : 0.4	
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CCO} \rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CO}$ 2-BUTENE, 2-METHYL-, + CARBON OXIDE(C ₂ O) 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 100. NOTE: k _{ref} : CH ₂ =CH ₂ + CCO	298	-	-	-		
$(\text{CH}_3)_3\text{CCH}_2 \cdot \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3 \cdot$ PROPYL, 2,2-DIMETHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	762	1.0(+14)	0	18875		
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2 \cdot + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH}(\text{CH}_2)_3\text{CH}_2 \cdot$ BUTYL, 3-METHYL-, FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	340-413	1.2(+10)	0	3235		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \cdot + \text{OH}$ PENTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7	1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{OH}$ PENTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	8.0(+13)	0	2320	0.7	1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \cdot + \text{CH}_4$ PENTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	4.8(+11)	0	5800±250	0.7	1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4$ PENTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	6.0(+11)	0	4830±250	0.7	1.3
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{O} \rightarrow [\text{C}_5\text{H}_{11} \cdot] + \text{OH}$ BUTANE, 2-METHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	307	8.0(+10)	-	-	0.7	1.4
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_4$ BUTANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.6(+10)	0	3975±250	0.7	1.3
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3 + \text{CH}_4$ BUTANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	2.0(+11)	0	4830±250	0.7	1.3
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2 \cdot$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 + \text{CH}_4$ BUTANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	7.1(+11)	0	5800±250	0.7	1.3
$(\text{CH}_3)_4\text{C} \rightarrow (\text{CH}_3)_3\text{C} \cdot + \text{CH}_3 \cdot$ PROPANE, 2,2-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	803-1200	5.0(+16)	0	40465		

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F	
$(\text{CH}_3)_4\text{C} + \text{O} \rightarrow (\text{CH}_3)_3\text{CCH}_2\cdot + \text{OH}$ PROPANE, 2,2-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7	1.4
$(\text{CH}_3)_4\text{C} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\cdot + \text{CH}_4$ PROPANE, 2,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	8.3(+11)	0	5940±350	0.6	1.4
$\text{CH}_2=\text{CHOCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CHO}$ 1-PROPENE, 3-ETHENYLOXY- 70 BEN/O'N REACTION ORDER: 1.	440-473	5.0(+11)	0	15400		
$\text{cis-CH}_3\text{CH}=\text{CHCOOCH}_3 \rightarrow \text{trans-CH}_3\text{CH}=\text{CHCOOCH}_3$ cis-2-BUTENOIC ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	673-833	1.6(+11)	0	29090		
$\text{trans-CH}_3\text{CH}=\text{CHCOOCH}_3 \rightarrow \text{cis-CH}_3\text{CH}=\text{CHCOOCH}_3$ trans-2-BUTENOIC ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	673-833	4.0(+12)	0	29190		
$\text{CH}_3\text{COOCH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ACETIC ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	308-448	2.5(+11)	0	3900		
$(\text{CH}_3\text{COO})_2\text{CH}_2 \rightarrow (\text{CH}_3\text{CO})_2\text{O} + \text{HCHO}$ METHANEDIOL, DIACETATE 70 BEN/O'N REACTION ORDER: 1.	493-578	5.0(+10)	0	18300		
$(\text{CH}_3)_2\text{CHOCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ PROPANE, 2-(ETHENYLOXY)- 70 BEN/O'N REACTION ORDER: 1.	720-794	3.8(+12)	0	21920		
$\text{CH}_2=\text{CHCH}_2\text{CH}(\text{OH})\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ 4-PENTEN-2-OL 70 BEN/O'N REACTION ORDER: 1.	625-663	8.5(+11)	0	20600		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\cdot + \text{CH}_4$ PENTANAL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3000±500	0.4	1.6
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\cdot + \text{CH}_4$ BUTANAL, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3200±500	0	2 .0
$(\text{CH}_3)_2\text{CHCH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{O})\cdot + \text{CH}_4$ BUTANAL, 3-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3070±500	0.4	1.6
$(\text{CH}_3)_3\text{CCHO} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{C}(\text{O})\cdot + \text{CH}_4$ PROPANAL, 2,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	3170±500	0.5	2.0
$(\text{CH}_3\text{CH}_2)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{COCH}_2\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3 + \text{CH}_4$ 3-PENTANONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-450	1.9(+11)	0	3675±500	0.5	1.5
$(\text{CH}_3\text{CD}_2)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{COCOD}_2\text{CH}_2\cdot + \text{CH}_4$ 3-PENTANONE-2,2,4,4-d ₄ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	500-600	2.0(+11)	0	5535±500	0.5	2.0
$(\text{CH}_3\text{CD}_2)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{COCOD}(\cdot)\text{CH}_3 + \text{CH}_4$ 3-PENTANONE-2,2,4,4-d ₄ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	500-600	1.3(+11)	0	4200±500	0.5	2.0
$(\text{CH}_3\text{CH}_2)_2\text{CO} + \text{CH}_3\text{CH}_2\cdot \rightarrow \cdot\text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3 + \text{CH}_3\text{CH}_3$ 3-PENTANONE + ETHYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-520	2.8(+11)	0	3986±100	0.4	2.2

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{HCOO}(\text{CH}_2)_3\text{CH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{COO}(\text{CH}_2)_3\text{CH}_3 + \text{HCOOCH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ $+ \text{HCOOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{HCOOCH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{HCOO}(\text{CH}_2)_3\text{CH}_2\cdot + \text{CH}_4$ FORMIC ACID BUTYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.5(+11)	0	4980±500	0.5 2.0
$\text{HCOOC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HCOOH}$ FORMIC ACID 1,1-DIMETHYLETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	503-573	7.9(+12)	0	19730	
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID PROPYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: RELIABILITY NO BETTER THAN AN ORDER OF MAGNITUDE.	725-810	2.5(+12)	0	24006	
$\text{CH}_3\text{COOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-METHYLETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	586-801	1.0(+13)	0	22645	
$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{COOH} + \text{CH}_2=\text{CH}_2$ PROPANOIC ACID ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	778-875	5.6(+12)	0	24400	
$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{COOCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}(\cdot)\text{CH}_3 + \cdot\text{CH}_2\text{CH}_2\text{COOCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_2\cdot + \text{CH}_4$ PROPANOIC ACID ETHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-650	2.5(+11)	0	4125±500	0.5 1.5
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_2=\text{CHOCH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID (2-METHOXYETHYL) ESTER 70 BEN/O'N REACTION ORDER: 1.	725-810	1.6(+12)	0	24460	
$\text{CH}_3\text{CH}_2\text{OCOOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ CARBONIC ACID DIETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	573-648	7.9(+12)	0	21800	
$(\text{CH}_3\text{CH}_2)\text{C}(\text{CH}_3)_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $+ \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 + \text{H}_2\text{O}$ 2-BUTANOL, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	757-799	3.2(+13)	0	30200	
$(\text{CH}_3)_3\text{CCN} \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CN} + \text{CH}_3\cdot$ PROPANENITRILE, 2,2-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	875-925	1.4(+15)	0	35330	
$(\text{CH}_3\text{CH}_2)_2\text{NCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2 + (\text{CH}_3\text{CH}_2)_2\text{NCH}_2\cdot + \text{CH}_4$ ETHANAMINE, N-ETHYL-N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	420	3.0(+ 7)	-	-	0.5 2.0
$(\text{CH}_3)_2\text{NCON}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2(\text{CH}_3)\text{NCON}(\text{CH}_3)_2 + \text{CH}_4$ UREA, TETRAMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-550	2.0(+11)	0	3975±500	0.5 1.5
$\text{CH}_2=\text{CHCH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{cy-CH}_2\text{CH}=\text{CHCH}=\text{CHCH}_2$ cis-1,3,5-HEXATRIENE 70 BEN/O'N REACTION ORDER: 1.	390-463	7.1(+11)	0	15050	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} + \text{N} \rightarrow \text{products}$ 1-HEXYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 14.0	320-550 435	4.6(+11) -	0 -	1233 -	
NOTE: k _{ref} : CHCH + N.					
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_2\text{CH}_3 + \text{N} \rightarrow \text{products}$ 3-HEXYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 14.0	320-550 435	3.4(+11) -	0 -	1102 -	
NOTE: k _{ref} : CH=CH + N					

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{cis-CH}_2=\text{CHCH}=\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_3$ cis-1,3-HEXADIENE 70 BEN/O'N REACTION ORDER: 1.	474-518	6.3(+10)	0	16355	
$\text{CD}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CD}_2 \rightarrow \text{CH}_2=\text{CHCD}_2\text{CD}_2\text{CH}=\text{CH}_2$ $\text{1,5-HEXADIENE-1,1,6,6-D}_4$ 70 BEN/O'N REACTION ORDER: 1.	530	1.3(+11)	0	17865	
$(\text{CH}_3)_2\text{C}=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CHCH}_3$ $\text{1,3-PENTADIENE, 4-METHYL-}$ 70 BEN/O'N REACTION ORDER: 1.	473-510	5.2(+11)	0	18199	
$\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ $+ \cdot\text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ $\text{1,3-BUTADIENE, 2,3-DIMETHYL-}, + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	318-414	1.6(+11)	0	2265	
$\text{cis-CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}=\text{CH}_2$ $\text{cis-1,3-PENTADIENE, 2-METHYL-}$ 70 BEN/O'N REACTION ORDER: 1.	473	1.7(+11)	0	16485	
$\text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2 + \text{O} \rightarrow \text{cy-}[\text{CH}_3(\text{CH}_2)_3]\text{CHCH}_2\text{O}$ $\text{1-HEXENE} + \text{OXYGEN ATOM}$ 73 HER/HUI REACTION ORDER: 2.	298	3.1(+12)	-	-	0.7 1.3
$\text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_3)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ $\text{1-HEXENE} + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	338-435	3.9(+10)	0	3400	
$\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ $\text{cis-2-HEXENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
$\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-HEXENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4150	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_3$ $\text{1-PENTENE, 2-METHYL-}, + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	3450	
$\text{cis-}(\text{CH}_3)_2\text{CHCH}=\text{CHCH}_3 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}(\text{CH}_3)_2$ $\text{cis-2-PENTENE, 4-METHYL-}, + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4390	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{O} \rightarrow \text{products}$ $\text{2-BUTENE, 2,3-DIMETHYL-}, + \text{OXYGEN ATOM}$ 73 HER/HUI REACTION ORDER: 2.	298-400	3.4(+12)	0	-790	0.8 1.2
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{H} \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ $\text{2-BUTENE, 2,3-DIMETHYL-}, + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 0.84	298 300	7.8(+11) -	- -	- -	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{S} \rightarrow \text{cy-}[(\text{CH}_3)_2]\text{CC}(\text{CH}_3)_2\text{S}$ $\text{2-BUTENE, 2,3-DIMETHYL-}, + \text{SULFUR ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	8.5(+13)	-	-	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{N} \rightarrow \text{products}$ $\text{2-BUTENE, 2,3-DIMETHYL-}, + \text{NITROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 3.5	320-550 435	1.7(+11) -	0 -	690 -	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{N} \rightarrow \text{products}$ $\text{2-BUTENE, 2,3-DIMETHYL-}, + \text{METHYLENE FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 2.16	297	-	-	-	
NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + \text{N}$					
NOTE: k _{ref} : $\text{CH}_2=\text{CH}_2 + \text{N}$					

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + {}^3\text{CH}_2 \rightarrow \text{products}$ 2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 2.74 NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$	297	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}=(\text{CH}_3)\text{CCH}_2 + \text{CH}_4$ 2-BUTENE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	403-614	7.8(+11)	0	4400±500	0.6 1.4
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{CC}(\cdot)(\text{CH}_3)_2$ 2-BUTENE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	403-453	1.0(+10)	0	3400	
NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$ k/k_{ref} : 0.2	453	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CCO} \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}$ 2-BUTENE, 2,3-DIMETHYL-, + CARBON OXIDE(C_2O) 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 250. NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	298	-	-	-	
$\text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ PENTYL, 1-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	822	2.0(+14)	0	13800	
$\text{CH}_3(\text{CH}_2)_4\text{CH}_3 + \text{O} \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot + \text{OH}$ HEXANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\text{CH}_3(\text{CH}_2)_4\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3 + \text{OH}$ HEXANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	1.1(+14)	0	2250	0.7 1.3
$\text{CH}_3(\text{CH}_2)_4\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot + \text{CH}_4$ HEXANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	4.8(+11)	0	5800±250	0.7 1.3
$\text{CH}_3(\text{CH}_2)_4\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4$ HEXANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	7.9(+11)	0	4830±250	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH}\cdot + (\text{CH}_3)_2\text{CH}\cdot$ BUTANE, 2,3-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	1000-1200	3.2(+16)	0	39250	
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot$ BUTANE, 2,3-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	1000-1200	1.0(+17)	0	41800	
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 + \text{O} \rightarrow \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{OH}$ BUTANE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 + \text{O} \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{OH}$ BUTANE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	3.1(+13)	0	1650	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.5(+11)	0	5800±250	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	1.9(+11)	0	3975±250	0.7 1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{CHC}(\cdot)(\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-500	5.0(+10)	0	3445	
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 + \text{CD}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CD}_3\text{H}$ BUTANE, 2,3-DIMETHYL-, + METHYL-d ₃ FREE RADICAL 72 KON REACTION ORDER: 2.	439-566	4.7(+11)	0	4525	
$\text{CH}_2=\text{C}(\text{CH}_3)\text{OCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ 1-PROPENE, 3-(1-METHYLETHENYLOXY)- 70 BEN/O'N REACTION ORDER: 1.	416-467	5.4(+11)	0	14745	
$\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{OCH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CHO}$ 1-PROPENE, 2-METHYL-3(ETHENYLOXY)- 70 BEN/O'N REACTION ORDER: 1.	423-461	1.4(+11)	0	14645	
$\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{OCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CHO}$ 1-PROPENE, 3-METHYL-3(ETHENYLOXY)- 70 BEN/O'N REACTION ORDER: 1.	423-461	2.1(+11)	0	14025	
$\text{CH}_2=\text{CHC}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ 3-BUTENOIC ACID, 2,2-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	511-548	1.4(+11)	0	18400	
$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow$ $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ PROPANOIC ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	352-453	2.5(+11)	0	3875	
$(\text{CH}_3\text{COO})_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{COOCOCH}_3 + \text{CH}_3\text{CHO}$ 1,1-ETHANEDIOL, DIACETATE 70 BEN/O'N REACTION ORDER: 1.	493-541	1.9(+10)	0	16560	
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OOC}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{O} \cdot + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{O} \cdot$ PEROXIDE, BIS(1-OXOPROPYL)- 70 BEN/O'N REACTION ORDER: 1.	373-464	2.5(+14)	0	15100	
$\text{CH}_2=\text{CHCH}_2\text{C}(\text{OH})(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CO}$ 4-PENTEN-2-OL, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	607-643	1.4(+12)	0	20500	
$\text{CH}_2=\text{CHO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ BUTANE, 1-(ETHENYLOXY)- 70 BEN/O'N REACTION ORDER: 1.	590-650	1.4(+11)	0	21330	
$\text{CH}_2=\text{CHO}(\text{CH}_2)_3\text{CH}_3 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{O}(\text{CH}_3)_3\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{O}(\text{CH}_2)_3\text{CH}_3$ BUTANE, 1-ETHENYLOXY-, + ETHYL FREE RADICAL 70 BEN/O'N REACTION ORDER: 2.	303-435	2.5(+10)	0	3070	
$\text{CH}_3\text{COO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID BUTYL ESTER 72 KER/PAR REACTION ORDER: 1.	725-810	1.6(+12)	0	23150	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$ $+ \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$ ACETIC ACID 1-METHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 57% 1-BUTENE: trans/cis-2-BUTENE = 0.64.	576-710	2.0(+13)	0	23450	
$\text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 2-METHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-810	7.9(+11)	0	23800	
$\text{CH}_3\text{COOC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,1-DIMETHYLETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	514-564	1.4(+13)	0	20130	
$(\text{CH}_3)_2\text{C}(\text{OH})\text{CH}_2\text{COCH}_3 \rightarrow (\text{CH}_3)_2\text{CO} + (\text{CH}_3)_2\text{CO}$ 2-PENTANONE, 4-HYDROXY-4-METHYL- 70 BEN/O'N REACTION ORDER: 1.	495-528	4.3(+11)	0	16255	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{OCH}_3$ + cis- and trans- $\text{CH}_3\text{CH}=\text{CHOCH}_3$ 2-PROPANOL, 1-METHOXY-, ACETATE 70 BEN/O'N REACTION ORDER: 1. NOTE: 58% PROPENE, 3-METHOXY-	650-710	1.1(+13)	0	23450	
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHOCH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ETHANOL, 2-ETHOXY-, ACETATE 70 BEN/O'N REACTION ORDER: 1.	725-810	1.2(+12)	0	24100	
$(\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CHOH}$ PROPANE, 2,2'-OXYBIS- 70 BEN/O'N REACTION ORDER: 1. NOTE: SUSPECT RATE CONSTANT.	696-760	4.2(+14)	0	31960	
$(\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OCH}(\text{CH}_3)_2$ + $\cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OCH}(\text{CH}_3)_2 + \text{CH}_4$ PROPANE, 2,2'-OXYBIS-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	2.1(+11)	0	4100±500	0.5 2.0
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{O}\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{O}\cdot$ PEROXIDE, DIPROPYL 70 BEN/O'N REACTION ORDER: 1.	420-428	4.0(+15)	0	18700	
$(\text{CH}_3)_2\text{CHOOCH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OOCH}(\text{CH}_3)_2$ + $\cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OOCH}(\text{CH}_3)_2 + \text{CH}_2\cdot + \text{CH}_4$ PEROXIDE, BIS(1-METHYLETHYL)-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-450	2.3(+11)	0	4100±500	0.5 1.5
$\text{CH}_3\text{CH}=\text{NC}(\text{CH}_3)_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\cdot)=\text{NC}(\text{CH}_3)_3$ + $\cdot\text{CH}_2\text{CH}=\text{NC}(\text{CH}_3)_3 + \text{CH}_3\text{CH}=\text{NC}(\text{CH}_3)_2\text{CH}_2\cdot + \text{CH}_4$ 2-PROPANIMINE, N-ETHYLIDENE-2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	8.9(+10)	0	3925±500	0.5 1.5
$(\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHN}=\text{N}\cdot + (\text{CH}_3)_2\text{CH}\cdot$ DIAZENE, BIS(1-METHYLETHYL)- 70 BEN/O'N REACTION ORDER: 1.	523-563	2.5(+16)	0	23900	
$(\text{CH}_3)_2\text{CHNHCH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHN}(\cdot)\text{CH}(\text{CH}_3)_2$ + $(\text{CH}_3)_2\text{C}(\cdot)\text{NHCH}(\text{CH}_3)_2 + \text{CH}_2\text{CH}(\text{CH}_3)\text{NHCH}(\text{CH}_3)_2 + \text{CH}_4$ 2-PROPANAMINE, N-(1-METHYLETHYL)-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	2.0(+11)	0	3370±750	
$(\text{CH}_3\text{CH}_2)_3\text{N} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$ + $\cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2 + \text{CH}_4$ ETHANAMINE, N,N-DIETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-600	5.0(+11)	0	4000±500	0 2.0
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHC}(=\text{CH}_2)\text{CH}_2\text{CH}=\text{CH}_2$ 1,2,6-HEPTATRIENE 70 BEN/O'N REACTION ORDER: 1.	445-491	9.3(+ 9)	0	14330	
$\text{CH}_3(\text{CH}_2)_4\text{CCH} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{C}(\cdot)=\text{CHCH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH}\cdot$ 1-HEPTYNE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.		3.9(+11)	0	4430	
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_2\text{CH}=\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ 1,5-HEPTADIENE 70 BEN/O'N REACTION ORDER: 1.	451-523	1.3(+11)	0	16355	
$\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$ 1,5-HEXADIENE, 3-METHYL- 70 BEN/O'N REACTION ORDER: 1.	451-523	7.1(+10)	0	17590	
$(\text{CH}_3)_2\text{C}=\text{C}=\text{C}(\text{CH}_3)_2 + \text{CCO} \rightarrow (\text{CH}_3)_2\text{C}=\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}$ 2,3-PENTADIENE, 2,4-DIMETHYL-, + CARBON OXIDE(C_2O) 70 BEN/O'N REACTION ORDER: 2. k/k_{ref} : 113. NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	304	-	-	-	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ 1-HEPTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	359-439	6.2(+10)	0	3500	
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2\cdot$ $+ (\text{CH}_3)_3\text{CC}(\cdot)(\text{CH}_3)_2$ 1-BUTENE, 2,3,3-TRIMETHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE BASED ON REACTION $(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}$	298	1.6(+12)	-	-	
$\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ 1-BUTENE, 2,3,3-TRIMETHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	322-364	7.8(+ 9)	0	2800	
$\text{CH}_3(\text{CH}_2)_5\text{CH}_3 + \text{O} \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2\cdot + \text{OH}$ HEPTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\text{CH}_3(\text{CH}_2)_5\text{CH}_3 + \text{O} \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)((\text{CH}_2)_2\text{CH}_3)$ $+ \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3 + \text{OH}$ HEPTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	1.2(+14)	0	2190	0.7 1.3
$(\text{CH}_3)_3\text{C}(\text{CH}_2)_2\text{CH}_3 + \text{O} \rightarrow \text{products}$ PENTANE, 2,2-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	307	6.5(+10)	-	-	0.7 1.4
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)_2 + \text{O} \rightarrow \text{products}$ PENTANE, 2,4-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	307	1.0(+11)	-	-	0.7 1.4
$(\text{CH}_3\text{CH}_2)_3\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3\text{CH}_2)_3\text{C}\cdot + \text{CH}_4$ PENTANE, 3-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$(\text{CH}_3\text{CH}_2)_3\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3\text{CH}_2)_2\text{CHCH}(\cdot)\text{CH}_3 + \text{CH}_4$ PENTANE, 3-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	6.0(+11)	0	4830±250	0.7 1.3
$(\text{CH}_3\text{CH}_2)_3\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3\text{CH}_2)_2\text{CHCH}_2\text{CH}_2\cdot + \text{CH}_4$ PENTANE, 3-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{C}\cdot + (\text{CH}_3)_2\text{CH}\cdot$ BUTANE, 2,2,3-TRIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	1069-1197	1.1(+16)	0	36335	
$\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_2\text{COOH} \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ 3-BUTENOIC ACID 2,2,3-TRIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	447-488	7.1(+10)	0	16560	
$\text{trans-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ $\text{trans-3-PENTENOIC ACID, 2,2-DIMETHYL-}$ 70 BEN/O'N REACTION ORDER: 1.	526-564	5.5(+11)	0	20300	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ $+ \text{cis-}, \text{ and trans-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ ACETIC ACID 1-METHYL-3-BUTENYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: trans/cis-1,3-PENTADIENE = 7/3; 1,4-PENTADIENE/1,3-PENTADIENE = 1/2.	564-628	2.0(+13)	0	22345	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{COCH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHCOCH}_3 + \text{CH}_3\text{COOH}$ 2-2-PENTANONE, 4-ACETYLOXY- 70 BEN/O'N REACTION ORDER: 1.	529-570	7.9(+11)	0	18800	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3\text{CH}_2\text{COO})_2\text{CH}_2 \rightarrow (\text{CH}_3\text{CH}_2\text{CO})_2\text{O} + \text{HCHO}$ METHANEDIOL, DIPROPANOATE 70 BEN/O'N REACTION ORDER: 1.	493-578	5.0(+10)	0	18300	
$\text{CH}_3\text{COO}(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID PENTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-810	1.6(+12)	0	23350	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{cis-}, \text{ and trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-METHYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 55% 1-PENTENE.	650-710	5.0(+12)	0	21995	
$\text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_3)_2 \rightarrow \text{cis-}, \text{ and trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$ $+ \text{CH}_3\text{COOH}$ ACETIC ACID 1-ETHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1.	650-710	1.2(+13)	0	22500	
$\text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 2-METHYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-810	7.9(+11)	0	23500	
$\text{CH}_3\text{COOC}[(\text{CH}_3)_2]\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $+ (\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,1-DIMETHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 75% 1-BUTENE, 2-METHYL-.	501-562	2.5(+13)	0	20300	
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 3-METHYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-810	1.6(+12)	0	23350	
$(\text{CH}_3)_3\text{CCOOCH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_3\text{CCOOH} + \text{CH}_2=\text{CH}_2$ PROPANOIC ACID, 2,2-DIMETHYL-, ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	635-694	4.0(+12)	0	24200	
$\text{CH}_3\text{CH}_2\text{COOC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{COOH}$ PROPANOIC ACID, 1,1-DIMETHYLETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	513-569	6.3(+12)	0	19730	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{N}(\text{CH}_3)_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{N}(\text{CHO})_2$ $+ \text{cis-}, \text{ and trans-CH}_3\text{CH}=\text{CHN}(\text{CH}_3)_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-METHYL-2-DIMETHYLAMINOETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	650-710	6.3(+12)	0	22245	
$(\text{CH}_3)_2\text{C}=\text{CHCH}=\text{C}(\text{CH}_3)_2 + 3\text{CH}_3\text{CH}_2 \rightarrow$ $(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)=\text{C}(\text{CH}_3)_2$ $+ (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}=\text{C}(\text{CH}_3)_2$ 2,4-HEXADIENE, 2,5-DIMETHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	328-420	6.2(+10)	0	3300	
$\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ 1-OCTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	339-425	1.2(+11)	0	3825	
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow$ $(\text{CH}_3)_3\text{CCH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ (\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ 1-PENTENE, 2,4,4-TRIMETHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	309-364	1.9(+10)	0	2870	
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{O} \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_2 \cdot + \text{OH}$ OCTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{O} \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3 + \text{OH}$ OCTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	9.3(+13)	0	2030	0.7 1.3

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot + \text{CH}_4$ OCTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	4.8(+11)	0	5800±250	0.7 1.3
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4$ OCTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	1.2(+12)	0	4830±250	0.7 1.3
$(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + 0 \rightarrow \text{products}$ PENTANE, 2,2,4-TRIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	307	5.5(+10)	-	-	0.6 1.5
$(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	2.0(+11)	0	4830±250	0.7 1.3
$(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{C}(\cdot)(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ $+ \text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + 0 \rightarrow \text{products}$ PENTANE, 2,3,4-TRIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	307	3.0(+10)	-	-	0.6 1.5
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow$ $\cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow$ $(\text{CH}_3)_2\text{CHC}(\cdot)(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	2.9(+11)	0	3975±250	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow [\text{C}_8\text{H}_{17}\cdot] + \text{CH}_4$ PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	414-605	4.7(+11)	0	4575	
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{C}\cdot + (\text{CH}_3)_3\text{C}\cdot$ BUTANE, 2,2,3,3-TETRAMETHYL- 70 BEN/O'N REACTION ORDER: 1.	985-1119	5.0(+16)	0	33800	
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 + 0 \rightarrow \text{products}$ BUTANE, 2,2,3,3-TETRAMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	8.0(+ 9)	-	-	0.6 1.5
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{CC}(\text{CH}_3)_2 + \text{CH}_4$ BUTANE, 2,2,3,3-TETRAMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-800	1.4(+12)	0	5800±250	0.7 1.3
$(\text{CH}_3\text{COO})_2\text{CHCH}=\text{CHCH}_3 \rightarrow (\text{CH}_3\text{CO})_2\text{O} + \text{cis-CH}_3\text{CH}=\text{CHCHO}$ 2-BUTENE-1,1-DIOL, DIACETATE 70 BEN/O'N REACTION ORDER: 1. NOTE: PROBABLY RELIABLE k.	492-533	1.3(+11)	0	16600	
$(\text{CH}_3\text{COO})_2\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow (\text{CH}_3\text{CO})_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$ 1,1-BUTANEDIOL, DIACETATE 70 BEN/O'N REACTION ORDER: 1. NOTE: PROBABLY RELIABLE k.	484-538	3.0(+10)	0	16560	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	T/K	A	B	E/R (in K)	k factors f F
$(\text{CH}_3\text{CH}_2\text{COO})_2\text{CHCH}_3 \rightarrow (\text{CH}_3\text{CH}_2\text{CO})_2\text{O} + \text{CH}_3\text{CHO}$ 1,1-ETHANEDIOL, DIPROPANOATE 70 BEN/O'N REACTION ORDER: 1.	484-538	2.5(+10)	0	16560	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OOC}(\text{O})\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{O}.$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{O}.$ PEROXIDE, BIS(1-OXOBUTYL) 70 BEN/O'N REACTION ORDER: 1.	370-452	2.0(+14)	0	14900	
$\text{CH}_3\text{COOC}(\text{CH}_2\text{CH}_3)_2\text{CH}_3 \rightarrow \text{cis-}, \text{ and } \text{trans-CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ $+ \text{CH}_2=\text{C}(\text{CH}_2\text{CH}_3)_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-ETHYL-1-METHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 65% 1-BUTENE, 2-ETHYL-.	560-610	1.4(+13)	0	19400	
$\text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 2-ETHYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-810	7.9(+11)	0	23050	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ $+ \text{cis-}, \text{ and } \text{trans-CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,2-DIMETHYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 76% 1-PENTENE, 3-METHYL-.	650-710	4.0(+12)	0	21740	
$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ (\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,1-DIMETHYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 72% 1-PENTENE, 2-METHYL-.	560-610	1.5(+13)	0	19525	
$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$ $+ \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,1,2-TRIMETHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 90% 1-BUTENE, 2,3-DIMETHYL-.	560-610	1.3(+13)	0	19075	
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{CHO} + (\text{CH}_3)_3\text{CO}.$ PEROXIDE, BIS(1,1-DIMETHYLETHYL) 70 BEN/O'N REACTION ORDER: 1.	403-443	4.0(+15)	0	18800	
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 + \text{CH}_3. \rightarrow .\text{CH}_2\text{C}(\text{CH}_3)_2\text{OOC}(\text{CH}_3)_3 + \text{CH}_4$ PEROXIDE, BIS(1,1-DIMETHYLETHYL)-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.8(+12)	0	5900±150	0.3 3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{N}.$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2.$ DIAZENE, DIBUTYL- 70 BEN/O'N REACTION ORDER: 1.	473-673	3.2(+16)	0	25165	
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{NCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{N}.$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3).$ DIAZENE, BIS(1-METHYLPROPYL)- 70 BEN/O'N REACTION ORDER: 1.	539-618	4.0(+16)	0	23500	
$(\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{NCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{N}.$ $+ (\text{CH}_3)_2\text{CHCH}_2.$ DIAZENE, BIS(2-METHYLPROPYL)- 70 BEN/O'N REACTION ORDER: 1.	473-673	1.7(+16)	0	24660	
$(\text{CH}_3)_3\text{CN}=\text{NC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{CN}=\text{N} + (\text{CH}_3)_3\text{C}.$ DIAZENE, BIS(1,1-DIMETHYLETHYL)- 70 BEN/O'N REACTION ORDER: 1.	473-673	1.4(+17)	0	21900	
$(\text{CH}_3\text{CH}_2)_2\text{NN}=\text{NN}(\text{CH}_2\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{NN}=\text{N} + (\text{CH}_3\text{CH}_2)_2\text{N}.$ 2-TETRAZENE, 1,1,4,4-TETRAETHYL- 70 BEN/O'N REACTION ORDER: 1.	471-508	2.5(+14)	0	17365	
$(\text{CH}_3)_2\text{CHCH}_2\text{N}(\text{O})\text{N}(\text{O})\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{NO}$ $+ (\text{CH}_3)_2\text{CHCH}_2\text{NO}$ PROPANE, 1-NITROSO-2-METHYL-, DIMERIC 70 BEN/O'N REACTION ORDER: 1.	374-402	2.5(+14)	0	12900	

Table of Arrhenius parameters for chemical reactions occurring in combustion—Continued

Chemical reactions	<i>T</i> /K	<i>A</i>	<i>B</i>	<i>E</i> / <i>R</i> (in K)	<i>k</i> factors <i>f</i> <i>F</i>
$\text{CH}_3\text{CH}=\text{C}(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)_2\text{COOH} \rightarrow (\text{CH}_3\text{CH}_2)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ PENTANOIC ACID, 2,2-DIMETHYL-3-ETHYLIDENE- 70 BEN/O'N REACTION ORDER: 1. NOTE: RELIABLE <i>k</i> .	468-502	4.8(+11)	0	18100	
$(\text{CH}_3\text{CH}_2\text{CH}_2\text{COO})_2\text{CH}_2 \rightarrow (\text{CH}_3\text{CH}_2\text{CH}_2\text{CO})_2\text{O} + \text{HCHO}$ METHANEDIOL, DIBUTANOATE 70 BEN/O'N REACTION ORDER: 1.	493-578	5.0(+10)	0	18300	
$\text{CH}_3\text{COOCH}(\text{CH}_3)(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2$ + <i>cis</i> -, and <i>trans</i> - $\text{CH}_3\text{CH}=\text{CH}(\text{CH}_2)_3\text{CH}_3$ ACETIC ACID 1-METHYLHEXYL ESTER 70 BEN/O'N REACTION ORDER: 1. NOTE: 58% 1-HEPTENE.	650-710	5.4(+12)	0	21995	
$\text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}(\text{CH}_2)_3\text{CH}_3$ + <i>cis</i> -, and <i>trans</i> - $\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-ETHYLPENTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	650-710	5.6(+12)	0	21740	
$\text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_2\text{CH}_3)_2 \rightarrow$ + <i>cis</i> -, and <i>trans</i> - $\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-PROPYLBUTYL ESTER 70 BEN/O'N REACTION ORDER: 1.	50-710	4.0(+12)	0	21500	
$\text{CH}_3\text{COOCH}[\text{CH}(\text{CH}_3)_2]_2 \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\text{CH}_3)_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-(1'-METHYLETHYL)-2-METHYLPROPYL ESTER 70 BEN/O'N REACTION ORDER: 1.	650-710	6.9(+12)	0	22500	
$(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow$ <i>cis</i> - $[\text{CH}_2=\text{C}(\text{CH}_3)]\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ 1,6-OCTADIENE, 3,7-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	656-682	1.2(+ 9)	0	17700	
$(\text{CH}_3\text{CH}_2\text{CH}_2\text{COO})_2\text{CHCH}_3 \rightarrow (\text{CH}_3\text{CH}_2\text{CH}_2\text{CO})_2\text{O} + \text{CH}_3\text{CHO}$ 1,1-ETHANEDIOL, DIBUTANOATE 70 BEN/O'N REACTION ORDER: 1. NOTE: PROBABLY RELIABLE <i>k</i> .	473-573	1.8(+10)	0	16600	
$(\text{CH}_3\text{COO})_2\text{CH}(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CHO} + (\text{CH}_3\text{CO})_2\text{O}$ 1,1-HEPTANEDIOL, DIACETATE 70 BEN/O'N REACTION ORDER: 1. NOTE: PROBABLY RELIABLE <i>k</i> .	473-573	3.0(+10)	0	16600	

3. Sources of Recommended Rate Constants

- Baulch, D. L., Drysdale, D. D., Horne, D. G., and Lloyd, A. C., "Evaluated Kinetics Data for High Temperature Reactions, Vol. 1: Homogeneous Gas Phase Reactions of the H_2 - O_2 System," (Butterworths, London, 1972).
- Baulch, D. L., Drysdale, D. D., Horne, D. G., "Evaluated Kinetic Data for High Temperature Reactions, Vol. 2: Homogeneous Gas Phase Reactions of the H_2 - N_2 - O_2 System," (Butterworths, London, 1973).
- Baulch, D. L., Drysdale, D. D., Duxbury, J., and Grant, S. J., "Evaluated Kinetic Data for High Temperature Reactions, Vol. 3: Homogeneous Gas Phase Reactions of the O_2 - O_3 System, the CO - O_2 - H_2 System, and of Sulphur-Containing Species," (Butterworths, London, 1976).
- Benson, S. W., Golden, D. M., Lawrence, R. W., Shaw, R., and Woolfolk, R. W., "Estimating the Kinetics of Combustion Including Reactions Involving Oxides of Nitrogen and Sulfur," Environmental Protection Agency Report No. EPA-600/2-75-019, August 1975.
- Benson, S. W., and O'Neal, H. E., "Kinetic Data on Gas Phase Unimolecular Reactions," NBS-NSRDS-21 (1970). (Supt. Doc., U.S. Govt. Printing Office, Washington, D.C. 20402).

- Engleman, V. S., "Survey and Evaluation of Kinetic Data on Reactions in Methane/Air Combustion," Environmental Protection Agency Report No. EPA-600/2-76-003, January 1976.
- Herron, J. T., and Huie, R. E., "Rate Constants for the Reactions of Atomic Oxygen (O^3P) with Organic Compounds in the Gas Phase," J. Phys. Chem. Ref. Data **2**, 467-518 (1973).
- Kerr, J. A., and Parsonage, M. J., "Evaluated Kinetic Data on Gas Phase Addition Reactions: Reactions of Atoms and Radicals with Alkenes, Alkynes and Aromatic Compounds," (Butterworths, London, 1972).
- Kerr, J. A., and Parsonage, M. J., "Evaluated Kinetic Data on Gas Phase Hydrogen Transfer Reactions of Methyl Radicals," (Butterworths, London 1976).
- Kondratiev, V. N., "Konstanty Skorosti Gazofaznykh Reaktsij Spravochnik," (Izdatelstvo "Nauka," Moskva, 1970); also issued as "Rate Constants of Gas Phase Reactions, Reference Book," R. M. Fristrom, Ed., Translated by L. J. Holtschlag COM-72-10014, Office of Standard Reference Data, NBS (1972) (Distributed by National Technical Information Service, Springfield, Virginia 22151).
- Lloyd, A. C., "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical," Int. J. Chem. Kinet. **6**, 169-228 (1974).

Appendix: Conversion Tables

Equivalent second order rate constants

<i>A</i>	<i>B</i>	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 ³ kN ⁻¹ s ⁻¹
1 cm ³ mol ⁻¹ s ⁻¹		1	10 ⁻³	10 ⁻⁶	1.66 × 10 ⁻²⁴	1.604 × 10 ⁻⁵ T ⁻¹	1.219 × 10 ⁻² T ⁻¹	2.453 × 10 ⁻⁹	1.203 × 10 ⁻⁴ T ⁻¹
1 dm ³ mol ⁻¹ s ⁻¹ =		10 ³	1	10 ⁻³	1.66 × 10 ⁻²¹	1.604 × 10 ⁻² T ⁻¹	12.19 T ⁻¹	2.453 × 10 ⁻⁶	1.203 × 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 × 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 × 10 ¹⁶ T ⁻¹	7.34 × 10 ²¹ T ⁻¹	1.478 × 10 ¹⁵	7.244 × 10 ¹⁹ T ⁻¹
1 (mm Hg) ⁻¹ s ⁻¹ =		6.236 × 10 ⁴ T	62.36 T	6.236 × 10 ⁻² T	1.035 × 10 ⁻¹⁹ T	1	760	4.56 × 10 ⁻²	7.500
1 atm ⁻¹ s ⁻¹ =		82.06 T	8.206 × 10 ⁻² T	8.206 × 10 ⁻⁵ T	1.362 × 10 ⁻²² T	1.316 × 10 ⁻³	1	6 × 10 ⁻⁵	9.969 × 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 ³ kN ⁻¹ s ⁻¹ =		8.314 T	8.314 T	8.314 × 10 ⁻³ T	1.38 × 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 cm³molecule⁻¹s⁻¹ to m³mol⁻¹s⁻¹ multiply by 6.023 × 10¹⁷.

Table adapted from Evaluated Kinetic Data for High Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the H₂-O₂ System, Butterworths, London, 1972.

Equivalent third order rate constants

<i>A</i>	<i>B</i>	cm ⁶ mol ⁻³ s ⁻¹	dm ⁶ mol ⁻³ s ⁻¹	m ⁶ mol ⁻³ s ⁻¹	cm ⁶ molecule ⁻³ s ⁻¹	(mm Hg) ⁻³ s ⁻¹	atm ⁻³ s ⁻¹	ppm ⁻³ min ⁻¹	m ⁶ kN ⁻³ s ⁻¹
1 cm ⁶ mol ⁻³ s ⁻¹ =		1	10 ⁻⁶	10 ⁻¹²	2.76 × 10 ⁻⁴⁶	2.57 × 10 ⁻¹⁰ T ⁻²	1.48 × 10 ⁻⁴ T ⁻²	1.003 × 10 ⁻¹⁹	1.447 × 10 ⁻⁶ T ⁻²
1 dm ⁶ mol ⁻³ s ⁻¹ =		10 ⁶	1	10 ⁻⁶	2.76 × 10 ⁻⁴²	2.57 × 10 ⁻⁴ T ⁻²	1.48 T ⁻²	1.003 × 10 ⁻¹³	1.447 × 10 ⁻² T ⁻²
1 m ⁶ mol ⁻³ s ⁻¹		10 ¹²	10 ⁶	1	2.76 × 10 ⁻³⁶	257 T ⁻²	1.48 × 10 ⁸ T ⁻²	1.003 × 10 ⁻⁷	1.447 × 10 ⁴ T ⁻²
1 cm ⁶ molecule ⁻³ s ⁻¹ =		3.628 × 10 ⁴⁷	3.628 × 10 ⁴¹	3.628 × 10 ³⁵	1	9.328 × 10 ³⁷ T ⁻²	5.388 × 10 ⁴³ T ⁻²	3.64 × 10 ²⁸	5.248 × 10 ³⁹ T ⁻²
1 (mm Hg) ⁻³ s ⁻¹ =		3.89 × 10 ⁹ T ²	3.89 T × 10 ³ T ²	3.89 × 10 ⁻³ T ²	1.07 × 10 ⁻³⁶ T ²	1	5.776 × 10 ⁵	3.46 × 10 ⁻⁵	56.25
1 atm ⁻³ s ⁻¹ =		6.733 × 10 ³ T ²	6.733 × 10 ⁻³ T ²	6.733 × 10 ⁻⁹ T ²	1.86 × 10 ⁻⁴⁴ T ²	1.73 × 10 ⁻⁶	1	6 × 10 ⁻¹¹	9.74 × 10 ⁻⁵
1 ppm ⁻³ 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 ⁶ kN ⁻³ s ⁻¹ =		6.91 T × 10 ⁷ T ²	69.1 T ²	6.91 × 10 ⁻⁵ T ²	1.904 × 10 ⁻⁴⁰ T ²	0.0178	1.027 × 10 ⁴	6.16 × 10 ⁻⁷	1

See note to Table for second order rate constants.

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET		1. PUBLICATION OR REPORT NO. NSRDS-NBS 67		2. Gov't. Accession No.		3. Recipient's Accession No.	
4. TITLE AND SUBTITLE Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion						5. Publication Date April 1980	
						6. Performing Organization Code	
7. AUTHOR(S) Francis Westley						8. Performing Organ. Report No.	
9. PERFORMING ORGANIZATION NAME AND ADDRESS NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, DC 20234						10. Project/Task/Work Unit No.	
						11. Contract/Grant No.	
12. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP) Department of Energy, Washington, DC 20545 and Office of Standard Reference Data, National Bureau of Standards, Washington, DC 20234						13. Type of Report & Period Covered N/A	
						14. Sponsoring Agency Code	
15. SUPPLEMENTARY NOTES Library of Congress Catalog Card Number: 79-607159 <input type="checkbox"/> Document describes a computer program; SF-185, FIPS Software Summary, is attached.							
16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.) A table of recommended rate constants for gas phase chemical reactions occurring in combustion is presented. Specifically, it gives in tabular form the values of the parameters for the modified Arrhenius equation $k = AT^B \exp(-E/RT)$. The table covers reactions occurring in the combustion, oxidation, and decomposition of aliphatic saturated or unsaturated C ₁ to C ₁₀ hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides and their free radicals, as well as the reactions of O, O ₂ , H, H ₂ , OH, H ₂ O, H ₂ O ₂ , N, N ₂ , NO, N ₂ O, NO ₂ , N ₂ O ₄ , N ₂ O ₅ , S, S ₂ , SH, SO, SO ₂ , SOH, NS, with each other. The table includes 169 first order reactions, 782 second order reactions, and 57 third order reactions. There are 1770 entries covering 1008 distinct chemical reactions. These recommendations have been taken from eleven evaluations and critical reviews published between 1970 and 1976. The papers examined by the evaluators extend from the nineteen fifties up to - and including - 1975.							
17. KEY WORDS (six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons) Arrhenius parameters; chemical kinetics; combustion; decomposition; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.							
18. AVAILABILITY <input checked="" type="checkbox"/> Unlimited <input type="checkbox"/> For Official Distribution. Do Not Release to NTIS <input checked="" type="checkbox"/> Order From Sup. of Doc., U.S. Government Printing Office, Washington, DC 20402, SD Stock No. SN003-003- <input type="checkbox"/> Order From National Technical Information Service (NTIS), Springfield, VA, 22161				19. SECURITY CLASS (THIS REPORT) UNCLASSIFIED		21. NO. OF PRINTED PAGES 119	
				20. SECURITY CLASS (THIS PAGE) UNCLASSIFIED		22. Price \$4.25	

**Where can you find
all the reference data
you need?**

Right in the Journal of Physical and Chemical Reference Data!

Now in its sixth year, this valuable publication has proved that it fills the important gaps for you in the literature of the physical sciences.

Published by the American Institute of Physics and the American Chemical Society for the National Bureau of Standards, this quarterly gives you quantitative numerical data, with recommended values and uncertainty limits chosen by experts in the field.

Critical commentary on methods of measurement and sources of error, as well as full references to the original literature, is an integral part of each of your four issues a year.

Can you afford to be without this prime source of reliable data on physical and chemical properties? To start receiving your copies, just fill in the order form and drop into the mail. If you do use a purchase order, please attach the printed form as this will help us to expedite your order. Send for complete list of reprints!



Journal of Physical and Chemical Reference Data
American Chemical Society
 1155 Sixteenth Street, N.W., Washington, D.C. 20036

Yes, I would like to receive the JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA at the one-year rate checked below:

Name

☐ Home

Street

☐ Business

City State Zip

Bill me ☐

Bill company or school ☐

Payment enclosed ☐

Members Nonmembers

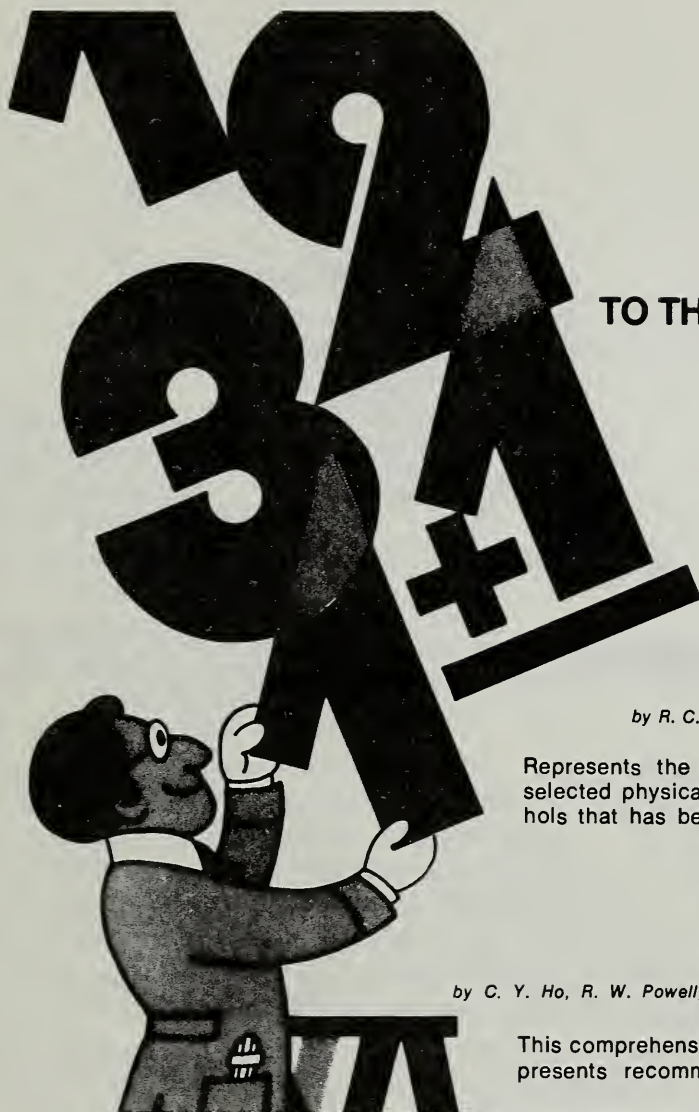
**U.S., Canada,
Mexico**

☐ \$25.00 ☐ \$100.00

Other Countries

☐ \$29.00 ☐ \$104.00

Please Attach This Order Form To Purchase Order.



Important Additions

TO THE JOURNAL OF PHYSICAL AND CHEMICAL REFERENCE DATA

Three comprehensive reference volumes, each, as the Journal itself, published by the American Institute of Physics and the American Chemical Society for the National Bureau of Standards . . . your triple assurance of their accuracy, immediacy, and usefulness.

Supplement No. 1 to Vol. 2

"PHYSICAL AND THERMODYNAMIC PROPERTIES OF ALIPHATIC ALCOHOLS"

by R. C. Wilhoit and B. J. Zwolinski, *Thermodynamics Research Center, Department of Chemistry, Texas A & M University*

Represents the most exhaustive review and critical analysis of selected physical and thermodynamic properties of aliphatic alcohols that has been published in the world literature of chemistry.

Supplement No. 1 to Vol. 3

"THERMAL CONDUCTIVITY OF THE ELEMENTS: A COMPREHENSIVE REVIEW"

by C. Y. Ho, R. W. Powell, and P. E. Liley, *Thermophysical Properties Research Center, Purdue University, West Lafayette, Indiana*

This comprehensive review of the world's thermal conductivity data presents recommended or estimated values for all 105 elements.

Supplement No. 1 to Vol. 6

ENERGETICS OF GASEOUS IONS

by H. M. Rosenstock, K. Draxl, B. Steiner, and J. T. Herron, *National Bureau of Standards*

Provides a comprehensive body of critically evaluated information on ionization potentials, appearance potentials, electron affinities and heats of formation of gaseous positive and negative ions. It is a complete revision and extension of the earlier reference work, "Ionization Potentials, Appearance Potentials and Heats for Formation of Gaseous Positive Ions," NSRDS-NBS 26.

Business Operations—Books and Journals Dept.
American Chemical Society
1155 16th Street, N.W.
Washington, D.C. 20036

Please send _____ copies of _____ at \$_____.

A. "PHYSICAL AND THERMODYNAMIC PROPERTIES OF ALIPHATIC ALCOHOLS." (First supplement to Vol. 2 of the *Journal of Physical and Chemical Reference Data*.) Hard Cover: \$33.00. Soft Cover: \$30.00.

B. "THERMAL CONDUCTIVITY OF THE ELEMENTS. A COMPREHENSIVE REVIEW." (First supplement to Vol. 3 of the *Journal of Physical and Chemical Reference Data*.) Hard Cover: \$60.00. Soft Cover: \$55.00.

C. "ENERGETICS OF GASEOUS IONS." (First supplement to Vol. 6 of the *Journal of Physical and Chemical Reference Data*.) Hard Cover: \$70.00. Soft Cover: \$65.00.

☐ I am enclosing a check ☐ I am enclosing a money order

Name _____

Address _____

City _____ State _____ Zip Code _____

Title _____ Employer _____

Please add \$1.50 extra for foreign postage and handling.

There's
a new
look
to...

DIMENSIONS

NBS

... the monthly magazine of the National Bureau of Standards. Still featured are special articles of general interest on current topics such as consumer product safety and building technology. In addition, new sections are designed to ... PROVIDE SCIENTISTS with illustrated discussions of recent technical developments and work in progress ... INFORM INDUSTRIAL MANAGERS of technology transfer activities in Federal and private labs. ... DESCRIBE TO MANUFACTURERS advances in the field of voluntary and mandatory standards. The new DIMENSIONS/NBS also carries complete listings of upcoming conferences to be held at NBS and reports on all the latest NBS publications, with information on how to order. Finally, each issue carries a page of News Briefs, aimed at keeping scientist and consumer alike up to date on major developments at the Nation's physical sciences and measurement laboratory.

(please detach here)

SUBSCRIPTION ORDER FORM

Enter my Subscription To DIMENSIONS/NBS at \$12.50. Add \$3.15 for foreign mailing. No additional postage is required for mailing within the United States or its possessions. Domestic remittances should be made either by postal money order, express money order, or check. Foreign remittances should be made either by international money order, draft on an American bank, or by UNESCO coupons.

Send Subscription to:

NAME-FIRST, LAST

COMPANY NAME OR ADDITIONAL ADDRESS LINE

STREET ADDRESS

CITY

STATE

ZIP CODE

PLEASE PRINT

☐ Remittance Enclosed
(Make checks payable
to Superintendent of
Documents)

☐ Charge to my Deposit
Account No.

MAIL ORDER FORM TO:
Superintendent of Documents
Government Printing Office
Washington, D.C. 20402

**Announcement of New Publications in
National Standard Reference Data Series**

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

Dear Sir:

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

Name_____

Company_____

Address_____

City_____State_____Zip Code_____

(Notification Key N-519)

NBS TECHNICAL PUBLICATIONS

PERIODICALS

JOURNAL OF RESEARCH—The Journal of Research of the National Bureau of Standards reports NBS research and development in those disciplines of the physical and engineering sciences in which the Bureau is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Bureau's technical and scientific programs. As a special service to subscribers each issue contains complete citations to all recent Bureau publications in both NBS and non-NBS media. Issued six times a year. Annual subscription: domestic \$17; foreign \$21.25. Single copy, \$3 domestic; \$3.75 foreign.

NOTE: The Journal was formerly published in two sections: Section A "Physics and Chemistry" and Section B "Mathematical Sciences."

DIMENSIONS/NBS—This monthly magazine is published to inform scientists, engineers, business and industry leaders, teachers, students, and consumers of the latest advances in science and technology, with primary emphasis on work at NBS. The magazine highlights and reviews such issues as energy research, fire protection, building technology, metric conversion, pollution abatement, health and safety, and consumer product performance. In addition, it reports the results of Bureau programs in measurement standards and techniques, properties of matter and materials, engineering standards and services, instrumentation, and automatic data processing. Annual subscription: domestic \$11; foreign \$13.75.

NONPERIODICALS

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

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

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

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

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NBS under the authority of the National Standard Data Act (Public Law 90-396).

NOTE: The principal publication outlet for the foregoing data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

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

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

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

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

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

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

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

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

BIBLIOGRAPHIC SUBSCRIPTION SERVICES

The following current-awareness and literature-survey bibliographies are issued periodically by the Bureau:

Cryogenic Data Center Current Awareness Service. A literature survey issued biweekly. Annual subscription: domestic \$25; foreign \$30.

Liquefied Natural Gas. A literature survey issued quarterly. Annual subscription: \$20.

Superconducting Devices and Materials. A literature survey issued quarterly. Annual subscription: \$30. Please send subscription orders and remittances for the preceding bibliographic services to the National Bureau of Standards, Cryogenic Data Center (736) Boulder, CO 80303.

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
Washington, O.C. 20234

OFFICIAL BUSINESS

Penalty for Private Use, \$300

POSTAGE AND FEES PAID
U.S. DEPARTMENT OF COMMERCE
COM-215



SPECIAL FOURTH-CLASS RATE
BOOK
