

# **Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion**

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## **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.



ERNEST AMBLER, *Director*

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# Table of Recommended Rate Constants for Chemical\* Reactions Occurring in Combustion

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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<sub>1</sub> to C<sub>10</sub> hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides and their free radicals, as well as the reactions of O, O<sub>2</sub>, H, H<sub>2</sub>, OH, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>, N, N<sub>2</sub>, NO, N<sub>2</sub>O, NO<sub>2</sub>, N<sub>2</sub>O<sub>4</sub>, N<sub>2</sub>O<sub>5</sub>, S, S<sub>2</sub>, SH, SO, SO<sub>2</sub>, 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  $k_o$  is the

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

$$fk_o < k < Fk_o \quad (1)$$

i.e., multiplication of the central value  $k_o$  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  $k_o$  is the central value of a rate constant, the statement that  $k_o$  is uncertain to a factor of  $F$  means that the uncertainty limits are defined by the relationship:

$$k_o/F < k < k_oF \quad (2)$$

which shows that division and multiplication of the central value  $k_o$  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  $\log_{10}k_o$ , and (c) Uncertainty expressed as a percentage of  $k_o$ . 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:

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

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

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:

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

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

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

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

then relationship (10) becomes:

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

which can take the form:

$$\log_{10}k_o/F < \log_{10}k < \log_{10}Fk_o$$

or  $k_o/F < k < Fk_o \quad (13)$

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  $k_o$ . 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  $k_o$  are defined by the relationship:

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

or  $(1 - p/100)k_o < k < (1 + p/100)k_o \quad (16)$

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

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

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

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

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

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 purposes. 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:  $fk_0 < k < Fk_0$ .

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  $cm^3mol^{-1}s^{-1}$

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

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:CO<sub>2</sub>. 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  $k/k_{\text{ref}}$  is given in the previous line, or other information pertinent to the reaction indicated above. The rate constant,  $k_{\text{ref}}$ , 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<sup>-1</sup> and  $R$  the gas constant with a value of 1.987 cal mol<sup>-1</sup>K<sup>-1</sup>, 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):  $f k_o < k < F k_o$ . 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 22<sup>1</sup>). 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, O<sub>2</sub>, O<sub>3</sub>.

(2) H-O system: H, H<sub>2</sub>, OH, HO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>.

(3) S-O-H system: S, S<sub>2</sub>, SO, SO<sub>3</sub>, SH, SH<sub>2</sub>, SOH.

(4) N-O-H-S system: N, N<sub>2</sub>, NO, NO<sub>2</sub>, NO<sub>3</sub>, N<sub>2</sub>O, N<sub>2</sub>O<sub>4</sub>, N<sub>2</sub>O<sub>5</sub>, NH, NH<sub>2</sub>, NH<sub>3</sub>, N<sub>2</sub>H<sub>4</sub>, HN<sub>3</sub>, HNO, HNO<sub>3</sub>, NS.

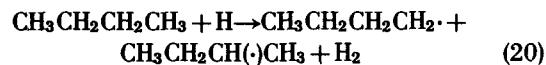
(5) C-O-H-S-N system: C<sub>1</sub> compounds: C, CO, CO<sub>2</sub>, CH, CH<sub>2</sub>, CH<sub>3</sub>, CH<sub>4</sub>, CHO, HCHO, CH<sub>3</sub>O·, CH<sub>3</sub>OH, CH<sub>3</sub>OOH, CS, CS<sub>2</sub>, COS, CH<sub>3</sub>S, CH<sub>3</sub>SH, CN, C(NO<sub>2</sub>)<sub>4</sub>, CHN, CH<sub>3</sub>NH<sub>2</sub>, CH=N≡N, CH<sub>3</sub>NHNH<sub>2</sub>, CH<sub>3</sub>NO, CH<sub>3</sub>NO<sub>2</sub>, CH<sub>3</sub>NO<sub>3</sub>, CH<sub>3</sub>ONH<sub>2</sub>. C<sub>2</sub> compounds: C<sub>2</sub>, C<sub>2</sub>O, CH=CH, CH<sub>2</sub>=CH<sub>2</sub>, CH<sub>3</sub>CH<sub>2</sub>·, CH<sub>3</sub>CH<sub>3</sub>, CH<sub>2</sub>=C=O, etc. C<sub>3</sub> compounds, etc., up to C<sub>10</sub> 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.

<sup>1</sup> 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 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 CH<sub>4</sub> + O → CH<sub>3</sub>· + OH, is inserted in the C-O-H-S-N system. This reaction may also be written as O + CH<sub>4</sub> → OH + CH<sub>3</sub>· 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 CH<sub>4</sub> 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 + NO<sub>2</sub> + O<sub>2</sub> → N<sub>2</sub>O<sub>5</sub>. This reaction will also be inserted under the forms: NO<sub>2</sub> + NO + O<sub>2</sub> → N<sub>2</sub>O<sub>5</sub> and O<sub>2</sub> + NO + NO<sub>2</sub> → N<sub>2</sub>O<sub>5</sub>. 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 O<sub>3</sub> + M → O + O<sub>2</sub> + M is inserted in the table only once, while reaction NO + O + M → NO<sub>2</sub> + M is inserted as such, and also under the form O + NO + M → NO<sub>2</sub> + 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

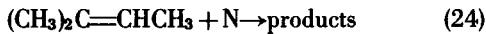


and  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{H}_2 \quad (22)$

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.:



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<sub>4</sub>, CH<sub>3</sub>CH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>.

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: CH<sub>3</sub>(CH<sub>2</sub>)<sub>4</sub>CH<sub>3</sub>, CH<sub>3</sub>(CH<sub>2</sub>)<sub>5</sub>CH<sub>3</sub>, CH<sub>3</sub>(CH<sub>2</sub>)<sub>6</sub>CH<sub>3</sub>, CH<sub>3</sub>(CH<sub>2</sub>)<sub>7</sub>CH<sub>3</sub>, CH<sub>3</sub>(CH<sub>2</sub>)<sub>8</sub>CH<sub>3</sub>.

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

Ethyne (Acetylene)	CH≡CH
1,2-Propadiene (Allene)	CH <sub>2</sub> =C=CH <sub>2</sub>
1,3-Butadiyne	CH≡CC≡CH
cis-2-Pentene	cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub>
1-Heptene	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH=CH <sub>2</sub>

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

Methyl free radical	CH <sub>3</sub> <sup>.</sup>
Ethyl, 1-methyl-, free radical (Isopropyl)	(CH <sub>3</sub> ) <sub>2</sub> CH <sup>.</sup>
Methyl, hydroxy-, free radical (Formyl) is written:	·CH <sub>2</sub> 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)	CH <sub>3</sub> CH <sub>2</sub> CH(-)CH <sub>3</sub>
Butyl, 1,1-dimethyl-, free radical (2-Methyl-2-pentyl)	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C(-)(CH <sub>3</sub> ) <sub>2</sub>
Methyl, oxo-, free radical (Formyl) is written:	·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: CH<sub>3</sub>O<sup>.</sup> 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: (CH<sub>3</sub>)<sub>2</sub>C(O<sup>.</sup>)CH<sub>2</sub>CH<sub>3</sub>.

*Peroxo, and other free radicals.* The rules for writing peroxy, and other free radicals are the same as for the oxy free radicals: CH<sub>3</sub>O<sub>2</sub><sup>.</sup>, CH<sub>3</sub>S<sup>.</sup>.

Atoms, like O, H, S, N, and simple radicals like OH, SH, NH, CH, CH<sub>2</sub>, are written without dot. Hydroperoxyl free radical is written HO<sub>2</sub><sup>.</sup> (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 <sub>2</sub> M: O <sub>2</sub> NOTE: k <sub>1</sub> = Kk <sub>-1</sub> . k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT ≈ 8000K.	190–4000 190–400 2000–10000	1.9(+13) 1.0(+14) 4.7(+23)	0 0 -2.5	-900±175 -720 0	0.8 1.2 0.5 1.5 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 <sub>2</sub> NOTE: M eff: O <sub>2</sub> (1.5) M: AR NOTE: M eff: Ar(1.0) M: N <sub>2</sub> NOTE: M eff: N <sub>2</sub> (1.4)	300 300	2.2(+14) 1.5(+14) 2.1(+14)	- - -	- - -	0.8 1.2 0.8 1.3 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 1500–2500	2.3(+13) 2.5(+13)	- 0	- 0	0.6 1.4 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	$38000 \pm 150$	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	$10400 \pm 1500$	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	$19500 \pm 150$	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	$-940 \pm 50$	0.8 1.2
Ar(0.1) AT 297K	M: Ar	200–500	1.1(+14)	0	$-940 \pm 50$
$H_2O(6.1)$ AT 297K	M: $H_2O$	200–500	6.7(+15)	0	$-940 \pm 15$
$D_2O(5.0)$ AT 297K	M: $D_2O$	200–500	5.5(+15)	0	$-940 \pm 50$
$SF_6(2.6)$ AT 297K	M: $SF_6$	200–500	2.9(+15)	0	$-940 \pm 50$
$N_2(1.4)$ AT 297K	M: $N_2$	200–500	1.5(+15)	0	$-940 \pm 50$
$N_2O(2.1)$ AT 297K	M: $N_2O$	200–500	2.3(+15)	0	$-940 \pm 50$
$CO_2(2.1)$ AT 297K	M: $CO_2$	200–500	2.3(+15)	0	$-940 \pm 50$
$CH_4(2.2)$ AT 297K	M: $CH_4$	200–500	2.4(+15)	0	$-940 \pm 50$
$CF_4(2.2)$ AT 297K	M: $CF_4$	200–500	2.4(+15)	0	$-940 \pm 50$
$O + NO_2 \rightarrow O_2 + NO$ OXYGEN ATOM + NITROGEN OXIDE( $NO_2$ ) 73 BAU/DRY REACTION ORDER: 2.	300–550	1.0(+13)	0	$300 \pm 100$	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	$500 \pm 250$	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: $k_O$ (LOW PRESSURE).	295	2.3(+16)	-	-	0.4 2.5
REACTION ORDER: 2. M: $N_2$ NOTE: LIMITING HIGH PRESSURE k.	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 <sub>2</sub> O → O <sub>2</sub> + N <sub>2</sub> OXYGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 73 BAU/DRY REACTION ORDER: 2.	1200–2000	1.0(+14)	0	14100±2000	0.4 2.5
O + N <sub>2</sub> O → NO + NO OXYGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 73 BAU/DRY REACTION ORDER: 2.	1200–2000	1.0(+14)	0	14100±1500	0.5 2.0
O + NH → OH + N OXYGEN ATOM + IMIDOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
O + NH → NO + H OXYGEN ATOM + IMIDOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
O + NH + M → HNO + M OXYGEN ATOM + IMIDOPEN FREE RADICAL 76 ENG REACTION ORDER: 3.	1500–2500	1.0(+16)	-0.5	0±2500	0.3 3.2
O + NH <sub>3</sub> → OH + NH <sub>2</sub> OXYGEN ATOM + AMMONIA 73 BAU/DRY REACTION ORDER: 2.	300–1000	1.5(+12)	0	3000±300	0.5 1.5
O + HNO → 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 → O <sub>2</sub> + 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 → NO <sub>2</sub> + 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 → SO + N OXYGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
O + NS → NO + S OXYGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
O + C + M → CO + M OXYGEN ATOM + CARBON ATOM 76 BAU/DRY REACTION ORDER: 3. NOTE: M = Ar, OR CO k <sub>1</sub> = Kk <sub>-1</sub>	7000–15000	3.3(+26)	-3.1	2114	0.3 1.8
O + CO → O <sub>2</sub> + C OXYGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	69300	
O + CO → CO + O OXYGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
O + CO + M → CO <sub>2</sub> + 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 <sub>2</sub> → O <sub>2</sub> + 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 <sub>1</sub> = Kk <sub>-1</sub>	1500–3000	1.7(+13)	0	26500±2500	0.5 2.0
O + CH → OH + C OXYGEN ATOM + METHYLIDENE 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
0 + CH → CO + H OXYGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
0 + CH + M → 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
0 + :CH <sub>2</sub> → H + .CHO OXYGEN ATOM + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	2000±2500	0.3 3.2
0 + :CH <sub>2</sub> → 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
0 + CH <sub>3</sub> → H + HCHO OXYGEN ATOM + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+13)	0	0	0.5 2.0
0 + CH <sub>4</sub> → OH + CH <sub>3</sub> . OXYGEN ATOM + METHANE 73 HER/HUI REACTION ORDER: 2. 76 ENG	350-1000 1500-2500	2.1(+13) 2.0(+13)	0	4550 4530±500	0.7 1.3 0.6 1.6
0 + .CHO → H + CO <sub>2</sub> OXYGEN ATOM + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	0	0±1500	
0 + .CHO → 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	
0 + HCHO → OH + .CHO OXYGEN ATOM + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	1.0	1750±1000	0.5 1.2
0 + HCHO → products OXYGEN ATOM + FORMALDEHYDE 73 HER/HUI REACTION ORDER: 2.	300	9.0(+10)	-	-	0.7 1.3
0 + HCDO → products OXYGEN ATOM + FORMALDEHYDE-d 73 HER/HUI REACTION ORDER: 2.	300	4.9(+10)	-	-	
0 + CH <sub>3</sub> O. → OH + HCHO OXYGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED	1500-2500	1.0(+14)	0	0±1500	
0 + CS → C + SO OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	28940	
0 + CS → 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
0 + CS <sub>2</sub> → S + COS OXYGEN ATOM + CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2.	302	2.2(+11)	-	-	0.5 1.5
0 + CS <sub>2</sub> → SO + CS OXYGEN ATOM + CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2.	200-1000	2.2(+13)	0	700±150	0.7 1.3
0 + COS → 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 → C + NO OXYGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	14545	
O + CN → 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 <sub>2</sub> → CO + C OXYGEN ATOM + CARBON DIMER 75 BEN/COL REACTION ORDER: 2.		6.3(+11)	0.5	0	
O + CH=CH → products OXYGEN ATOM + ETHYNE 73 HER/HUI REACTION ORDER: 2.	200–700	1.4(+13)	0	1500	0.8 1.2
O + CH <sub>2</sub> =CH <sub>2</sub> → cy-CH <sub>2</sub> CH <sub>2</sub> O OXYGEN ATOM + ETHÈNE 73 HER/HUI REACTION ORDER: 2.	200–500	3.3(+12)	0	565	0.8 1.2
O + CH <sub>3</sub> CH <sub>3</sub> → OH + CH <sub>2</sub> CH <sub>2</sub> . OXYGEN ATOM + ETHANE 73 HER/HUI REACTION ORDER: 2.	298–650	2.5(+13)	0	3200	0.7 1.3
O + CH <sub>2</sub> =C=O → products OXYGEN ATOM + ETHENONE 73 HER/HUI REACTION ORDER: 2.	298	5.3(+11)	-	-	0.7 1.3
O + CH <sub>3</sub> CHO → products OXYGEN ATOM + ACETALDEHYDE 73 HER/HUI REACTION ORDER: 2.	298–500	1.4(+13)	0	1140	0.5 2.0
O + cy-CH <sub>2</sub> CH <sub>2</sub> O → products OXYGEN ATOM + OXIRANE 73 HER/HUI REACTION ORDER: 2.	298	7.0(+8)	-	-	0.6 1.5
O + CH <sub>3</sub> CH <sub>2</sub> OH → products OXYGEN ATOM + ETHANOL 73 HER/HUI REACTION ORDER: 2.	298	8.7(+10)	-	-	0.6 1.5
O + CH <sub>3</sub> OCH <sub>3</sub> → products OXYGEN ATOM + METHANE, OXYBIS- 73 HER/HUI REACTION ORDER: 2.	200–500	5.9(+12)	0	1520	0.7 1.3
O + CH <sub>3</sub> C≡CH → products OXYGEN ATOM + PROPYNE 73 HER/HUI REACTION ORDER: 2.	298	4.0(+11)	-	-	0.5 2.0
O + CH <sub>3</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> )CHCH <sub>2</sub> O OXYGEN ATOM + 1-PROPENE 73 HER/HUI REACTION ORDER: 2.	200–500	2.5(+12)	0	38	0.8 1.2
O + CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> . + (CH <sub>3</sub> ) <sub>2</sub> CH. OXYGEN ATOM + PROPANE 73 HER/HUI REACTION ORDER: 2.	298	9.0(+9)	-	-	0.7 2
O + (CH <sub>3</sub> ) <sub>2</sub> CHOH → products OXYGEN ATOM + 2-PROPANOL 73 HER/HUI REACTION ORDER: 2.	298	1.3(+11)	-	-	0.6 1.5
O + (CH <sub>3</sub> ) <sub>2</sub> C≡CH → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> O OXYGEN ATOM + 1-PROPENE, 2-METHYL- 73 HER/HUI REACTION ORDER: 2.	298	1.2(+13)	-	-	0.7 1.3
O + CH=CC≡CH → products OXYGEN ATOM + 1,3-BUTADIYNE 73 HER/HUI REACTION ORDER: 2.	300	9.0(+11)	-	-	0.7 1.4
O + CH <sub>2</sub> =CHCH=CH <sub>2</sub> → 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 + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> CH <sub>2</sub> )CHCH <sub>2</sub> O OXYGEN ATOM + 1-BUTENE 73 HER/HUI REACTION ORDER: 2.	298	2.3(+12)	-	-	0.8 1.2
0 + cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → products OXYGEN ATOM + cis-2-BUTENE 73 HER/HUI REACTION ORDER: 2.	250-500	5.9(+12)	0	-165	0.8 1.2
0 + trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → products OXYGEN ATOM + trans-2-BUTENE 73 HER/HUI REACTION ORDER: 2.	298	1.4(+13)	-	-	0.7 1.3
0 + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . OXYGEN ATOM + BUTANE 73 HER/HUI REACTION ORDER: 2.	298-650	3.0(+13)	0	2920	0.7 1.3
0 + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> OXYGEN ATOM + BUTANE 73 HER/HUI REACTION ORDER: 2.	298-650	4.3(+13)	0	2410	0.7 1.3
0 + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> )CHCH <sub>2</sub> O OXYGEN ATOM + 1-PENTENE 73 HER/HUI REACTION ORDER: 2.	298	2.8(+12)	-	-	0.7 1.3
0 + cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> → products OXYGEN ATOM + cis-2-PENTENE 73 HER/HUI REACTION ORDER: 2.	298	1.1(+13)	-	-	0.7 1.3
0 + (CH <sub>3</sub> ) <sub>2</sub> C-CHCH <sub>3</sub> → 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 + CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . OXYGEN ATOM + PENTANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
0 + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>2</sub> CH <sub>3</sub> OXYGEN ATOM + PENTANE 73 HER/HUI REACTION ORDER: 2.	298-650	8.0(+13)	0	2320	0.7 1.3
0 + (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH <sub>3</sub> → OH + (CH <sub>3</sub> ) <sub>2</sub> C(.)CH <sub>2</sub> CH <sub>3</sub> + (CH <sub>3</sub> ) <sub>2</sub> CHCH(.)CH <sub>3</sub> + (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH <sub>2</sub> . + CH <sub>2</sub> CH(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>3</sub> OXYGEN ATOM + BUTANE, 2-METHYL- 73 HER/HUI REACTION ORDER: 2.	307	8.0(+10)	-	-	0.7 1.4
0 + (CH <sub>3</sub> ) <sub>4</sub> C → OH + (CH <sub>3</sub> ) <sub>3</sub> CCH <sub>2</sub> . OXYGEN ATOM + PROPANE, 2,2-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.4
0 + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> )CHCH <sub>2</sub> O OXYGEN ATOM + 1-HEXENE 73 HER/HUI REACTION ORDER: 2.	298	3.1(+12)	-	-	0.7 1.3
0 + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → 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 + CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>2</sub> . OXYGEN ATOM + HEXANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
0 + CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub> → OH + CH <sub>3</sub> CH(.)CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> OXYGEN ATOM + HEXANE 73 HER/HUI REACTION ORDER: 2.	298-650	1.1(+14)	0	2250	0.8 1.3
0 + (CH <sub>3</sub> ) <sub>2</sub> CHCH(CH <sub>3</sub> ) <sub>2</sub> → OH + CH <sub>2</sub> CH(CH <sub>3</sub> )CH(CH <sub>3</sub> ) <sub>2</sub> OXYGEN ATOM + BUTANE, 2,3-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.3
0 + (CH <sub>3</sub> ) <sub>2</sub> CHCH(CH <sub>3</sub> ) <sub>2</sub> → OH + (CH <sub>3</sub> ) <sub>2</sub> C(.)CH(CH <sub>3</sub> ) <sub>2</sub> 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
0 + $\text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3(\text{CH}_2)_5\text{CH}_2$ . OXYGEN ATOM + HEPTANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
0 + $\text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ OXYGEN ATOM + HEPTANE 73 HER/HUI REACTION ORDER: 2.	298-650	1.2(+14)	0	2190	0.7 1.3
0 + $(\text{CH}_3)_3\text{C}(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,2-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	6.5(+10)	-	-	0.7 1.4
0 + $(\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,4-DIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	1.0(+11)	-	-	0.7 1.4
0 + $\text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3(\text{CH}_2)_6\text{CH}_2$ . OXYGEN ATOM + OCTANE 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
0 + $\text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ OXYGEN ATOM + OCTANE 73 HER/HUI REACTION ORDER: 2.	298-650	9.3(+13)	0	2030	0.7 1.3
0 + $(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,2,4-TRIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	5.5(+10)	-	-	0.6 1.5
0 + $(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,3,4-TRIMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	3.0(+10)	-	-	0.6 1.5
0 + $(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow \text{products}$ OXYGEN ATOM + BUTANE, 2,2,3,3-TETRAMETHYL- 73 HER/HUI REACTION ORDER: 2.	307	8.0(+9)	-	-	0.6 1.5
$\text{O}_2 + \text{O} \rightarrow \text{O} + \text{O}_2$ OXYGEN MOLECULE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{O}_2 + \text{O} + \text{M} \rightarrow \text{O}_3 + \text{M}$ OXYGEN MOLECULE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: $\text{O}_2$ NOTE: M eff: $\text{O}_2(1.5)$	300	2.2(+14)	-	-	0.8 1.2
	M: Ar	300	1.5(+14)	-	0.8 1.3
	M: $\text{N}_2$	300	2.1(+14)	-	0.8 1.2
$\text{O}_2 + \text{H} \rightarrow \text{O} + \text{OH}$ 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 1.3 0.9 1.2
$\text{O}_2 + \text{D} \rightarrow \text{O} + \text{OD}$ OXYGEN MOLECULE + DEUTERIUM ATOM 72 BAU/DRY REACTION ORDER: 2.	800-1000	8.9(+13)	-	7500	
$\text{O}_2 + \text{H} + \text{M} \rightarrow \text{HO}_2 + \text{M}$ OXYGEN MOLECULE + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 3. M: $\text{H}_2$ NOTE: M eff: $\text{H}_2(1.0)$	300-2000	5.0(+15)	0	-500±250	0.5 1.5
	M: $\text{O}_2$	300-2000	2.0(+15)	0	-500±250
	M: $\text{H}_2\text{O}$	300-2000	3.2(+16)	0	-500±250
	M: He	300-2000	1.5(+15)	0	-500±250
	M: Ar	300-2000	1.5(+15)	0	-500±250
	M: $\text{N}_2$	300-2000	2.0(+15)	0	-500±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
$\text{CO}_2(1.5)$	M: $\text{CO}_2$	300–2000	7.5(+15)	0	-500±250
$\text{O}_2 + \text{H}_2 \rightarrow \text{OH} + \text{OH}$ OXYGEN MOLECULE + HYDROGEN MOLECULE 76 ENG	REACTION ORDER: 2.	1500–2500	2.5(+12)	0	$19630 \pm 5000$
$\text{O}_2 + \text{H}_2 \rightarrow \text{HO}_2 + \text{H}$ OXYGEN MOLECULE + HYDROGEN MOLECULE 72 BAU/DRY	REACTION ORDER: 2.	290–800	5.5(+13)	0	$29100 \pm 350$
$\text{O}_2 + \text{S} \rightarrow \text{O} + \text{SO}$ OXYGEN MOLECULE + SULFUR ATOM 76 BAU/DRY	REACTION ORDER: 2.	250–450	1.4(+12)	0	$0 \pm 50$
$\text{O}_2 + \text{SO} \rightarrow \text{O} + \text{SO}_2$ OXYGEN MOLECULE + SULFUR MONOXIDE 76 BAU/DRY	REACTION ORDER: 2.	440–2100	4.5(+11)	0	$3250 \pm 590$
$\text{O}_2 + \text{N} \rightarrow \text{O} + \text{NO}$ OXYGEN MOLECULE + NITROGEN ATOM 73 BAU/DRY	REACTION ORDER: 2.	300–3000	6.4(+ 9)	1.0	$3150 \pm 150$
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 3000K.					
$\text{O}_2 + \text{N}_2 \rightarrow \text{O} + \text{N}_2\text{O}$ OXYGEN MOLECULE + NITROGEN MOLECULE 73 BAU/DRY	REACTION ORDER: 2.	1200–2000	6.3(+13)	0	$55200 \pm 2000$
NOTE: $k_1 = Kk_{-1}$					
$\text{O}_2 + \text{NO} \rightarrow \text{O} + \text{NO}_2$ OXYGEN MOLECULE + NITROGEN OXIDE(NO) 73 BAU/DRY	REACTION ORDER: 2.	300–550	1.7(+12)	0	23400
NOTE: $k_1 = Kk_{-1}$					
$\text{O}_2 + \text{NO} + \text{NO} \rightarrow \text{NO}_2 + \text{NO}_2$ OXYGEN MOLECULE + NITROGEN OXIDE(NO) 73 BAU/DRY	REACTION ORDER: 3.	273–660	1.2(+ 9)	0	$-530 \pm 100$
$\text{O}_2 + \text{NO} + \text{NO}_2 \rightarrow \text{NO}_2 + \text{NO}_3$ OXYGEN MOLECULE + NITROGEN OXIDE(NO) + NITROGEN OXIDE( $\text{NO}_2$ ) 73 BAU/DRY	REACTION ORDER: 3.	300–500	2.9(+ 7)	0	$-400 \pm 500$
$\text{O}_2 + \text{C} \rightarrow \text{O} + \text{CO}$ OXYGEN MOLECULE + CARBON ATOM 75 BEN/GOL	REACTION ORDER: 2.		6.3(+11)	0.5	0
$\text{O}_2 + \text{CO} \rightarrow \text{O} + \text{CO}_2$ OXYGEN MOLECULE + CARBON MONOXIDE 76 BAU/DRY	REACTION ORDER: 2.	1500–3000	2.5(+12)	0	$24000 \pm 2500$
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K.					
$\text{O}_2 + \text{CH} \rightarrow \text{O} + \text{CHO}$ OXYGEN MOLECULE + METHYLIDYNE FREE RADICAL 76 ENG	REACTION ORDER: 2.	1500–2500	5.0(+11)	0.5	$3000 \pm 2500$
$\text{O}_2 + \text{CH}_2 \rightarrow \text{O} + \text{HCHO}$ OXYGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG	REACTION ORDER: 2.		5.0(+11)	0.5	$3500 \pm 2500$
$\text{O}_2 + \text{CH}_3 \cdot \rightarrow \text{O} + \text{CH}_3\text{O}\cdot$ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG	REACTION ORDER: 2.	1500–2500	3.2(+12)	0	$15100 \pm 1500$
NOTE: k ESTIMATED.					
$\text{O}_2 + \text{CH}_3 \cdot \rightarrow \text{OH} + \text{HCHO}$ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG	REACTION ORDER: 2.	1500–2500	3.2(+13)	0	$10000 \pm 5000$
$\text{O}_2 + \text{CH}_3 \cdot \rightarrow \text{HO}_2 \cdot + :\text{CH}_2$ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG	REACTION ORDER: 2.	1500–2500	3.2(+12)	0	$34975 \pm 1500$
NOTE: k ESTIMATED					

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
$O_2 + .CHO \rightarrow HO_2 + CO$ 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 + CYANOGEND 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 M: O <sub>2</sub> NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT ≈ 8000K. M: Ar 3000-18000	3.5(+25) 9.8(+24)	-2.5 -2.5	59380 59380	0.5 2.0 0.4 2.5
$O_3 + O \rightarrow O_2 + O_2$ OZONE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 AT ≈ 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
$O_3 + H2S \rightarrow SO_2 + H2O$ 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 <sub>2</sub> ) 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 <sub>2</sub> NOTE: M eff: H <sub>2</sub> (1.0)	300-2000	5.0(+15)	0	-500±250	0.5 1.5
M: O <sub>2</sub>	300-2000	2.0(+15)	0	-500±250	0.5 1.5
M: H <sub>2</sub> O	300-2000	3.2(+16)	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	
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 <sub>2</sub> (0.4)	M: N <sub>2</sub>	300-2000	2.0(+15)	0	-500±250	0.5 1.5	
CO <sub>2</sub> (1.5)	M: CO <sub>2</sub>	300-2000	7.5(+15)	0	-500±250	0.5 1.5	
H + O <sub>3</sub> → OH + O <sub>2</sub> HYDROGEN ATOM + OZONE 76 BAU/DRY	REACTION ORDER: 2.	300	1.6(+13)	-	-	0.5 2.0	
H + H + M → H <sub>2</sub> + M HYDROGEN ATOM 72 BAU/DRY	REACTION ORDER: 3.	M: H <sub>2</sub> M: H <sub>2</sub>	300 2500-5000	3.0(+15) 2.6(+15)	-1.0 -1.0	0 0	0.5 1.5 0.4 2.5
NOTE: M eff: H <sub>2</sub> (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 <sub>2</sub> → H <sub>2</sub> + H HYDROGEN ATOM + HYDROGEN MOLECULE 75 BEN/GOL	REACTION ORDER: 2.		6.3(+11)	0.5	4000		
H + D <sub>2</sub> → 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 <sub>2</sub> → 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 <sub>2</sub> O + 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 <sub>2</sub> O + M HYDROGEN ATOM + HYDROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 3.	M: H <sub>2</sub> O	1000-3000	1.4(+23)	-2.0	0	0.7 1.5
NOTE: M eff: H <sub>2</sub> 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 <sub>2</sub>	1000-3000	2.2(+22)	-2.0	0	0.5 2.0	
N <sub>2</sub> (0.16)							
H + HO <sub>2</sub> → O + H <sub>2</sub> 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 <sub>2</sub> → H <sub>2</sub> + O <sub>2</sub> HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2.	290-800	2.5(+13)	0	350±350	0.4 2.5	
76 ENG		1500-2500	2.5(+13)	0	350±350	0.5 2.0	
H + HO <sub>2</sub> → OH + OH HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2.	290-800	2.5(+14)	0	950±350	0.5 2.0	
76 ENG		1500-2500	2.5(+14)	0	950±500	0.5 2.0	
H + H <sub>2</sub> O → OH + H <sub>2</sub> 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 <sub>2</sub> O <sub>2</sub> → H <sub>2</sub> + HO <sub>2</sub> 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 <sub>2</sub> → SH + S HYDROGEN ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		7.9(+12)	0.5	8355	
H + SO → OH + S HYDROGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	11200	
H + SO → SH + O HYDROGEN ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	19930	
H + SO <sub>2</sub> + M → HSO <sub>2</sub> + M HYDROGEN ATOM + SULFUR DIOXIDE 76 BAU/DRY REACTION ORDER: 3.	1660–2120	5.1(+15)	–	–	0.5 1.5
H + SH → H <sub>2</sub> + S HYDROGEN ATOM + MERCAPTO FREE RADICAL 76 BAU/DRY REACTION ORDER: 2.	298	1.5(+13)	–	–	0.5 1.5
H + SH → SH + H HYDROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
H + H <sub>2</sub> S → H <sub>2</sub> + 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 → 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 <sub>2</sub> → NH + N HYDROGEN ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	75945	
H + NO → OH + N HYDROGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	24460	
H + NO → NH + O HYDROGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	38200	
H + NO + M → 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 → HNO + M HYDROGEN ATOM + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 3. M: H <sub>2</sub>	1500–2500	5.0(+15)	0	-300±150	0.5 2.0
H + NO <sub>2</sub> → OH + NO HYDROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT T = 633K.	298–630	3.5(+14)	0	740±500	0.5 1.5
H + NO <sub>2</sub> → OH + NO HYDROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+14)	0	750±500	0.5 2.0
H + N <sub>2</sub> O → OH + N <sub>2</sub> HYDROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 73 BAU/DRY REACTION ORDER: 2.	700–2500	7.6(+13)	0	7600±500	0.5 1.5
H + N <sub>2</sub> O → NH + NO HYDROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	15100±2500	0.3 3.2
H + NH → H <sub>2</sub> + 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 → NH + H HYDROGEN ATOM + IMIDOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
H + NH <sub>2</sub> + M → NH <sub>3</sub> + M HYDROGEN ATOM + AMIDOGEN FREE RADICAL 73 BAU/DRY REACTION ORDER: 3. M: Ar NOTE: k <sub>1</sub> = Kk <sub>-1</sub>	2000-3000	4.8(+14)	0	-8300±2500	0.5	2.0
H + NH <sub>2</sub> NH <sub>2</sub> → H <sub>2</sub> + NH <sub>2</sub> NH. HYDROGEN ATOM + HYDRAZINE 73 BAU/DRY REACTION ORDER: 2.	250-500	1.3(+13)	0	1260±100	0.5	2.0
H + HNO → H <sub>2</sub> + NO HYDROGEN ATOM + NITROSYL HYDRIDE 73 BAU/DRY REACTION ORDER: 2.	2000	4.8(+12)	-	-	0.5	1.5
H + HNO → 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 → SH + N HYDROGEN ATOM + NITROGEN SULFIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	15700		
H + NS → NH + S HYDROGEN ATOM + NITROGEN SULFIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	20735		
H + CO → OH + C HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	77755		
H + CO → CH + O HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		2.5(+13)	0.5	88020		
H + CO + M → .CHO + M HYDROGEN ATOM + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 3. M: H <sub>2</sub> NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 773K. 76 ENG	298-773 1500-2500	6.9(+14) 1.6(+20)	0 -1.5	850±500 0	0.7 0.3	1.3 3.2
H + CO <sub>2</sub> → 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 → H <sub>2</sub> + C HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000		
H + CH → CH + H HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
H + CH + M → CH <sub>2</sub> + 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 <sub>2</sub> → H <sub>2</sub> + 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 <sub>4</sub> → H <sub>2</sub> + CH <sub>3</sub> . HYDROGEN ATOM + METHANE 76 ENG REACTION ORDER: 2.	1500-2500	6.3(+13)	0	5990±150	0.5	2.0
D + CH <sub>4</sub> → DH + CH <sub>3</sub> . DEUTERIUM ATOM + METHANE 72 KON REACTION ORDER: 2.	523-673	8.3(+12)	0	5100		
H + .CHO → H <sub>2</sub> + 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
H + HCHO → H <sub>2</sub> + .CHO HYDROGEN ATOM + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500–2500	1.3(+10)	1.0	1600	0.3 3.2
H + CH <sub>3</sub> O. → H <sub>2</sub> + HCHO HYDROGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.0(+14)	0	0±1500	
H + CS → C + SH HYDROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		2.0(+13)	0.5	48870	
H + CS → CH + S HYDROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+13)	0.5	50930	
H + COS → HS + CO HYDROGEN ATOM + CARBON OXIDE SULFIDE 76 BAU/DRY REACTION ORDER: 2.	298	1.3(+10)	-	-	0.8 1.3
H + CN → C + NH HYDROGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.0(+13)	0.5	52745	
H + CN → CH + N HYDROGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+12)	0.5	49775	
H + CN + M → HCN + M HYDROGEN ATOM + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 3.	1500–2500	3.2(+16)	-0.5	0±2500	0.3 3.2
H + C <sub>2</sub> → CH + C HYDROGEN ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		1.6(+13)	0.5	30450	
H + CH <sub>2</sub> =CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> . HYDROGEN ATOM + ETHENE 72 KER/PAR REACTION ORDER: 2.	298	9.3(+13)	0	1410	
H + CH <sub>2</sub> =CH <sub>2</sub> + M → CH <sub>3</sub> CH <sub>2</sub> . + M HYDROGEN ATOM + ETHENE 72 KON REACTION ORDER: 3.	298–813	5.6(+17)	0.5	495	
H + CH <sub>3</sub> CH <sub>3</sub> → H <sub>2</sub> + CH <sub>3</sub> CH <sub>2</sub> . HYDROGEN ATOM + ETHANE 72 KON REACTION ORDER: 2.	285–1440	1.0(+14)	0	4815±70	0.8 1.2
H + CH <sub>3</sub> C≡CH → CH <sub>3</sub> CH=CH + CH <sub>3</sub> C(.)=CH <sub>2</sub> HYDROGEN ATOM + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. NOTE: k TAKEN AS LOWER LIMIT.	298	0.5(+11)	-	-	
H + CH <sub>3</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	298	7.2(+12)	0	1460	
H + CH <sub>3</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH(.)CH <sub>3</sub> 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	
H + CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub> → H <sub>2</sub> + (CH <sub>3</sub> ) <sub>2</sub> CH. + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + PROPANE 72 KON REACTION ORDER: 2.	333–933	1.0(+13)	0	3130±180	0.7 1.4
H + (CH <sub>3</sub> ) <sub>2</sub> CO → H <sub>2</sub> + CH <sub>3</sub> C(O)CH <sub>2</sub> . 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 <sub>2</sub> =CHCH=CH <sub>2</sub> → CH <sub>2</sub> =CHCH(.)CH <sub>3</sub> + CH <sub>2</sub> =CHCH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGED RATE CONSTANT.	298	4.10(+13)	0	655	
H + CH <sub>2</sub> =CHCH=CH <sub>2</sub> → CH <sub>2</sub> =CHCH(.)CH <sub>3</sub> + CH <sub>2</sub> =CHCH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 4.9 NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub>	300	-	-	-	
H + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.03 NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub>	300	-	-	-	
H + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . 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	8.7(+11)	-	-	
H + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> 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 + cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> HYDROGEN ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION. k/k <sub>ref</sub> : 0.47 NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub> .	298	4.6(+11)	-	-	
H + trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> HYDROGEN ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGE k k/k <sub>ref</sub> : 0.59 NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub> .	298	5.6(+11)	-	-	
H + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>3</sub> C. HYDROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	3.10(+13)	0	755	
H + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> . 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 <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> .	298	1.3(+11)	-	-	
H + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>3</sub> C. + (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> . HYDROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 2.52 NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub>	300	-	-	-	
H + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → H <sub>2</sub> + CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + BUTANE 72 KON REACTION ORDER: 2.	320-930	4.1(+12)	0	2637±320	0.5 2.0
H + (CH <sub>3</sub> ) <sub>3</sub> CH → H <sub>2</sub> + (CH <sub>3</sub> ) <sub>3</sub> C. + (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> . HYDROGEN ATOM + PROPANE, 2-METHYL- 72 KON REACTION ORDER: 2.	300-800	1.9(+13)	0	2680±85	0.8 1.2
H + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . HYDROGEN ATOM + 1-PENTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.89 NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub> .	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
H + cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> HYDROGEN ATOM + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.39	298 300	3.8(+11) -	-	-	
NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub> .					
H + trans-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> HYDROGEN ATOM + trans-2-PENTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.44	298 300	4.1(+11) -	-	-	
NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub> .					
H + CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> C(.)CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH <sub>2</sub> HYDROGEN ATOM + 1-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	9.1(+11)	-	-	
D + CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> C(.)CH <sub>3</sub> D + CH <sub>3</sub> CH <sub>2</sub> CD(CH <sub>3</sub> )CH <sub>2</sub> DEUTERIUM ATOM + 1-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	2.0(+12)	-	-	
H + (CH <sub>3</sub> ) <sub>2</sub> CHCH=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHCH(.)CH <sub>3</sub> + (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH <sub>2</sub> HYDROGEN ATOM + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	7.4(+11)	-	-	
D + (CH <sub>3</sub> ) <sub>2</sub> CHCH=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHCH(.)CH <sub>2</sub> D + (CH <sub>3</sub> ) <sub>2</sub> CHCHDCH <sub>2</sub> DEUTERIUM ATOM + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	7.6(+11)	-	-	
H + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHCH(.)CH <sub>3</sub> + (CH <sub>3</sub> ) <sub>2</sub> C(.)CH <sub>2</sub> CH <sub>3</sub> HYDROGEN ATOM + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.03	298 300	9.1(+11) -	-	-	
NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub>					
H + (CH <sub>3</sub> ) <sub>2</sub> C(CH <sub>3</sub> ) <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHC(.)CH <sub>3</sub> HYDROGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.84	298 300	7.8(+11) -	-	-	
NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub>					
H + (CH <sub>3</sub> ) <sub>3</sub> CC(CH <sub>3</sub> )=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>3</sub> CCH(CH <sub>3</sub> )CH <sub>2</sub> + (CH <sub>3</sub> ) <sub>3</sub> CC(.)CH <sub>3</sub> HYDROGEN ATOM + 1-BUTENE, 2,3,3,-TRIMETHYL- 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE VALUE BASED ON REACTION: H + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>	298	1.6(+12)	-	-	
H <sub>2</sub> + O → H + OH HYDROGEN MOLECULE + OXYGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	400-2000	1.8(+10)	1.0	4480±150	0.7 1.3
D <sub>2</sub> + O → D + OD DEUTERIUM MOLECULE + OXYGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	416-968	2.0(+13)	0	5500	0.5 2.0
H <sub>2</sub> + O <sub>2</sub> → H + HO <sub>2</sub> HYDROGEN MOLECULE + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2.	290-800	5.5(+13)	0	29100±350	0.4 2.5
H <sub>2</sub> + O <sub>2</sub> → OH + OH HYDROGEN MOLECULE + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500-2500	2.5(+12)	0	19630±5000	0.1 10.
H <sub>2</sub> + H → H + H <sub>2</sub> 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
H <sub>2</sub> + D → H + HD HYDROGEN MOLECULE + DEUTERIUM ATOM 72 KON REACTION ORDER: 2.	400–1000	5.0(+13)	0	3890±40	0.9 1.1
D <sub>2</sub> + H → D + DH DEUTERIUM MOLECULE + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	1000	3.1(+13)	0	4485±250	0.6 1.6
H <sub>2</sub> + OH → H + H <sub>2</sub> 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
D <sub>2</sub> + OH → D + DHO DEUTERIUM MOLECULE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.	300–623	1.9(+13)	0	2904±280	0.5 2.0
H <sub>2</sub> + HO <sub>2</sub> → H + H <sub>2</sub> O <sub>2</sub> HYDROGEN MOLECULE + HYDROPEROXYL FREE RADICAL 72 BAU/DRY REACTION ORDER: 2.	300–800	7.3(+11)	0	9400±250	0.5 2.0
H <sub>2</sub> + S → H + SH HYDROGEN MOLECULE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k <sub>1</sub> = Kk <sub>-1</sub> 75 BEN/GOL	298	1.3(- 1) 2.5(+12)	0.5	13640	0.5 1.5
H <sub>2</sub> + N → H + NH HYDROGEN MOLECULE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	18700	
H <sub>2</sub> + C → H + CH HYDROGEN MOLECULE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	15700	
H <sub>2</sub> + CO <sub>2</sub> → H <sub>2</sub> O + CO HYDROGEN MOLECULE + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+ 9)	0.5	7550±2500	0.3 3.2
H <sub>2</sub> + CH <sub>2</sub> → H + CH <sub>3</sub> . HYDROGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	3525±1500	
H <sub>2</sub> + CH <sub>3</sub> . → H + CH <sub>4</sub> HYDROGEN MOLECULE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	370–700	8.5(+11)	0	5500±500	0.7 1.3
H <sub>2</sub> + CD <sub>3</sub> H → H + CD <sub>3</sub> H HYDROGEN MOLECULE + METHYL-D <sub>3</sub> -FREE RADICAL 72 KON REACTION ORDER: 2.	400–570	7.4(+11)	0	5250±235	0.6 1.7
DH + CH <sub>3</sub> . → H + CH <sub>2</sub> D DEUTERIUM HYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–700	2.4(+11)	0	5635±500	0.5 1.5
DH + CH <sub>3</sub> . → D + CH <sub>4</sub> DEUTERIUM HYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–700	2.1(+11)	0	5300±500	0.5 1.5
D <sub>2</sub> + CH <sub>3</sub> . → D + CH <sub>3</sub> D DEUTERIUM MOLECULE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300–700	7.1(+11)	0	5990±250	0.7 1.3
H <sub>2</sub> + CN → H + HCN HYDROGEN MOLECULE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	2500±1500	
H <sub>2</sub> + CH <sub>3</sub> CH <sub>2</sub> . → H + CH <sub>3</sub> CH <sub>3</sub> 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
$H_2 + M \rightarrow H + H + M$ 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
$OH + O \rightarrow O + OH$ HYDROXYL FREE RADICAL + OXYGEN ATOM 75 BEN/GOL	REACTION ORDER: 2.	6.3(+11)	0.5	4000	
$OH + O \rightarrow H + O_2$ 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
$OH + O \rightarrow H + O_2$ HYDROXYL FREE RADICAL + OXYGEN ATOM 76 ENG	REACTION ORDER: 2. 1500-2500	2.5(+13)	0	0	0.5 2.0
$OH + O + M \rightarrow HO_2 + M$ HYDROXYL FREE RADICAL + OXYGEN ATOM 76 ENG	REACTION ORDER: 3. 1500-2500	1.0(+17)	0	0	0.01 100.
$OH + O_3 \rightarrow HO_2 + O_2$ HYDROXYL FREE RADICAL + OZONE 76 BAU/DRY	REACTION ORDER: 2. 300	3.9(+10)	-	-	0.5 1.5
$OH + H \rightarrow O + H_2$ HYDROXYL FREE RADICAL + HYDROGEN ATOM 72 BAU/DRY	REACTION ORDER: 2. 400-2000	8.3(+9)	1.0	3500±150	0.7 1.3
$OH + H \rightarrow H + OH$ HYDROXYL FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2.	6.3(+11)	0.5	0	
$OH + H + M \rightarrow H_2O + M$ HYDROXYL FREE RADICAL + HYDROGEN ATOM 72 BAU/DRY	REACTION ORDER: 3. M: $H_2O$ 1000-3000	1.4(+23)	-2.0	0	0.7 1.5
NOTE: M eff: $H_2O(1.0)$ . $k_1 = Kk_{-1}$	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
$N_2(0.16)$					
$OH + H_2 \rightarrow H_2O + H$ HYDROXYL FREE RADICAL + HYDROGEN MOLECULE 72 BAU/DRY	REACTION ORDER: 2. 300-2500	2.2(+13)	0	2590±100	0.8 1.2
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 FOR T > 300K					
$OH + D_2 \rightarrow DHO + D$ HYDROXYL FREE RADICAL + DEUTERIUM MOLECULE 72 KON	REACTION ORDER: 2. 300-623	1.9(+13)	0	2904±280	0.5 2.0
$OH + OH \rightarrow HO_2 + H$ HYDROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2. 290-800	1.2(+13)	0	20200±350	0.5 2.0
$OH + OH \rightarrow H_2O + O$ HYDROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 2. 300-2000	6.3(+12)	0	550±200	0.7 1.5
$OH + OH + M \rightarrow H_2O_2 + M$ HYDROXYL FREE RADICAL 72 BAU/DRY	REACTION ORDER: 3. M: $N_2$ 700-1500	9.1(+14)	0	2550±1000	0.8 1.3
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 1500K.					
$OH + H_2O_2 \rightarrow H_2O + HO_2$ HYDROXYL FREE RADICAL + HYDROGEN PEROXIDE 72 BAU/DRY	REACTION ORDER: 2. 300-800	1.0(+13)	0	910±150	0.5 1.5
$OH + S \rightarrow O + SH$ 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
OH + S → H + SO HYDROXYL FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
OH + H <sub>2</sub> S → H <sub>2</sub> O + 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
OH + N → O + NH HYDROXYL FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	17765		
OH + N → H + NO HYDROXYL FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
OH + N + M → HNO + M HYDROXYL FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+15)	-0.5	0		
OH + NO <sub>2</sub> + M → HNO <sub>3</sub> + M HYDROXYL FREE RADICAL + NITROGEN OXIDE(NO <sub>2</sub> ) 73 BAU/DRY REACTION ORDER: 3.	300	5.0(+17)	-	-	0.4	1.6
OH + N <sub>2</sub> O → HO <sub>2</sub> + N <sub>2</sub> HYDROXYL FREE RADICAL + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+13)	0	7550		
OH + NH → H <sub>2</sub> O + N HYDROXYL FREE RADICAL AND IMIDOPEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	1000±2500	0.3	3.2
OH + HNO → H <sub>2</sub> O + NO HYDROXYL FREE RADICAL + NITROSYL HYDRIDE 73 BAU/DRY REACTION ORDER: 2.	2000	3.6(+13)	-	-	0.5	1.5
OH + HNO <sub>3</sub> → H <sub>2</sub> O + NO <sub>3</sub> HYDROXYL FREE RADICAL + NITRIC ACID 73 BAU/DRY REACTION ORDER: 2.	300	8.0(+10)	-	-	0.5	2.0
OH + C → O + CH HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		7.9(+11)	0.5	14800		
OH + C → H + CO HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0		
OH + CO → H + CO <sub>2</sub> 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: $\log(k) \text{ccmol}^{-1}\text{s}^{-1} = 10.83 + 3.94 \cdot 10^{-4}T$	250-2000	1.5(+7)	1.3	- 385	0.8	1.2
OH + CH → H + .CHO HYDROXYL FREE RADICAL AND METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.		5.0(+11)	0.5	5000±2500	0.3	3.2
OH + CH <sub>2</sub> → O + CH <sub>3</sub> . 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
OH + CH <sub>2</sub> → H + HCHO HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+13)	0	2517		
OH + CH <sub>2</sub> → H <sub>2</sub> O + 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
$\text{OH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{H}_2\text{O} + \text{CH}_2=\text{CH}_2$ . 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	
$\text{OH} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{OH} + \text{CH}_3\text{CH(OH)}\text{CH}_2$ . 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 2.5 0.5 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 2.0 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
$\text{HO}_2 + \text{H} \rightarrow \text{H}_2\text{O} + \text{O}$ 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
$\text{HO}_2 + \text{SO}_3 \rightarrow \text{OH} + \text{SO}_3$ 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
$\text{HO}_2 + \text{CH}_3 \rightarrow \text{O}_2 + \text{CH}_4$ 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 <sub>ref</sub> FOR $\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$ . k FACTORS MIGHT BE HIGHER.	300	1.0(+ 7)	-	-	0.1	10.
$\text{HO}_2 + \text{CH}_3\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2$ HYDROPEROXYL RADICAL + ETHANE 74 LLO REACTION ORDER: 2. NOTE: E ESTIMATED. UPPER LIMIT RECOMMENDED. k <sub>ref</sub> IS FOR $\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$ .	300–1000	1.0(+12)	0	7000	0.1	10.
$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_2\text{CH}$ HYDROPEROXYL FREE RADICAL + PROPANE 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k <sub>ref</sub> 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.
$\text{HO}_2 + (\text{CHO})_3\text{CH} \rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_3\text{C}$ . 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	$23000 \pm 250$	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	$9240 \pm 200$	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	$10250 \pm 100$	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	$16500 \pm 500$	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	$1500 \pm 2500$	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	$12900 \pm 1000$	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: $\text{H}_2\text{O}$ NOTE: M eff: $\text{H}_2\text{O}(1.0)$ . $k_1 = Kk_{-1}$ Ar(0.06) M: Ar N <sub>2</sub> (0.16) M: N <sub>2</sub>	2000–6000	2.2(+16)	0	$52900 \pm 2500$	0.7 1.5
$\text{H}_2\text{O}_2 + \text{H} \rightarrow \text{HO}_2 + \text{H}_2$ HYDROGEN PEROXIDE + HYDROGEN ATOM 72 BAU/DRY REACTION ORDER: 2.	300–800	1.7(+12)	0	$1900 \pm 250$	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	$910 \pm 150$	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 <sub>2</sub> NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 1500K.	700–1500	1.20(+17)	0	$22900 \pm 1000$	0.8 1.3
$\text{S} + \text{O}_2 \rightarrow \text{SO} + \text{O}$ 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: $k_1 = Kk_{-1}$ 75 BEN/GOL	298	1.3(-1)	-	-	0.5 1.5
$\text{S} + \text{OH} \rightarrow \text{SO} + \text{H}$ SULFUR ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	13640	
		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 → SH + O SULFUR ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	12700	
S + S <sub>2</sub> → S <sub>2</sub> + S SULFUR ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S + SO → S <sub>2</sub> + O SULFUR ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	11500	
S + SO → SO + S SULFUR ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S + SH → S <sub>2</sub> + H SULFUR ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S + SH → SH + S SULFUR ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
S + N <sub>2</sub> → NS + N SULFUR ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	55200	
S + NO → SO + N SULFUR ATOM + NITROGEN OXIDE (NO) 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	17260	
S + NO → NS + O SULFUR ATOM + NITROGEN OXIDE (NO) 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	17465	
S + NH → SH + N SULFUR ATOM + IMIDOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
S + NH → NS + H SULFUR ATOM + IMIDOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S + NS → S <sub>2</sub> + N SULFUR ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	10870	
S + NS → NS + S SULFUR ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S + CO → SO + C SULFUR ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	66530	
S + CO → CS + O SULFUR ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	37600	
S + CH → SH + C SULFUR ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
S + CH → CS + H SULFUR ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S + CS → S <sub>2</sub> + 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 <sub>2</sub> + M SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 76 BAU/DRY REACTION ORDER: 3. NOTE: k <sub>1</sub> = k <sub>k-1</sub>	1800–3700	8.7(+13)	0	4370	0.5 1.5
S + CS <sub>2</sub> → S <sub>2</sub> + CS SULFUR ATOM + CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2.	298	3.9(+11)	-	-	0.5 1.5
S + COS → S <sub>2</sub> + 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 <sub>2</sub> → 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 <sub>2</sub> =CH <sub>2</sub> → cy-CH <sub>2</sub> CH <sub>2</sub> S SULFUR ATOM + ETHENE 72 KER/PAR REACTION ORDER: 2.	298	8.1(+11)	-	-	
S + CH <sub>3</sub> C≡CH → cy-(CH <sub>3</sub> )C=CHS SULFUR ATOM + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2.	298	1.1(+12)	-	-	
S + CH <sub>3</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> )CHCH <sub>2</sub> S SULFUR ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 6.9	298 298	5.8(+12) -	-	-	
NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>					
S*( <sup>1</sup> D) + CH <sub>3</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> )CHCH <sub>2</sub> S SULFUR ATOM ( <sup>1</sup> D) + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.7	300	-	-	-	
NOTE: k <sub>ref</sub> : S*( <sup>1</sup> D) + CH <sub>2</sub> =CH <sub>2</sub>					
S + CH <sub>3</sub> C≡CCH <sub>3</sub> → cy-(CH <sub>3</sub> )C=C(CH <sub>3</sub> )S SULFUR ATOM + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2.	298	1.9(+13)	-	-	
S + CH <sub>2</sub> =CHCH=CH <sub>2</sub> → cy-(CH <sub>2</sub> =CH)CHCH <sub>2</sub> S SULFUR ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2.	298	6.0(+13)	-	-	
S + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> CH <sub>2</sub> )CHCH <sub>2</sub> S SULFUR ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 10.0	298 298	9.3(+12) -	-	-	
NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>					
S + cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → cy-(CH <sub>3</sub> )CHCH(CH <sub>3</sub> )S SULFUR ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 16.0	298 298	1.4(+13) -	-	-	
NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>					

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 + trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → cy-(CH <sub>3</sub> )CHCH(CH <sub>3</sub> )S SULFUR ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 20.0	298 298	1.4(+13) -	-	-	
NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>					
S + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> S SULFUR ATOM + 1-PROPENE, 2-METHYL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 50.0	298 298	4.0(+13) -	-	-	
NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>					
S* <sup>(1)D</sup> + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> S SULFUR ATOM <sup>(1)D</sup> + 1-PROPENE, 2-METHYL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5	300	-	-	-	
NOTE: k <sub>ref</sub> : S* <sup>(1)D</sup> + CH <sub>2</sub> =CH <sub>2</sub>					
S + CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> CH=CH <sub>2</sub> → cy-CH <sub>3</sub> (CH <sub>2</sub> )CHCH <sub>2</sub> S SULFUR ATOM + 1-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	8.1(+12)	-	-	
S + CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> → cy-CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )CH <sub>2</sub> S SULFUR ATOM + 1-BUTENE, 2-METHYL 72 KER/PAR REACTION ORDER: 2.	298	7.4(+13)	-	-	
S + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH(CH <sub>3</sub> )S SULFUR ATOM + 2-BUTENE, 2-METHYL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 56.	298 298	6.5(+13) -	-	-	
NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>					
S + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → cy-(CH <sub>3</sub> ) <sub>2</sub> CC(CH <sub>3</sub> ) <sub>2</sub> S SULFUR ATOM + 2-BUTENE, 2,3-DIMETHYL 72 KER/PAR REACTION ORDER: 2.	298	8.5(+13)	-	-	
S <sub>2</sub> + O → S + SO SULFUR DIMER + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S <sub>2</sub> + H → S + SH SULFUR DIMER + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		7.9(+12)	0.5	8355	
S <sub>2</sub> + S → S + S <sub>2</sub> SULFUR DIMER + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
S <sub>2</sub> + N → S + NS SULFUR DIMER + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
S <sub>2</sub> + C → S + CS SULFUR DIMER + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
SO + O → O + SO SULFUR MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
SO + O → S + O <sub>2</sub> SULFUR MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	2770	
SO + O + M → SO <sub>2</sub> + M SULFUR MONOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3.	298	6.7(+13)	-	-	0.7 1.3
SO + O <sub>2</sub> → SO <sub>2</sub> + 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 → 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 kref 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/COL 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/COL 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: $\text{N}_2$	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 → NH + S NITROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	9060	
N + SH → NS + H NITROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	403	
N + N + M → N <sub>2</sub> + M NITROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: N <sub>2</sub> 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 <sub>2</sub> → N <sub>2</sub> + N NITROGEN ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
N + NO → N <sub>2</sub> + 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 → NO + N NITROGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
N + NO <sub>2</sub> → N <sub>2</sub> + O <sub>2</sub> NITROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+12)	0	0±1500	
N + NO <sub>2</sub> → NO + NO NITROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	1500–2500	4.0(+12)	0	0±1500	0.2 5.0
N + NO <sub>2</sub> → N <sub>2</sub> O + O NITROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+12)	0	0±1500	0.5 2.0
N + N <sub>2</sub> O → NO + N <sub>2</sub> NITROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+ 8)	0	5000±2500	0.3 3.2
N + NH → N <sub>2</sub> + H NITROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
N + NH → NH + N NITROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
N + HNO → H + N <sub>2</sub> O NITROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+10)	0.5	1500±2500	
N + HNO → NH + NO NITROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	1000±2500	
N + NS → N <sub>2</sub> + S NITROGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
N + NS → NS + N NITROGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
N + CO → NO + C NITROGEN ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	57300	
N + CO → 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
N + CO <sub>2</sub> → NO + CO NITROGEN ATOM + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500–2500	2.00(+11)	0.5	1500±10000	0.1 10.
N + CH → NH + C NITROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	6995	
N + CH → CN + H NITROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
N + CH <sub>2</sub> → NH + CH NITROGEN ATOM + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	6.3(+11)	0.67	20400±2500	0.3 3.2
N + CHO → O + HCN NITROGEN ATOM + FORMYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+14)	0	0	
NOTE: k ESTIMATED.					
N + CHO → NH + CO NITROGEN ATOM + FORMYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	2.0(+11)	0.5	1000±2500	
N + CH <sub>3</sub> O → NH + HCHO NITROGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+14)	0	0±1500	
N + CS → C + NS NITROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		4.0(+12)	0.5	37200	
N + CS → CN + S NITROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	1160	
N + CN → N <sub>2</sub> + C NITROGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
N + C <sub>2</sub> → CN + C NITROGEN ATOM + CARBON DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
N + CH≡CH → C <sub>2</sub> H <sub>2</sub> N NITROGEN ATOM + ETHYNE 72 KER/PAR REACTION ORDER: 2.	440	2.0(+ 9)	-	-	
NOTE: UPPER LIMIT.					
N + CH <sub>2</sub> =CH <sub>2</sub> → products NITROGEN ATOM + ETHENE 72 KER/PAR REACTION ORDER: 2.	320–550	2.0(+10)	0	353	
N + CH <sub>3</sub> C≡CH → products NITROGEN ATOM + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 6.5	320–550 435	6.9(+10) -	0 -	745 -	
NOTE: k <sub>ref</sub> : N + CH≡CH					
N + CH <sub>3</sub> CH=CH <sub>2</sub> → products NITROGEN ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 2.8	320–550 435	1.2(+11) -	0 -	655 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub>					
N + CH <sub>3</sub> CH <sub>2</sub> C≡CH → products NITROGEN ATOM + 1-BUTYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 13.0	320–550 435	3.5(+11) -	0 -	1125 -	
NOTE: k <sub>ref</sub> : 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
N + CH <sub>3</sub> C≡CCH <sub>3</sub> → products NITROGEN ATOM + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 12.0	320–550 435	1.9(+11) -	0 -	926 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + CH <sub>2</sub> =CHCH=CH <sub>2</sub> → products NITROGEN ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2.	340	3.5(+10)	-	-	
N + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → products NITROGEN ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.4	320–550 435	1.6(+11) -	0 -	660 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → products NITROGEN ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 2.4	320–550 435	2.3(+11) -	0 -	995 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → products NITROGEN ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.0	320–550 435	3.4(+11) -	0 -	1055 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → products NITROGEN ATOM + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 4.1	320–550 435	7.8(+10) -	0 -	277 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C≡CH → products NITROGEN ATOM + 1-PENTYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 14.0	320–550 435	3.0(+11) -	0 -	1047 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → products NITROGEN ATOM + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5	320–550 435	9.3(+10) -	0 -	433 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> C≡CH → products NITROGEN ATOM + 1-HEXYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 14.0	320–55 435	4.6(+11) -	0 -	1233 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + CH <sub>3</sub> CH <sub>2</sub> C≡CCH <sub>2</sub> CH <sub>3</sub> → products NITROGEN ATOM + 3-HEXYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 14.0	320–550 435	3.4(+11) -	0 -	1102 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → products NITROGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5	320–550 435	1.7(+11) -	0 -	690 -	
NOTE: k <sub>ref</sub> : N + CH <sub>2</sub> =CH <sub>2</sub> .					
N <sub>2</sub> + O → N + 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 <sub>1</sub> = Kk <sub>1</sub>					
N <sub>2</sub> + O + M → N <sub>2</sub> O + 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 + MÉTHYLIDYNE 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 Ar(0.1) AT 297K $H_2O(6.1)$ AT 297K $D_2O(5.0)$ AT 297K $SF_6(2.6)$ AT 297K $N_2(1.4)$ AT 297K $N_2O(2.1)$ AT 297K $CO_2(2.1)$ AT 297K $CH_4(2.2)$ AT 297K $CF_4(2.2)$ AT 297K	200–500 200–500 200–500 200–500 200–500 200–500 200–500 200–500 200–500 200–500 200–500	1.1(+15) 1.1(+14) 6.7(+15) 5.5(+15) 2.9(+15) 1.5(+15) 2.3(+15) 2.3(+15) 2.4(+15) 2.4(+15)	0 0 0 0 0 0 0 0 0 0	-940±50 -940±50 -940±50 -940±50 -940±50 -940±50 -940±50 -940±50 -940±50 -940±50	0.8 1.2 0.8 1.2 0.8 1.2 0.8 1.2 0.8 1.2 0.8 1.2 0.8 1.2 0.8 1.2 0.8 1.2 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
NO + O <sub>2</sub> → NO <sub>2</sub> + O NITROGEN OXIDE(NO) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: k <sub>1</sub> = Kk <sub>-1</sub>	300-550	1.7(+12)	0	23400	0.8 1.3
NO + O <sub>3</sub> → NO <sub>2</sub> + O <sub>2</sub> NITROGEN OXIDE(NO) + OZONE 73 BAU/DRY REACTION ORDER: 2.	200-350	8.9(+11)	0	1330±130	0.5 1.5
NO + H → O + NH NITROGEN OXIDE(NO) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		5.0(+12)	0.5	38200	
NO + H → N + OH NITROGEN OXIDE(NO) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	24460	
NO + H + M → HNO + M NITROGEN OXIDE(NO) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: H <sub>2</sub> 76 ENG M: H <sub>2</sub>	230-700 1500-2500	5.4(+15) 5.0(+15)	0 0	-300±100 -300±150	0.5 1.5 0.5 2.0
NO + S → O + NS NITROGEN OXIDE(NO) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	17465	
NO + S → N + SO NITROGEN OXIDE(NO) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	17260	
NO + N → O + N <sub>2</sub> 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
NO + N → N + NO NITROGEN OXIDE(NO) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NO + NO → N <sub>2</sub> + O <sub>2</sub> NITROGEN OXIDE(NO <sub>2</sub> ) + OXYGEN MOLECULE 72 KON REACTION ORDER: 2.	1370-4300	1.3(+14)	0	38060±720	0.7 1.5
NO + NO → N <sub>2</sub> O + O NITROGEN OXIDE (NO) 73 BAU/DRY REACTION ORDER: 2.	1200-2000	1.3(+12)	0	32100±1500	0.5 2.0
NO + NO + O <sub>2</sub> → NO <sub>2</sub> + NO <sub>2</sub> NITROGEN OXIDE(NO) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 3.	273-660	1.2(+ 9)	0	-530±100	0.5 1.5
NO + NO <sub>2</sub> → N <sub>2</sub> O + O <sub>2</sub> NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	1500-2500	1.0 (+12)	0	30200	0.01 100.
NO + NO <sub>2</sub> + O <sub>2</sub> → NO <sub>2</sub> + NO <sub>3</sub> NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO <sub>2</sub> ) + OXYGEN MOLECULE 73 BAU/DRY REACTION ORDER: 3.	300-500	2.9(+ 7)	0	-400±500	0.4 2.5
NO + NO <sub>3</sub> → NO <sub>2</sub> + NO <sub>2</sub> NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO <sub>3</sub> ) 72 KON REACTION ORDER: 2.	298-547	1.5(+14)	0	1163±115	0.7 1.4
NO + N <sub>2</sub> O → NO <sub>2</sub> + N <sub>2</sub> NITROGEN OXIDE(NO) + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+14)	0	25000	0.1 1.0
NO + HNO → N <sub>2</sub> O + 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
NO + C → O + CN NITROGEN OXIDE(NO) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NO + C → N + CO NITROGEN OXIDE(NO) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NO + CH → O + HCN NITROGEN OXIDE(NO) + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	2.0(+12)	0	0±1000	
NO + CH → N + .CHO NITROGEN OXIDE(NO) + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.6(+13)	0	5000±3000	
NO + CH <sub>2</sub> → N + HCHO NITROGEN OXIDE(NO) + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.6(+12)	0	3500±2000	
NO + .CHO → HNO + 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
NO + CN → N <sub>2</sub> + CO NITROGEN OXIDE(NO) + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+11)	0	0±2500	0.3 3.2
NO + M → N + O + M NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: M = Ar, OR N <sub>2</sub> OR O <sub>2</sub> . GIVEN WITH CAUTION. 72 KON	1500–2500 M: Ar 3000–8000	4.0(+20) 8.00(+ 2)	-1.5 -1.5	75500±2500 75500	0.3 3.2
NO <sub>2</sub> + O → NO + O <sub>2</sub> NITROGEN OXIDE(NO <sub>2</sub> ) + 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
NO <sub>2</sub> + O + M → NO <sub>3</sub> + M NITROGEN OXIDE(NO <sub>2</sub> ) + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2. M: N <sub>2</sub> NOTE: LIMITING HIGH PRESSURE k REACTION ORDER: 3. k <sub>O</sub> (LOW PRESSURE).	295 295	1.1(+13) 2.3(+16)	- -	- -	0.4 0.4 2.5 2.5
NO <sub>2</sub> + O <sub>3</sub> → NO <sub>3</sub> + O <sub>2</sub> NITROGEN OXIDE(NO <sub>2</sub> ) + OZONE 73 BAU/DRY REACTION ORDER: 2.	286–302	5.9(+12)	0	3500	0.5 2.0
NO <sub>2</sub> + H → NO + OH NITROGEN OXIDE(NO <sub>2</sub> ) + 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
NO <sub>2</sub> + OH + M → HNO <sub>3</sub> + M NITROGEN OXIDE(NO <sub>2</sub> ) + HYDROXYL FREE RADICAL 73 BAU/DRY REACTION ORDER: 3. M: He	300	5.0(+17)	-	-	0.4 1.6
NO <sub>2</sub> + N → O + N <sub>2</sub> O NITROGEN OXIDE(NO <sub>2</sub> ) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+12)	0	0±1500	0.5 2.0
NO <sub>2</sub> + N → O <sub>2</sub> + N <sub>2</sub> NITROGEN OXIDE(NO <sub>2</sub> ) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+12)	0	0±1500	0.5 2.0
NO <sub>2</sub> + N → NO + NO NITROGEN OXIDE(NO <sub>2</sub> ) + 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( $\text{NO}_2$ ) + 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( $\text{NO}_2$ ) + 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( $\text{NO}_2$ ) REACTION ORDER: 2. 73 BAU/DRY 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( $\text{NO}_2$ ) REACTION ORDER: 3. M: $\text{N}_2$ 73 BAU/DRY NOTE: CORRECTED k VALUE (PERSONAL COMMUNICATION FROM DR. BAULCH TO DR. HAMPSON). $k_1 = \text{Kk}_{-1}$	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( $\text{NO}_2$ ) + NITROGEN OXIDE( $\text{NO}_3$ ) REACTION ORDER: 2. 73 BAU/DRY	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( $\text{NO}_2$ ) + NITROGEN OXIDE( $\text{NO}_3$ ) REACTION ORDER: 2. 73 BAU/DRY NOTE: LIMITING HIGH PRESSURE k M IS A $\text{N}_2\text{O}_5$ + NO MIXTURE	300	2.3(+12)	-	-	0.4 2.5
$\text{NO}_2 + \text{NH} \rightarrow \text{NO} + \text{HNO}$ NITROGEN OXIDE( $\text{NO}_2$ ) + IMIDOPEN FREE RADICAL REACTION ORDER: 2. 76 ENG	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( $\text{NO}_2$ ) + CARBON MONOXIDE REACTION ORDER: 2. 72 KON 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( $\text{NO}_2$ ) 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( $\text{NO}_3$ ) + NITROGEN OXIDE(NO) REACTION ORDER: 2. 72 KON	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( $\text{NO}_3$ ) + NITROGEN OXIDE( $\text{NO}_2$ ) REACTION ORDER: 2. 73 BAU/DRY	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( $\text{NO}_3$ ) + NITROGEN OXIDE( $\text{NO}_2$ ) REACTION ORDER: 2. 72 BAU/DRY NOTE: LIMITING HIGH-PRESSURE k. M IS A $\text{N}_2\text{O}_5$ + NO MIXTURE. $k_1 = \text{Kk}_{-1}$ REACTION ORDER: 3. k <sub>o</sub> (LOW PRESSURE). M IS A $\text{N}_2\text{O}_5$ + NO MIXTURE.	300	2.3(+12)	-	-	0.4 2.5
$\text{NO}_3 + \text{M} \rightarrow \text{NO} + \text{O}_2 + \text{M}$ NITROGEN OXIDE( $\text{NO}_3$ ) REACTION ORDER: 2. M: $\text{NO}_2$ 72 KON	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( $\text{N}_2\text{O}$ ) + OXYGEN ATOM REACTION ORDER: 2. 73 BAU/DRY	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( $\text{N}_2\text{O}$ ) + OXYGEN ATOM REACTION ORDER: 2. 73 BAU/DRY 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 f	f F
$\text{N}_2\text{O} + \text{H} \rightarrow \text{N}_2 + \text{OH}$ NITROGEN OXIDE( $\text{N}_2\text{O}$ ) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	700-2500	7.6(+13)	0	$7600 \pm 500$	0.5	1.5
$\text{N}_2\text{O} + \text{H} \rightarrow \text{NO} + \text{NH}$ NITROGEN OXIDE( $\text{N}_2\text{O}$ ) + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0.5	$15100 \pm 2500$	0.3	3.2
$\text{N}_2\text{O} + \text{OH} \rightarrow \text{N}_2 + \text{HO}_2$ NITROGEN OXIDE( $\text{N}_2\text{O}$ ) + 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( $\text{N}_2\text{O}$ ) + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+ 8)	0	$5000 \pm 2500$	0.3	3.2
$\text{N}_2\text{O} + \text{NO} \rightarrow \text{N}_2 + \text{NO}_2$ NITROGEN OXIDE( $\text{N}_2\text{O}$ ) + 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( $\text{N}_2\text{O}$ ) + CARBON MONOXIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0	$10000 \pm 1500$	0.5	2.0
$\text{N}_2\text{O} + \text{M} \rightarrow \text{N}_2 + \text{O} + \text{M}$ NITROGEN OXIDE( $\text{N}_2\text{O}$ ) 73 BAU/DRY REACTION ORDER: 2.	1300-2500	5.0(+14)	0	$29000 \pm 1500$	0.7	1.5
$\text{N}_2\text{O}_4 \rightarrow \text{NO}_2 + \text{NO}_2$ NITROGEN OXIDE( $\text{N}_2\text{O}_4$ ) 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( $\text{N}_2\text{O}_4$ ) 73 BAU/DRY REACTION ORDER: 2. M: $\text{N}_2$	250-350	2.5(+17)	0	$5550 \pm 500$	0.7	1.3
$\text{N}_2\text{O}_5 + \text{M} \rightarrow \text{NO}_2 + \text{NO}_3 + \text{M}$ NITROGEN OXIDE ( $\text{N}_2\text{O}_5$ ) 73 BAU/DRY REACTION ORDER: 1. NOTE: LIMITING HIGH-PRESSURE k. M IS A $\text{N}_2\text{O}_5 + \text{NO}$ MIXTURE. REACTION ORDER: 2. k <sub>o</sub> (LOW PRESSURE). M IS A $\text{N}_2\text{O}_5 + \text{NO}$ MIXTURE.	300-340	5.7(+14)	0	10600	0.4	2.5
$\text{NH} + \text{O} \rightarrow \text{H} + \text{NO}$ 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	$0 \pm 2500$	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	$1000 \pm 2500$	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	$1500 \pm 2500$	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
NH + S → H + NS IMIDODEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NH + S → N + SH IMIDODEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NH + N → H + N <sub>2</sub> IMIDODEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NH + N → N + NH IMIDODEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NH + NO <sub>2</sub> → HNO + NO IMIDODEN FREE RADICAL + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	1500–2500	2.0(+11)	0.5	2500±2500	0.3 3.2
NH + NH → H <sub>2</sub> + N <sub>2</sub> IMIDODEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+13)	0	0	0.1 10.
NH + C → H + CN IMIDODEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NH + C → N + CH IMIDODEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NH + CN → N + HCN IMIDODEN FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	1000±25000	
NH <sub>2</sub> + H + M → NH <sub>3</sub> + M AMIDODEN FREE RADICAL + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: Ar NOTE: k <sub>1</sub> = Kk <sub>-1</sub>	2000–3000	4.8(+14)	0	-8300±2500	0.5 2.0
NH <sub>3</sub> + O → NH <sub>2</sub> + OH AMMONIA + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	300–1000	1.5(+12)	0	3020±300	0.5 1.5
NH <sub>3</sub> + CH <sub>3</sub> · → NH <sub>2</sub> + CH <sub>4</sub> AMMONIA + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–650	1.0(+11)	0	5100±500	0.3 1.3
ND <sub>3</sub> + CH <sub>3</sub> · → ND <sub>2</sub> + CH <sub>3</sub> D AMMONIA-D <sub>3</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+11)	0	5535±500	0.3 1.3
NH <sub>3</sub> + M → H + NH <sub>2</sub> + M AMMONIA 73 BAU/DRY REACTION ORDER: 2. M: Ar	2000–3000	9.2(+15)	0	42400±2500	0.5 2.0
NH <sub>2</sub> NH <sub>2</sub> + H → NH <sub>2</sub> NH <sub>·</sub> + H <sub>2</sub> HYDRAZINE + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2.	250–500	1.3(+13)	0	1260±100	0.5 2.0
NH <sub>2</sub> NH <sub>2</sub> + CH <sub>3</sub> · → NH <sub>2</sub> NH <sub>·</sub> + CH <sub>4</sub> HYDRAZINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+11)	0	2515±500	0.5 2.0
ND <sub>2</sub> ND <sub>2</sub> + CH <sub>3</sub> · → ND <sub>2</sub> ND <sub>·</sub> + CH <sub>3</sub> D HYDRAZINE-D <sub>4</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–500	7.2(+10)	0	3200±500	0.5 2.0
NH <sub>2</sub> NH <sub>2</sub> + M → NH <sub>2</sub> · + NH <sub>2</sub> · + 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
$\text{NH}_2\text{NH}_2 + \text{M} \rightarrow \text{NH}_2\cdot + \text{NH}_2 + \text{M}$ HYDRAZINE 73 BAU/DRY NOTE: $k_0$ (LOW PRESSURE).	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.	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
$\text{HNO} + \text{CH}_2\cdot \rightarrow \text{NO} + \text{CH}_3$ 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
$\text{HNO} + \text{CHO} \rightarrow \text{NO} + \text{HCHO}$ 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
HNO <sub>3</sub> + M → NO <sub>2</sub> + OH + M NITRIC ACID 73 BAU/DRY REACTION ORDER: 2. M: Ar	800-1200	1.6(+15)	0	15400±1500	0.4 2.5
NS + O → S + NO NITROGEN SULFIDE(NS) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NS + O → N + SO NITROGEN SULFIDE(NS) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NS + H → S + NH NITROGEN SULFIDE(NS) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	20735	
NS + H → N + SH NITROGEN SULFIDE(NS) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	15700	
NS + S → S + NS NITROGEN SULFIDE(NS) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NS + S → N + S <sub>2</sub> NITROGEN SULFIDE(NS) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+11)	0.5	10870	
NS + N → S + N <sub>2</sub> NITROGEN SULFIDE(NS) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NS + N → N + NS NITROGEN SULFIDE(NS) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
NS + C → S + CN NITROGEN SULFIDE(NS) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
NS + C → N + CS NITROGEN SULFIDE(NS) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
C + O + M → CO + M CARBON ATOM + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 3. NOTE: M = Ar, OR CO k <sub>1</sub> = Kk <sub>-1</sub>	7000-14000	3.3(+26)	-3.1	-2114	0.3 1.8
C + O <sub>2</sub> → CO + O CARBON ATOM + OXYGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + H <sub>2</sub> → CH + H CARBON ATOM + HYDROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	15700	
C + OH → CO + H CARBON ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + OH → CH + O CARBON ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		7.9(+11)	0.5	14800	
C + S <sub>2</sub> → CS + S CARBON ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + SO → CO + 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 → CS + O CARBON ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + SH → CH + S CARBON ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		4.0(+11)	0.5	6090	
C + SH → CS + H CARBON ATOM + MERCAPTO FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + N <sub>2</sub> → CN + N CARBON ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	22750	
C + NO → CO + N CARBON ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
C + NO → CN + O CARBON ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + NH → CH + N CARBON ATOM + IMIDOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
C + NH → CN + H CARBON ATOM + IMIDOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + NS → CS + N CARBON ATOM ATOM + NITRIC SULFIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
C + NS → CN + S CARBON ATOM + NITRIC SULFIDE 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + CO → C <sub>2</sub> + O CARBON ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	58025	
C + CH → CH + C CARBON ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
C + CH → C <sub>2</sub> + H CARBON ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + CS → CS + C CARBON ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + CS → C <sub>2</sub> + S CARBON ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		5.0(+11)	0.5	20435	
C + CN → CN + C CARBON ATOM + CYANOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C + CN → C <sub>2</sub> + N CARBON ATOM + CYANOPEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		2.5(+11)	0.5	19300	
C + C <sub>2</sub> → C <sub>2</sub> + 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 <sub>2</sub> 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 <sub>2</sub> ) 72 KON 76 ENG REACTION ORDER: 2.	500-800 1500-2500	1.9(+12) 2.0(+12)	0 0	14726±385 15000±1500	0.5 1.9 0.5 2.0
$\text{CO} + \text{N}_2\text{O} \rightarrow \text{CO}_2 + \text{N}_2$ CARBON MONOXIDE + NITROGEN OXIDE(N <sub>2</sub> 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
CO + C → O + C <sub>2</sub> CARBON MONOXIDE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	58025	
CO + CH <sub>3</sub> · → CH <sub>3</sub> C(O). CARBON MONOXIDE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	273–400	3.8(+ 8)	0	1965	
CO + M → C + O + M CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 OVER 1000K. M = Ar OR CO	7000–15000	8.8(+29)	-3.5	128700±1800	0.3 1.8
CO <sub>2</sub> + O → CO + O <sub>2</sub> CARBON DIOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K. k <sub>1</sub> = Kk <sub>-1</sub>	1500–3000	1.7(+13)	0	26500±2500	0.5 2.0
CO <sub>2</sub> + H → CO + OH CARBON DIOXIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	1000–3000	1.5(+14)	0	13300±150	0.8 1.2
CO <sub>2</sub> + H <sub>2</sub> → CO + H <sub>2</sub> O CARBON DIOXIDE + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+ 9)	0.5	7550±2500	0.3 3.2
CO <sub>2</sub> + N → CO + NO CARBON DIOXIDE + NITROGEN ATOM 76 ENG REACTION ORDER: 2.	1500–2500	2.0(+11)	0.5	15000±10000	0.1 1.0
CO <sub>2</sub> + CH → CO + .CHO CARBON DIOXIDE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+10)	0.5	3000±2500	0.3 3.2
CO <sub>2</sub> + M → CO + O + M CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+15)	0	50000±2500	0.5 2.0
CH + O → H + CO METHYLIDYNE FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CH + O → C + OH METHYLIDYNE FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
CH + O + M → .CHO + M METHYLIDYNE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 3.	1500–2500	1.0(+16)	-0.5	0±2500	0.3 3.2
CH + O <sub>2</sub> → .CHO + O METHYLIDYNE FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+11)	0.5	3000±2500	0.3 3.2
CH + H → H + CH METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CH + H → C + H <sub>2</sub> METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
CH + H + M → CH <sub>2</sub> + M METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 3.	1500–2500	1.00(+19)	-1.0	0	0.3 3.2
CH + OH → .CHO + 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
CH + HO <sub>2</sub> → CH <sub>2</sub> + O <sub>2</sub> METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+10)	0.5	7550±2500	0.3 3.2
CH + HO <sub>2</sub> → .CHO + 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
CH + S → H + CS METHYLIDYNE FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CH + S → C + SH METHYLIDYNE FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
CH + N → H + CN METHYLIDYNE FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CH + N → C + NH METHYLIDYNE FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+12)	0.5	6995	
CH + N <sub>2</sub> → CN + NH METHYLIDYNE FREE RADICAL + NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+14)	0	46300±10000	
CH + N <sub>2</sub> → HCN + N METHYLIDYNE FREE RADICAL + NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: REVISED ESTIMATE.	1500–2500	1.0(+11)	0	9560	
CH + NO → .CHO + N METHYLIDYNE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.6(+13)	0	5000±3000	
CH + NO → HCN + O METHYLIDYNE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	2.0(+12)	0	0±1000	
CH + HNO → CH <sub>2</sub> + NO METHYLIDYNE FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	6.3(+11)	0.5	0±2500	0.3 3.2
CH + C → H + C <sub>2</sub> METHYLIDYNE FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CH + C → C + CH METHYLIDYNE FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
CH + CO <sub>2</sub> → .CHO + CO METHYLIDYNE FREE RADICAL + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+10)	0.5	3000±2500	0.3 3.2
CH + CH <sub>4</sub> → CH <sub>2</sub> + CH <sub>3</sub> . METHYLIDYNE FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2.	1500–2500	2.5(+11)	0.7	3000±2500	0.3 3.2
CH + .CHO → CH <sub>2</sub> + 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
CH + HCHO → CH <sub>2</sub> + .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	$13000 \pm 2500$	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	$2000 \pm 2500$	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	$3500 \pm 2500$	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	$2500 \pm 2500$	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	$3525 \pm 1500$	
$\text{CH}_2 + \text{OH} \rightarrow \text{CH} + \text{H}_2\text{O}$ METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	5.0(+11)	0.5	$3000 \pm 2500$	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	$3000 \pm 2500$	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	$20400 \pm 2500$	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	$35230 \pm 10000$	
$\text{CH}_2 + \text{NO} \rightarrow \text{HCHO} + \text{N}$ METHYLENE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.6(+12)	0	$3500 \pm 2000$	
$\text{CH}_2 + \text{HNO} \rightarrow \text{CH}_3\cdot + \text{NO}$ METHYLENE FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	6.3(+11)	0.5	$0 \pm 2500$	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	$3000 \pm 2500$	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	$10000 \pm 2500$	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	$500 \pm 2500$	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	$3270 \pm 1500$	
$\text{CH}_2 + \text{CN} \rightarrow \text{CH} + \text{HCN}$ METHYLENE FREE RADICAL + CYANOCEN FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	$2500 \pm 1500$	

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. $k/k_{\text{ref}}$ : 1.27 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 1.0 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 1.63 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 1.6 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 1.37 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.94 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^1\text{CH}_2 + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 1.39 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$^3\text{CH}_2 + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.89 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 1.96 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 2.86 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 2.12 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 1.83 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 2.16 NOTE: $k_{\text{ref}}: ^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$	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. $k/k_{\text{ref}}$ : 2.74 NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$	297	-	-	-	
$\text{CH}_3\cdot + \text{O} \rightarrow \text{HCHO} + \text{H}$ 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
$\text{CH}_3\cdot + \text{O}_2 \rightarrow \text{CH}_2\cdot + \text{HO}_2$ 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	
$\text{CH}_3\cdot + \text{H}_2 \rightarrow \text{CH}_4\cdot + \text{H}$ METHYL FREE RADICAL + HYDROGEN MOLECULE 72 KER/PAR REACTION ORDER: 2.	370–700	8.5(+11)	0	5500±500	0.7 1.3
$\text{CH}_3\cdot + \text{HD} \rightarrow \text{CH}_3\text{D} + \text{H}$ METHYL FREE RADICAL + DEUTERIUM HYDRIDE 76 KER/PAR REACTION ORDER: 2.	400–700	2.4(+11)	0	5635±500	0.5 1.5
$\text{CH}_3\cdot + \text{HD} \rightarrow \text{CH}_4\cdot + \text{D}$ METHYL FREE RADICAL + DEUTERIUM HYDRIDE 76 KER/PAR REACTION ORDER: 2.	400–700	2.1(+11)	0	5300±500	0.5 1.5
$\text{CH}_3\cdot + \text{D}_2 \rightarrow \text{CH}_3\text{D} + \text{D}$ METHYL FREE RADICAL + DEUTERIUM MOLECULE 76 KER/PAR REACTION ORDER: 2.	300–700	7.1(+11)	0	5990±250	0.7 1.3
$\text{CD}_3\cdot + \text{H}_2 \rightarrow \text{CD}_3\text{H} + \text{H}$ METHYL-D <sub>3</sub> FREE RADICAL + HYDROGEN MOLECULE 72 KON REACTION ORDER: 2.	400–570	7.4(+11)	0	5250±235	0.6 1.7
$\text{CH}_3\cdot + \text{OH} \rightarrow \text{CH}_2\cdot + \text{H}_2\text{O}$ METHYL FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	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.	1500–2500	6.3(+12)	0	0	
$\text{CH}_3\cdot + \text{HO}_2 \rightarrow \text{CH}_4\cdot + \text{O}_2$ 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
$\text{CH}_3\cdot + \text{H}_2\text{S} \rightarrow \text{CH}_4\cdot + \text{SH}$ 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
$\text{CH}_3\cdot + \text{NH}_3 \rightarrow \text{CH}_4\cdot + \text{NH}_2$ 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 <sub>3</sub> 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+11)	0	5535±500	0.3 1.8
$\text{CH}_3\cdot + \text{NH}_2\text{NH}_2 \rightarrow \text{CH}_4\cdot + \text{NH}_2\text{NH}$ METHYL FREE RADICAL + HYDRAZINE 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+11)	0	2500±500	0.5 2.0
$\text{CH}_3\cdot + \text{ND}_2\text{ND}_2 \rightarrow \text{CH}_3\text{D} + \text{ND}_2\text{ND}$ METHYL FREE RADICAL + HYDRAZINE-d <sub>4</sub> 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
$\text{CH}_3\cdot + \text{CO} \rightarrow \text{CH}_3\text{C}(0)$ . METHYL FREE RADICAL + CARBON MONOXIDE 72 KON REACTION ORDER: 2.	273-400	3.8(+8)	0	1968	
$\text{CH}_3\cdot + \text{CH}_4 \rightarrow \text{CH}_4 + \text{CH}_3$ . METHYL FREE RADICAL + METHANE 76 KER/PAR REACTION ORDER: 2.	450-800	4.0(+11)	0	7045±250	0.7 1.3
$\text{CH}_3\cdot + \text{CHD}_3 \rightarrow \text{CH}_4 + \text{CD}_3$ . METHYL FREE RADICAL + METHANE-d <sub>3</sub> 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400-650	1.1(+11)	0	6995±250	0.7 1.3
$\text{CH}_3\cdot + \text{CD}_4 \rightarrow \text{CH}_3\text{D} + \text{CD}_3$ . METHYL FREE RADICAL + METHANE-d <sub>4</sub> 76 KER/PAR REACTION ORDER: 2.	400-650	2.5(+11)	0	7700±500	0.5 1.5
$\text{CD}_3\cdot + \text{CH}_3\text{D} \rightarrow \text{CD}_4 + \text{CH}_3$ . METHYL-d <sub>3</sub> -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
$\text{CD}_3\cdot + \text{CD}_4 \rightarrow \text{CD}_4 + \text{CD}_3$ . METHYL-d <sub>3</sub> -FREE RADICAL + METHANE-d <sub>4</sub> 72 KON REACTION ORDER: 2.	473-623	4.1(+12)	0	8960±250	
$\text{CH}_3\cdot + \text{.CHO} \rightarrow \text{CH}_4 + \text{CO}$ 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
$\text{CH}_3\cdot + \text{HCHO} \rightarrow \text{CH}_4 + \text{.CHO}$ METHYL FREE RADICAL + FORMALDEHYDE 76 KER/PAR REACTION ORDER: 2.	300-500	1.1(+11)	0	3070±500	0.5 1.5
$\text{CH}_3\cdot + \text{HCHO} \rightarrow \text{CH}_4 + \text{.CHO}$ METHYL FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+10)	0.5	3000±2500	0.3 3.2
$\text{CH}_3\cdot + \text{DCDO} \rightarrow \text{CH}_3\text{D} + \text{.CDO}$ METHYL FREE RADICAL + FORMALDEHYDE-d <sub>2</sub> 76 KER/PAR REACTION ORDER: 2.	300-500	1.4(+11)	0	3975±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{O}$ . METHYL FREE RADICAL + METHANOL 76 KER/PAR REACTION ORDER: 2.	350-550	6.2(+10)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{.CH}_2\text{OH}$ METHYL FREE RADICAL + MÉTHANOL 76 KER/PAR REACTION ORDER: 2.	350-500	1.9(+11)	0	5035±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{O} + \text{.CH}_2\text{OH}$ METHYL FREE RADICAL + METHANOL 76 KER/PAR REACTION ORDER: 2.	350-550	2.3(+11)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CD}_3\text{OH} \rightarrow \text{CH}_3\text{D} + \text{.CD}_2\text{OH}$ METHYL FREE RADICAL + METHAN-d <sub>3</sub> -OL 76 KER/PAR REACTION ORDER: 2.	370-550	2.0(+11)	0	5940±500	0.6 1.4
$\text{CH}_3\cdot + \text{CD}_3\text{OH} \rightarrow \text{CH}_4 + \text{CD}_3\text{O}$ . METHYL FREE RADICAL + METHAN-d <sub>3</sub> -OL 76 KER/PAR REACTION ORDER: 2.	370-550	6.2(+10)	0	4900±500	0.6 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{OD} \rightarrow \text{CD}_3\text{H} + \text{.CH}_2\text{OD}$ METHYL-d <sub>3</sub> 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 <sub>3</sub> 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
$\text{CH}_3\cdot + \text{CH}_3\text{SH} \rightarrow \text{CH}_4 + \text{CH}_3\text{S}\cdot + \text{CH}_2\text{SH}$ 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 <sub>3</sub> -THIOL 76 KER/PAR REACTION ORDER: 2.	400–500	1.1(+11)	0	2050±500	0.5	2.0
$\text{CH}_3\cdot + \text{CD}_3\text{SH} \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{SH}$ METHYL FREE RADICAL + METHANE-d <sub>3</sub> -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
$\text{CH}_3\cdot + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + METHANAMINE 72 KON REACTION ORDER: 2.	388–617	5.4(+11)	0	5020±500	0.3	3.0
$\text{CH}_3\cdot + \text{CH}_3\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{NH} + \text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + MÉTHANAMINE 76 KER/PAR REACTION ORDER: 2.	350–650	2.1(+11)	0	4330±500	0.7	1.3
$\text{CH}_3\cdot + \text{CH}_3\text{ND}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{ND}_2$ METHYL FREE RADICAL + METHANAMINE-d <sub>2</sub> 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 <sub>2</sub> 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350–450	2.0(+11)	0	5135±1000	0.5	1.5
$\text{CH}_3\cdot + \text{CD}_3\text{NH}_2 \rightarrow \text{CH}_4 + \text{CD}_3\text{NH}$ METHYL FREE RADICAL + MÉTHAN-d <sub>3</sub> -AMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	400–500	2.0(+11)	0	4530±750	0.5	2.0
$\text{CH}_3\cdot + \text{CD}_3\text{NH}_2 \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{NH}_2$ METHYL FREE RADICAL + MÉTHAN-d <sub>3</sub> -AMINE 76 KER/PAR REACTION ORDER: 2.	400–500	7.2(+10)	0	5100±500	0.5	1.5
$\text{CH}_3\cdot + \text{CH}_2\text{NNH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}(\cdot)\text{NH}_2 + \text{CH}_3\text{NNH}_2$ + .CH_2\text{NNH}_2 METHYL FREE RADICAL + HYDRAZINE, METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	420	6.3(+ 8)	-	-		
$\text{CH}_3\cdot + \text{HCONH}_2 \rightarrow \text{CH}_4 + \text{HCONH} + \text{CONH}_2$ METHYL FREE RADICAL + FORMAMIDE 76 KER/PAR REACTION ORDER: 2.	350–500	3.6(+10)	0	3300±500	0.5	1.5
$\text{CH}_3\cdot + \text{HCOND}_2 \rightarrow \text{CH}_4 + \text{COND}_2$ METHYL FREE RADICAL + FORMAMIDE-N,N-d <sub>2</sub> 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 <sub>2</sub> 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350–500	2.0(+11)	0	4900±500	0.5	2.0
$\text{CH}_3\cdot + \text{CH}_3\text{NO}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{NO}_2$ 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
$\text{CH}_3\cdot + \text{CH}_3\text{ONH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{ONH}$ 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 reaction	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 <sub>2</sub> , O-METHYL- 76 KER/PAR REACTION ORDER: 2.	300-500	3.5(+10)	0	2970±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}=\text{CH} \rightarrow \text{CH}_4 + \text{CH}\equiv\text{C}$ . 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
$\text{CH}_3\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2$ . METHYL FREE RADICAL + ETHANE 76 KER/PAR REACTION ORDER: 2.	400-800	5.6(+11)	0	5840±250	0.7 1.3
$\text{CH}_3\cdot + \text{CD}_3\text{CD}_3 \rightarrow \text{CH}_3\text{D} + \text{CD}_3\text{CD}_2$ . METHYL FREE RADICAL + ETHANE-d <sub>6</sub> 76 KER/PAR REACTION ORDER: 2.	500-900	5.6(+11)	0	6600±250	0.7 1.3
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}_2$ . METHYL-d <sub>3</sub> FREE RADICAL + ETHANE 72 KON REACTION ORDER: 2.	390-800	1.0(+12)	0	6085±165	0.7 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{CD}_3 \rightarrow \text{CD}_3\text{H} + \text{CD}_3\text{CH}_2$ . METHYL-d <sub>3</sub> FREE RADICAL + ETHANE-1,1,1-d <sub>3</sub> 76 KER/PAR REACTION ORDER: 2.	500-750	3.0(+11)	0	5900±250	0.7 1.3
$\text{CD}_3\cdot + \text{CH}_3\text{CD}_3 \rightarrow \text{CD}_4 + \text{CH}_3\text{CD}_2$ . METHYL-d <sub>3</sub> FREE RADICAL + ETHANE-1,1,1-d <sub>3</sub> 76 KER/PAR REACTION ORDER: 2.	500-750	4.3(+11)	0	6845±250	0.7 1.3
$\text{CD}_3\cdot + \text{CD}_3\text{CD}_3 \rightarrow \text{CD}_4 + \text{CD}_3\text{CD}_2$ . METHYL-d <sub>3</sub> FREE RADICAL + ETHANE-d <sub>6</sub> 72 KON REACTION ORDER: 2.	550-760	4.6(+11)	0	6405	
$\text{CH}_3\cdot + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(0)$ . METHYL FREE RADICAL + ACETALDEHYDE 76 KER/PAR REACTION ORDER: 2.	300-525	8.5(+10)	0	3000±250	0.4 1.6
$\text{CH}_3\cdot + \text{CH}_3\text{CDO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{C}(0)$ . 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
$\text{CH}_3\cdot + \text{HCOOCH}_3 \rightarrow \text{CH}_4 + \text{COOCH}_3$ . 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
$\text{CH}_3\cdot + \text{HCOOCH}_3 \rightarrow \text{CH}_4 + \text{HCOOCH}_2$ . 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
$\text{CH}_3\cdot + \text{HCOOCH}_3 \rightarrow \text{CH}_4 + \text{COOCH}_3 + \text{HCOOCH}_2$ . 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
$\text{CH}_3\cdot + \text{DCOOCH}_3 \rightarrow \text{CH}_3\text{D} + \text{COOCH}_3$ 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
$\text{CH}_3\cdot + \text{DCOOCH}_3 \rightarrow \text{CH}_4 + \text{DCOOCH}_2$ 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
$\text{CH}_3\cdot + \text{CH}_3\text{COOD} \rightarrow \text{CH}_4 + \text{CH}_2\text{COOD}$ METHYL FREE RADICAL + ACETIC ACID-d 76 KER/PAR REACTION ORDER: 2.	300-600	1.6(+11)	0	5135±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{O}$ 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{O} + \text{CH}_3\text{CH}(\cdot)\text{OH}$ + .CH_2\text{CH}_2\text{OH}	400-625	5.1(+11)	0	4900±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CD}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{O} + \text{CH}_2\text{CD}_2\text{OH}$ METHYL FREE RADICAL + ETHAN-1,1-d <sub>2</sub> -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 <sub>2</sub> -OL 76 KER/PAR REACTION ORDER: 2.	400-550	4.1(+11)	0	5735±500	0.6 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_2\text{OD} \rightarrow \text{CD}_2\text{H} + \text{CH}_3\text{CH}(\cdot)\text{OD} + \text{CH}_2\text{CH}_2\text{OD}$ METHYL-d <sub>3</sub> FREE RADICAL + ETHANOL-d 76 KER/PAR REACTION ORDER: 2.	400-525	4.4(+11)	0	4900±500	0.6 1.4
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_2\text{OD} \rightarrow \text{CD}_4 + \text{CH}_3\text{CH}_2\text{O}$ METHYL-d <sub>3</sub> FREE RADICAL + ETHANOL-d 76 KER/PAR REACTION ORDER: 2.	400-525	6.2(+10)	0	5135±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{OCH}_2$ METHYL FREE RADICAL + METHANE, OXYBIS- 76 KER/PAR REACTION ORDER: 2.	300-550	4.2(+11)	0	5035±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{OOCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{OOCH}_2$ 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 <sub>3</sub> FREE RADICAL + THIIRANE 76 KER/PAR REACTION ORDER: 2.	300-500	2.2(+11)	0	4800±500	0.5 2.0
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{S} + \text{CH}_3\text{CH}(\cdot)\text{SH}$ + .CH_2\text{CH}_2\text{SH}	303	3.5(+ 7)	-	-	0.5 2.0
METHYL FREE RADICAL + ETHANETHIOL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + \text{CH}_3\text{CN} \rightarrow \text{CH}_4 + \text{CH}_2\text{CN}$ METHYL FREE RADICAL + ACETONITRILE 76 KER/PAR REACTION ORDER: 2.	350-600	5.4(+11)	0	5100±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{NH} + \text{CH}_3\text{CH}(\cdot)\text{NH}_2$ + .CH_2\text{CH}_2\text{NH}_2	350-500	2.9(+11)	0	4200±500	0.5 2.0
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 <sub>3</sub> -AMINE 76 KER/PAR REACTION ORDER: 2.	350–500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\cdot + \text{CD}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CD}_3\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + ETHAN-2,2,2-d <sub>3</sub> -AMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	423	4.0(+ 5)	-	-	
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N} + \cdot\text{CH}_2\text{NHCH}_3$ METHYL FREE RADICAL + METHANAMINE, N-METHYL- 76 KER/PAR REACTION ORDER: 2.	350–650	1.6(+11)	0	3500±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N}$ 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{ND} \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{N}$ 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 <sub>3</sub> FREE RADICAL + DIAZENE, DI(METHYL-d <sub>3</sub> )- 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 <sub>2</sub> )- 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 <sub>2</sub> )- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350–500	3.2(+11)	0	5100±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NNH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{NNH}$ 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NNH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{NNH} + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{NH}_2$ 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 <sub>2</sub> , 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{NND}$ METHYL FREE RADICAL + HYDRAZINE-d <sub>2</sub> , 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
$\text{CH}_3\cdot + \text{CH}_3\text{NNHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}(\cdot)\text{NHCH}_3 + \cdot\text{CH}_2\text{NNHCH}_3$ 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 <sub>2</sub> , 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
$\text{CH}_3\cdot + \text{HCONHCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CONHCH}_3 + \text{HCON}(\cdot)\text{CH}_3$ 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
$\text{CD}_3\cdot + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_3\text{H} + \text{CD}_3\text{CONH}$ METHYL FREE RADICAL + ACETAMIDE-2,2,2-d <sub>3</sub> 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 <sub>3</sub> 76 KER/PAR REACTION ORDER: 2.	350-600	1.4(+11)	0	5800±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow (\text{CH}_3)_2\text{C}\equiv\text{CH} \cdot + \text{CH}_3\text{C}(\cdot)=\text{CHCH}_3$ METHYL FREE RADICAL + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. CH <sub>3</sub> 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 <sub>ref</sub> : 0.72	353-453 453	1.7(+11) -	0 -	3700 -	
NOTE: k <sub>ref</sub> : CH <sub>3</sub> · + CH <sub>2</sub> =CH <sub>2</sub>					
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CH}\cdot$ 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 <sub>3</sub> FREE RADICAL + PROPANE-2,2-d <sub>2</sub> 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 <sub>3</sub> FREE RADICAL + PROPANE-2,2-d <sub>2</sub> 76 KER/PAR REACTION ORDER: 2.	550-750	2.5(+11)	0	5735±250	0.7 1.3
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{C}(0)\cdot$ 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_3\text{C(O)CH}_2$ . METHYL FREE RADICAL + 2-PROPANONE 76 KER/PAR REACTION ORDER: 2.	350-700	3.5(+11)	0	4900±250	0.8 1.3
$\text{CD}_3\cdot + (\text{CD}_3)_2\text{CO} \rightarrow \text{CD}_4 + \text{CD}_3\text{C(O)CD}_2$ . METHYL-d <sub>3</sub> FREE RADICAL + 2-PROPANONE-1,1,1,3,3,3-d <sub>6</sub> 76 KER/PAR REACTION ORDER: 2.	350-800	4.8(+11)	0	5735±250	0.8 1.3
$\text{CH}_3\cdot + \text{HCOOCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{.COOCH}_2\text{CH}_3 + \text{HCOOCH}(\cdot)\text{CH}_3$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{COOCH}_3 \rightarrow \text{CH}_4 + \text{.CH}_2\text{COOCH}_3 + \text{CH}_3\text{COOCH}_2$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{COOCd}_3 \rightarrow \text{CH}_4 + \text{.CH}_2\text{COOCd}_3$ . METHYL FREE RADICAL + ACETIC ACID METHYL-d <sub>3</sub> ESTER 76 KER/PAR REACTION ORDER: 2.	350-650	1.9(+11)	0	5035±500	0.4 1.6
$\text{CH}_3\cdot + \text{CD}_3\text{COOCH}_3 \rightarrow \text{CH}_4 + \text{CD}_3\text{COOCH}_2$ . METHYL FREE RADICAL + ACETIC-d <sub>3</sub> ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	400-600	1.7(+11)	0	5990±500	0.5 1.5
$\text{CH}_3\cdot + \text{CH}_3\text{OCOOCH}_3 \rightarrow \text{CH}_4 + \text{.CH}_2\text{OCOOCH}_3$ . 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
$\text{CD}_3\cdot + (\text{CH}_3)_2\text{CHOD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{C}(\cdot)\text{OD} + \text{.CH}_2\text{CH(CH}_3\text{)OD}$ . METHYL-d <sub>3</sub> 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHSH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHS} + (\text{CH}_3)_2\text{C}(\cdot)\text{SH}$ . + .CH <sub>2</sub> CH(CH <sub>3</sub> )SH METHYL FREE RADICAL + 2-PROPANETHIOL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	4.1(+ 7)	-	-	0.5 2.0
$\text{CD}_3\cdot + \text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}(\cdot)\text{CN} + \text{.CH}_2\text{CH}_2\text{CN}$ . METHYL-d <sub>3</sub> FREE RADICAL + PROPANENITRILE 76 KER/PAR REACTION ORDER: 2.	400-600	3.6(+11)	0	4330±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{N} \rightarrow \text{CH}_4 + \text{.CH}_2\text{N}(\text{CH}_3)_2$ . 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
$\text{CH}_3\cdot + \text{HCON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{.CON}(\text{CH}_3)_2 + \text{HCO-(CH}_3\text{)NCH}_2$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{C=CH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{C=CH}$ . + .CH <sub>2</sub> CH <sub>2</sub> C≡CH + CH <sub>3</sub> CH <sub>2</sub> C≡C. 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
$\text{CH}_3\cdot + \text{CH}_3\text{C=CCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C=CCH}_2$ . 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	
$\text{CH}_3\cdot + \text{CH}_2=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$ + . $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 12.0	453	—	—	—	
NOTE: $k_{\text{ref}}: \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{CH}=\text{CH}_2$ METHYL FREE RADICAL + 1-BUTENE 76 KER/PAR REACTION ORDER: 2.	350–650	2.5(+11)	0	4200±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CHCH}_3$ + $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ . METHYL FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.7	353–453 453	1.0(+11) —	0 —	3600 —	
NOTE: $k_{\text{ref}}: \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3\cdot + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHCH}_2$ . METHYL FREE RADICAL + cis-2-BUTENE 76 KER/PAR REACTION ORDER: 2.	350–650	1.8(+11)	0	4100±500	0.6 1.4
$\text{CH}_3\cdot + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.2	353–453 453	4.5(+10) —	0 —	3675 —	
NOTE: $k_{\text{ref}}: \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3\cdot + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHCH}_2$ . METHYL FREE RADICAL + trans-2-BUTENE 76 KER/PAR REACTION ORDER: 2.	350–500	1.0(+12)	0	4830±500	0.6 1.4
$\text{CH}_3\cdot + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.4	353–453 453	1.4(+11) —	0 —	4075 —	
NOTE: $k_{\text{ref}}: \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ . 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	353–453 453	1.4(+11) —	0 —	3475 —	
NOTE: $k_{\text{ref}}: \text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ 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 <sub>3</sub> FREE RADICAL + BUTANE-2,2,3,3-d <sub>4</sub> 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 <sub>3</sub> FREE RADICAL + BUTANE-2,2,3,3-d <sub>4</sub> 76 KER/PAR REACTION ORDER: 2.	600–750	4.5(+11)	0	5735±250	0.7 1.3
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C} \cdot + (\text{CH}_3)_2\text{CHCH}_2$ . 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
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C}$ . METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KER/PAR REACTION ORDER: 2.	550-750	9.6(+10)	0	3975±250	0.7 1.3
$\text{CD}_3\cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{CDCH}_2$ . METHYL-d <sub>3</sub> 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
$\text{CD}_3\cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_4 + (\text{CH}_3)_3\text{C}$ . METHYL-d <sub>3</sub> 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{CHCHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHC(O)}$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{COCOCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{COCOCH}_2$ . METHYL FREE RADICAL + 2,3-BUTANEDIONE 76 KER/PAR REACTION ORDER: 2.	300-800	2.2(+11)	0	4300±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3\text{CO})_2\text{O} \rightarrow \text{CH}_4 + \text{CH}_3\text{COOCCH}_2$ . METHYL FREE RADICAL + ACETIC ACID ANHYDRIDE 76 KER/PAR REACTION ORDER: 2.	300-500	1.8(+11)	0	4830±500	0.6 1.4
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C(O)}$ . 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCHO} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHC(O)}$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{COCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{COCH}_3 + \text{CH}_2\text{CH}_2\text{COCH}_3$ . METHYL FREE RADICAL + 2-BUTANONE 76 KER/PAR REACTION ORDER: 2.	300-500	8.2(+10)	0	3700±500	0.5 1.5
$\text{CH}_3\cdot + \text{HCOOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COOCH}_2\text{CH}_2\text{CH}_3$ . METHYL FREE RADICAL + FORMIC ACID PROPYL ESTER 72 KON REACTION ORDER: 2.	347-455	1.3(+10)	0	3675	
$\text{CH}_3\cdot + \text{HCOOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COOCH}_2\text{CH}_2\text{CH}_3$ . $+ \text{HCOOCH}(\cdot)\text{CH}_2\text{CH}_3 + \text{HCOOCH}_2\text{CH}(\cdot)\text{CH}_3$ . $+ \text{HCOOCH}_2\text{CH}_2\text{CH}_2$ . 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
$\text{CH}_3\cdot + \text{HCOOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COOCH}(\text{CH}_3)_2$ . $+ \text{HCOOC}(\cdot)(\text{CH}_3)_2 + \text{HCOOCH}(\text{CH}_3)\text{CH}_2$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{OCH}(\cdot)\text{CH}_3$ . $+ \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2$ . 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CSH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CS} + \text{CH}_2\text{C}(\text{CH}_3)_2\text{SH}$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{NN=CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\cdot)=\text{NN=CHCH}_3$ . $+ \text{CH}_2\text{CH}=\text{NN=CHCH}_3$ . 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}\cdot$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{NH}_2 + \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + 1-BUTANAMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	426	3.2(+ 7)	-	-	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{N}\cdot$ $+ \text{CH}_3\text{CH}(\cdot)\text{NHCH}_2\text{CH}_3 + \text{CH}_2\text{CH}_2\text{NHCH}_2\text{CH}_3$ 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
$\text{CH}_3\cdot + \text{CH}_3\text{CON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{CON}(\text{CH}_3)_2$ $- \text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2\cdot$ METHYL FREE RADICAL + ACETAMIDE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-600	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. NOTE: TENTATIVE k VALUE.	450-650	4.5(+11)	0	4500±500	0.6 1.4
$\text{CH}_3\cdot + \text{cis}-\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	298	-	-	4060	
$\text{CH}_3\cdot + \text{cis}-\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	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. NOTE: TENTATIVE k VALUE.	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. NOTE: TENTATIVE k VALUE.	450-600	4.4(+11)	0	4225±7500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}=\text{CH}_2\text{CH}_2\cdot$ $+ \text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3$ 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
$\text{CH}_3\cdot - (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}_3$ $+ (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.4 NOTE: k <sub>ref</sub> : CH <sub>3</sub> · + CH <sub>2</sub> =CH <sub>2</sub> TENTATIVE k VALUE.	453	-	-	-	
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ + .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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(0)\cdot$ 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(0)\cdot$ 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{C}(0)\cdot$ 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
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCHO} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CC}(0)\cdot$ 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
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{COCH}_3\text{CH}_3$ + .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
$\text{CH}_3\cdot + (\text{CH}_3\text{CD}_2)_2\text{CO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{COCD}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d <sub>4</sub> 76 KER/PAR REACTION ORDER: 2.	500-600	2.0(+11)	0	5535±500	0.5 2.0
$\text{CH}_3\cdot + (\text{CH}_3\text{CD}_2)_2\text{CO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CD}_2\text{COCD}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d <sub>4</sub> 76 KER/PAR REACTION ORDER: 2.	500-600	1.3(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\cdot + \text{HCOO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_4 + .\text{COO}(\text{CH}_2)_3\text{CH}_3$ + HCOOCH(·)(CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub> + HCOOCH <sub>2</sub> CH(·)CH <sub>2</sub> CH <sub>3</sub> + HCOOCH <sub>2</sub> CH <sub>2</sub> CH(·)CH <sub>3</sub> + HCOO(CH <sub>2</sub> ) <sub>3</sub> CH <sub>2</sub> 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{COOCH}_2\text{CH}_3$ + CH <sub>3</sub> CH <sub>2</sub> COOCH(·)CH <sub>3</sub> + .CH <sub>2</sub> CH <sub>2</sub> COOCH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> COOCH <sub>2</sub> CH <sub>2</sub> METHYL FREE RADICAL + PROPAPIOIC ACID ETHYL ESTER 76 KER/PAR REACTION ORDER: 2.	300-650	2.5(+11)	0	4125±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_2\text{NCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)\text{CH}_3$ + .CH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> CH <sub>3</sub> )CH <sub>3</sub> + (CH <sub>2</sub> CH <sub>2</sub> ) <sub>2</sub> NCH <sub>2</sub> 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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{NCON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{N}(\text{CH}_3)\text{CON}(\text{CH}_3)_2$ METHYL FREE RADICAL + UREA TETRAMETHYL- 76 KER/PAR REACTION ORDER: 2.	350-550	2.0(+11)	0	3975±500	0.5 1.5
$\text{CH}_3\cdot + \text{cis}-\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + cis-2-HEXENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
$\text{CH}_3\cdot + \text{cis}-\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ 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. $k/k_{\text{ref}}$ : 0.2	453	-	-	-	
NOTE: $k_{\text{ref}}$ : $\text{CH}_3\cdot + \text{CH}_2=\text{CH}_2$					
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ 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.					
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ 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.					
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ 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.					
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHC}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KON REACTION ORDER: 2.	300-500	5.0(+10)	0	3445	
$\text{CD}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL-d <sub>3</sub> FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KON REACTION ORDER: 2.	439-566	4.7(+11)	0	4525	
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{OCH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PROPANE, 2,2'-OXYBIS-	400-600	2.1(+11)	0	4100±500	0.5 2.0
76 KER/PAR REACTION ORDER: 2.					
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHOOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{OOCH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PEROXIDE, BIS(1-METHYLETHYL)-	300-450	2.3(+11)	0	4100±500	0.5 1.5
76 KER/PAR REACTION ORDER: 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
$\text{CH}_3\cdot + \text{CH}_3\text{CH}=\text{NC(CH}_3)_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\cdot)=\text{NC(CH}_3)_3$ + .\text{CH}_2\text{CH}=\text{NC(CH}_3)_3 + \text{CH}_3\text{CH}=\text{NC(CH}_3)_2\text{CH}_2\cdot METHYL FREE RADICAL + PROPANIMINE, N-ETHYLDENE-2-METHYL-					
76 KER/PAR REACTION ORDER: 2.	350-500	8.9(+10)	0	3925±500	0.5 1.5
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHNHCH(CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHN}(\cdot)\text{CH}(\text{CH}_3)_2$ + (\text{CH}_3)_2\text{C}(\cdot)\text{NHCH(CH}_3)_2 METHYL FREE RADICAL + 2-PROPANAMINE, N-(1-METHYLETHYL)-					
76 KER/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	3370±750	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{N} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$ + .\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.	350-600	5.0(+11)	0	4000±500	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_3\text{C}$ METHYL FREE RADICAL + PENTANE, 3-ETHYL-					
76 KER/PAR REACTION ORDER: 2.	350-750	9.5(+10)	0	3975±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + PENTANE, 3-ETHYL-					
76 KER/PAR REACTION ORDER: 2.	350-750	6.0(+11)	0	4830±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{CHCH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + PENTANE, 3-ETHYL-					
76 KER/PAR REACTION ORDER: 2.	350-750	7.1(+11)	0	5800±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot$ METHYL FREE RADICAL + OCTANE					
76 KER/PAR REACTION ORDER: 2.	350-800	4.8(+11)	0	5800±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3 METHYL FREE RADICAL + OCTANE					
76 KER/PAR REACTION ORDER: 2.	350-800	1.2(+12)	0	4830±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL-					
76 KER/PAR REACTION ORDER: 2.	350-750	2.0(+11)	0	4830±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\text{C}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL-					
76 KER/PAR REACTION ORDER: 2.	350-750	9.5(+10)	0	3975±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ + .\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.	350-750	1.2(+12)	0	5800±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CHO})\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4$ + .\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.	350-750	1.2(+12)	0	5800±250	0.7 1.3
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4$ + (\text{CH}_3)_2\text{CH}(\cdot)(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + (\text{CH}_3)\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.	350-750	2.9(+11)	0	3975±250	0.7 1.3
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
$\text{CH}_3\cdot + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + [\text{C}_8\text{H}_{17}\cdot]$ 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
$\text{CH}_4 + \text{CH} \rightarrow \text{CH}_3\cdot + :\text{CH}_2$ METHANE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.5(+11)	0.7	3000±2500	0.3 3.2
$\text{CH}_4 + \text{CH}_2 \rightarrow \text{CH}_3\cdot + \text{CH}_3$ 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 <sub>3</sub> 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 <sub>3</sub> + 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 <sub>4</sub> + 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 <sub>4</sub> + METHYL-d <sub>3</sub> 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 70 BEN/0'N REACTION ORDER: 1.	298	5.0(+13)	0	9560	
.CHO + O → CO <sub>2</sub> + H METHYL, OXO-, FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	0	0±1500	
.CHO + O → CO + OH METHYL, OXO-, FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	1.0	250±1500	
.CHO + O <sub>2</sub> → CO + HO <sub>2</sub> METHYL, OXO-, FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.6(+12)	0	3500±1500	
.CHO + H → CO + H <sub>2</sub> 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 <sub>2</sub> O METHYL, OXO-, FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+10)	1.0	0±1500	
.CHO + HO <sub>2</sub> → HCHO + O <sub>2</sub> METHYL, OXO-, FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	1500±1500	
.CHO + N → HCN + O METHYL, OXO-, FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(+14)	0	0±1000	
.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 <sub>2</sub> 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 <sub>2</sub> → CO + CH <sub>3</sub> . 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 <sub>3</sub> . → CO + CH <sub>4</sub> . 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 <sub>2</sub> FORMALDEHYDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 2.	1500–2500	1.3(+10)	1.0	1600	0.3 3.2
HCHO + OH → .CHO + H <sub>2</sub> 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 <sub>2</sub> → .CHO + H <sub>2</sub> O <sub>2</sub> 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 <sub>2</sub> FORMALDEHYDE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.7	2000±2500	0.3 3.2
HCHO + CH <sub>2</sub> → .CHO + CH <sub>3</sub> FORMALDEHYDE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	2.0(+11)	0	3270±1500	- -
HCHO + CH <sub>3</sub> → .CHO + CH <sub>4</sub> 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 <sub>3</sub> → .CDO + CH <sub>3</sub> 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 <sub>3</sub> OH → HCHO + H METHYL, HYDROXY-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 2.	673–773	1.1(+13)	0	14600	
CH <sub>3</sub> 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 <sub>3</sub> O. + O <sub>2</sub> → HCHO + HO <sub>2</sub> METHOXY FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.0(+12)	0	3000±1500	
CH <sub>3</sub> O. + H → HCHO + H <sub>2</sub> METHOXY FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	1.0(+14)	0	0±1500	
CH <sub>3</sub> O. + OH → HCHO + H <sub>2</sub> O METHOXY FREE RADICAL + HYDROXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+13)	0	0±1500	
CH <sub>3</sub> 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 f	f F
$\text{CH}_3\text{O} \cdot + \text{M} \rightarrow \text{HCHO} + \text{H} + \text{M}$ METHOXY FREE RADICAL 76 ENG 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 <sub>3</sub> 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 <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–500	3.2(+10)	0	5700±1000	0.5	2.0
NOTE: GIVEN WITH CAUTION.						
$\text{CD}_3\text{OH} + \text{CH}_3 \cdot \rightarrow \cdot\text{CD}_2\text{OH} + \text{CH}_3\text{D}$ METHAN-d <sub>3</sub> -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 <sub>3</sub> -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.	565–651	7.9(+14)	0	21640		
NOTE: RATE CONSTANTS MAY BE SLIGHTLY LOW.						
$\text{CS} + \text{O} \rightarrow \text{S} + \text{CO}$ 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.	1800–3700	8.7(+13)	0	4370	0.5	1.5
NOTE: $k_1 = \text{Kk}_{-1}$						

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 <sub>2</sub> 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 <sub>2</sub> + 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 <sub>2</sub> + O → COS + S CARBON DISULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2.	302	2.2(+11)	-	-	0.5 1.5
CS <sub>2</sub> + S → CS + S <sub>2</sub> CARBON DISULFIDE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2.	298	3.9(+11)	-	-	0.5 1.5
CS <sub>2</sub> + 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 <sub>2</sub> CARBON OXIDE SULFIDE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2.	230-2600	1.7(+12)	0	2050±230	0.3 3.0
CH <sub>3</sub> S· + CH=CH → CH <sub>3</sub> SCH=CH. METHYLTHIO FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2.	298-333	7.9(+ 7)	-	-	
CH <sub>3</sub> S· + CH <sub>2</sub> =CH <sub>2</sub> → CH <sub>3</sub> SCH <sub>2</sub> CH <sub>2</sub> . METHYLTHIO FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	298	4.8(+ 8)	-	-	
CH <sub>3</sub> S· + CH <sub>3</sub> CH=CHCH <sub>3</sub> → CH <sub>3</sub> CH(SCH <sub>3</sub> )CH(.)CH <sub>3</sub> METHYLTHIO FREE RADICAL + 2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: cis-trans EQUILIBRIUM - WEIGHTED k.	298-333	1.6(+ 9)	-	-	
CH <sub>3</sub> SH → CH <sub>3</sub> · + SH METHANETHIOL 70 BEN/O'N REACTION ORDER: 1.	1005-1102	3.2(+15)	0	38550	
CH <sub>3</sub> SH + CH <sub>3</sub> · → CH <sub>3</sub> S· + .CH <sub>2</sub> SH + CH <sub>4</sub> METHANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	303	1.2(+ 8)	-	-	0.5 2.0
CD <sub>3</sub> SH + CH <sub>3</sub> · → CD <sub>3</sub> S· + CH <sub>4</sub> METHANE-d <sub>3</sub> -THIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-500	1.1(+11)	0	2065±500	0.5 2.0
CD <sub>3</sub> SH + CH <sub>3</sub> · → .CD <sub>2</sub> SH + CH <sub>3</sub> D METHANE-d <sub>3</sub> -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
CN + O → N + CO CYANOCEN FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+12)	0	0±2500	0.3 3.2
CN + O → NO + C CYANOCEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.3(+12)	0.5	14545	
CN + O <sub>2</sub> → NO + CO CYANOCEN FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+11)	0	0±5000	0.3 3.2
CN + H → N + CH CYANOCEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+12)	0.5	49775	
CN + H → NH + C CYANOCEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.0(+13)	0.5	52745	
CN + H + M → HCN + M CYANOCEN FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 3.	1500–2500	3.2(+16)	-0.5	0±2500	0.3 3.2
CN + H <sub>2</sub> → HCN + H CYANOCEN FREE RADICAL + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	2500±1500	
CN + OH → HCN + O CYANOCEN FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	1500±1500	
CN + S → N + CS CYANOCEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CN + S → C + NS CYANOCEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		2.0(+12)	0.5	32010	
CN + N → C + N <sub>2</sub> CYANOCEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CN + NO → CO + N <sub>2</sub> CYANOCEN FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+11)	0	0±2500	0.3 3.2
CN + NH → HCN + N CYANOCEN FREE RADICAL + IMIDOGEN FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	1.0(+11)	0.5	1000±2500	0.3 3.2
CN + HNO → HCN + NO CYANOCEN FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2.	1500–2500	4.0(+11)	0.5	0±2500	0.3 3.2
CN + C → N + C <sub>2</sub> CYANOCEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+11)	0.5	19300	
CN + C → C + CN CYANOCEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CN + CH <sub>2</sub> → HCN + CH CYANOCEN FREE RADICAL + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500–2500	3.2(+12)	0	2500±1500	
CN + CH <sub>3</sub> → HCN + CH <sub>2</sub> CYANOCEN 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
CN + CH <sub>4</sub> → HCN + CH <sub>3</sub> CYANOPEN FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2.	1500–2500	3.2(+11)	0.7	2500±2500	0.3 3.2
CN + CHO → CO + HCN CYANOPEN FREE RADICAL + METHYL, OXO-, FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	2.0(+11)	0.5	0±2500	0.3 3.2
CN + HCHO → HCN + CHO CYANOPEN FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500–2500	1.3(+11)	0.7	1500±2500	0.3 3.2
C(NO <sub>2</sub> ) <sub>4</sub> → .C(NO <sub>2</sub> ) <sub>3</sub> + NO <sub>2</sub> METHANE, TETRANITRO- 70 BEN/O'N REACTION ORDER: 1.	443–506	3.4(+17)	0	20575	
HCN + OH → CN + H <sub>2</sub> O HYDROCYANIC ACID + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500–2500	2.0(+11)	0.6	2500±2500	0.3 3.2
CH <sub>3</sub> NH <sub>2</sub> + CH <sub>3</sub> · → CH <sub>3</sub> NH · + .CH <sub>2</sub> NH <sub>2</sub> + CH <sub>4</sub> METHANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–650	2.1(+11)	0	4330±500	0.7 1.3
CH <sub>3</sub> NH <sub>2</sub> + CH <sub>3</sub> · → .CH <sub>2</sub> NH <sub>2</sub> + CH <sub>4</sub> METHANAMINE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	388–617	5.4(+11)	0	5020±500	0.3 3.0
CH <sub>3</sub> ND <sub>2</sub> + CH <sub>3</sub> · → CH <sub>3</sub> ND · + CH <sub>3</sub> D METHANAMINE-d <sub>2</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–450	2.0(+11)	0	5135±1000	0.5 1.5
NOTE: TENTATIVE k VALUE.					
CH <sub>3</sub> ND <sub>2</sub> + CH <sub>3</sub> · → .CH <sub>2</sub> ND <sub>2</sub> + CH <sub>4</sub> METHANAMINE-d <sub>2</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–450	1.4(+11)	0	4530±500	0.7 1.3
CD <sub>3</sub> NH <sub>2</sub> + CH <sub>3</sub> · → .CD <sub>2</sub> NH <sub>2</sub> + CH <sub>3</sub> D METHAN-d <sub>3</sub> -AMINE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	400–500	7.2(+10)	0	5100±500	0.5 1.5
CD <sub>3</sub> NH <sub>2</sub> + CH <sub>3</sub> · → CD <sub>3</sub> NH · + CH <sub>4</sub> METHAN-d <sub>3</sub> -AMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–500	2.0(+11)	0	4530±750	0.5 2.0
NOTE: TENTATIVE k VALUE.					
CH <sub>2</sub> =N=N → CH <sub>2</sub> + N <sub>2</sub> METHANE, DIAZO- 70 BEN/O'N REACTION ORDER: 1.	498–723	1.0(+13)	0	17600	
CH <sub>3</sub> NHNH <sub>2</sub> → CH <sub>3</sub> NH · + NH <sub>2</sub> HYDRAZINE, METHYL- 70 BEN/O'N REACTION ORDER: 1.	746–862	5.0(+16)	-	32600	
NOTE: SUSPECT ARRHENIUS FACTORS.					
CH <sub>3</sub> NHNH <sub>2</sub> + CH <sub>3</sub> · → CH <sub>3</sub> N(·)NH <sub>2</sub> + CH <sub>3</sub> NHH. + .CH <sub>2</sub> NHNH <sub>2</sub> + CH <sub>4</sub> HYDRAZINE, METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	420	6.3(+ 8)	-	-	
NOTE: TENTATIVE k VALUE.					
CH <sub>3</sub> NO → CH <sub>2</sub> =NOH METHANE, NITROSO- 70 BEN/O'N REACTION ORDER: 1.	633–698	7.9(+12)	0	19800	
HCONH <sub>2</sub> + CH <sub>3</sub> · → HCONH · + .CONH <sub>2</sub> + CH <sub>4</sub> FORMAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–500	3.6(+10)	0	3300±5000	0.5 1.5
HCOND <sub>2</sub> + CH <sub>3</sub> · → HCOND · + CH <sub>3</sub> D FORMAMIDE-N,N-d <sub>2</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–500	2.0(+11)	0	4900±500	0.5 2.0
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
HCOND <sub>2</sub> + CH <sub>3</sub> · → .COND <sub>2</sub> + CH <sub>4</sub> FORMAMIDE-N,N-d <sub>2</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–500	5.5(+10)	0	3575±500	0.5 2.0
CH <sub>3</sub> ONO → CH <sub>3</sub> O · + NO NITROUS ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	453–513	4.0(+15)	0	20700	
CH <sub>3</sub> NO <sub>2</sub> → CH <sub>3</sub> · + NO <sub>2</sub> METHANE, NITRO- 70 BEN/O'N REACTION ORDER: 1.	660	4.0(+15)	0	29700	
CH <sub>3</sub> NO <sub>2</sub> + CH <sub>3</sub> · → .CH <sub>2</sub> NO <sub>2</sub> + CH <sub>4</sub> METHANE, NITRO- + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300–500	1.0(+11)	0	5100±750	0.4 2.5
NOTE: TENTATIVE k VALUE.					
CH <sub>3</sub> ONO <sub>2</sub> → CH <sub>3</sub> O · + NO <sub>2</sub> NITRIC ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	483–513	3.2(+15)	0	20030	
CH <sub>3</sub> ONH <sub>2</sub> + CH <sub>3</sub> · → CH <sub>3</sub> OH · + CH <sub>4</sub> HYDROXYLAMINE, O-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300–500	5.0(+10)	0	2265±500	0.5 1.5
CH <sub>3</sub> OND <sub>2</sub> + CH <sub>3</sub> · → CHO <sub>3</sub> ND · + CH <sub>3</sub> D HYDROXYLAMINE-N,N-d <sub>2</sub> , O-METHYL, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300–500	3.5(+10)	0	2970±500	0.5 1.5
C <sub>2</sub> + O → C + CO CARBON DIMER + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C <sub>2</sub> + H → C + CH CARBON DIMER + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+13)	0.5	30450	
C <sub>2</sub> + S → C + CS CARBON DIMER + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C <sub>2</sub> + N → C + CN CARBON DIMER + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
C <sub>2</sub> + C → C + C <sub>2</sub> CARBON DIMER + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
CCO + CH=CH → products CARBON OXIDE(C <sub>2</sub> O) + ETHYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.3 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	304	-	-	-	
CCO + CH <sub>3</sub> CH=CH <sub>2</sub> → CO + CH <sub>3</sub> CH=C=CH <sub>2</sub> CARBON OXIDE(C <sub>2</sub> O) + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 5.7 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	297	-	-	-	
CCO + CH <sub>3</sub> C≡CCH <sub>3</sub> → products CARBON OXIDE(C <sub>2</sub> O) + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 8.5 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	304	-	-	-	
CCO + CH <sub>2</sub> =CHCH=CH <sub>2</sub> → CO + CH <sub>2</sub> =C=CHCH=CH <sub>2</sub> CARBON OXIDE(C <sub>2</sub> O) + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 210. NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	298	-	-	-	
CCO + CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH=C=CH <sub>2</sub> + CO CARBON OXIDE(C <sub>2</sub> O) + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 7.0 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	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
CCO + cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → CO + cis-CH <sub>3</sub> CH=C=CHCH <sub>3</sub> CARBON OXIDE(C <sub>2</sub> O) + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 9.1 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	297	-	-	-	
CCO + trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → CO + trans-CH <sub>3</sub> CH=C=CHCH <sub>3</sub> CARBON OXIDE(C <sub>2</sub> O) + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 10.6 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	297	-	-	-	
CCO + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → CO + (CH <sub>3</sub> ) <sub>2</sub> C=C=CH <sub>2</sub> CARBON OXIDE(C <sub>2</sub> O) + 1-PROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 50.0 NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	297	-	-	-	
CCO + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → CO + (CH <sub>3</sub> ) <sub>2</sub> C=C=CHCH <sub>3</sub> CARBON OXIDE(C <sub>2</sub> O) + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 100. NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	298	-	-	-	
CCO + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → CO + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> CARBON OXIDE(C <sub>2</sub> O) + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 250. NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	298	-	-	-	
CCO + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → CO + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> CARBON OXIDE(C <sub>2</sub> O) + 2,3-PENTADIENE, 2,4-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 113. NOTE: k <sub>ref</sub> : CCO + CH <sub>2</sub> =CH <sub>2</sub>	304	-	-	-	
CH≡CH + O → products ETHYNE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	200-700	1.4(+13)	0	1500	0.8 1.2
CH≡CH + OH → CH≡C. + H <sub>2</sub> O ETHYNE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-2000	7.6(+12)	0	2335+400	0.5 2.1
CH≡CH + S → cy-CH=CHS ETHYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	1.7(+11)	-	-	
CH≡CH + N → C <sub>2</sub> H <sub>2</sub> N ETHYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: UPPER LIMIT.	440	2.0(+ 9)	-	-	
CH≡CH + CH <sub>3</sub> . → CH≡C. + CH <sub>4</sub> ETHYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: GIVEN WITH CAUTION.	473-773	-	-	7100	
CH≡CH + CH <sub>3</sub> . → CH <sub>3</sub> CH=CH. ETHYNE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2	371-479	2.5(+11)	0	3900	
CH≡CH + CH <sub>3</sub> S. → CH <sub>3</sub> SCH=CH. ETHYNE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298-333	7.9(+ 7)	-	-	
CH≡CH + CCO → products ETHYNE + CARBON OXIDE(C <sub>2</sub> O) 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.3 NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CCO	304	-	-	-	
CH≡CH + CH <sub>3</sub> CH <sub>2</sub> . → CH <sub>3</sub> CH <sub>2</sub> CH=CH. ETHYNE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	373-473	5.0(+10)	0	3500	
CH≡CH + (CH <sub>3</sub> ) <sub>2</sub> CH. → (CH <sub>3</sub> ) <sub>2</sub> 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
$\text{CH}=\text{CH} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}$ . ETHYNE + ETHYL, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	363-577	1.0(+11)	0	3875	
cis-CDH=CDH → trans-CDH=CHD cis-ETHENE-1,2-d <sub>2</sub> 70 BEN/O'N REACTION ORDER: 1.	723-823	1.0(+13)	0	32700	
$\text{CH}_2=\text{CH}_2 + \text{O} \rightarrow \text{cy-CH}_2\text{CH}_2\text{O}$ ETHÈNE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	200-500	3.3(+12)	0	565	0.8 1.2
$\text{CH}_2=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2$ . ETHÈNE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	9.3(+13)	0	1410	
$\text{CH}_2=\text{CH}_2 + \text{H} + \text{M} \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{M}$ ETHÈNE + HYDROGEN ATOM 72 KON REACTION ORDER: 3. M: H <sub>2</sub>	298-813	5.6(+17)	0.5	495	
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_2=\text{CH}\cdot + \text{H}_2\text{O}$ ETHÈNE + HYDROXYL FREE RADICAL 72 KON REACTION ORDER: 2.	3500-1400	1.6(+14)	0	2831+445	0.4 2.4
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_2\text{CH}_2\text{OH}$ ETHÈNE + HYDROXYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.		1.1(+12)	-	-	0.8 1.3
$\text{CH}_2=\text{CH}_2 + \text{HO}_2 \rightarrow \text{products}$ ETHÈNE + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: RATIO DATA VERSUS kref. FOR HO <sub>2</sub> + CO → CO <sub>2</sub> + OH k FACTORS MIGHT BE HIGH.	300	1.0(+ 7)	-	-	0.1 10.
$\text{CH}_2=\text{CH}_2 + \text{S} \rightarrow \text{cy-CH}_2\text{CH}_2\text{S}$ ETHÈNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	8.1(+11)	-	-	
$\text{CH}_2=\text{CH}_2 + \text{N} \rightarrow \text{products}$ ETHÈNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	320-550	2.0(+10)	0	353	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_2=\text{CH}\cdot + \text{CH}_4$ ETHÈNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	4.2(+11)	0	5600±500	0.5 1.5
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2$ . ETHÈNE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	353-453	3.3(+11)	0	3900	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot + (\text{CH}_3)_2\text{CH}$ . ETHÈNE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	350-705	2.0(+11)	0	3575±105	0.8 1.3
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{S}\cdot \rightarrow \text{CH}_3\text{SCH}_2\text{CH}_2$ . ETHÈNE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	4.8(+ 8)	-	-	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ ETHÈNE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	348-482	1.6(+11)	0	3675	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ ETHÈNE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	375-503	1.9(+10)	0	3070	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{CH}\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ . ETHÈNE + 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
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2$ ETHÈNE + BUTYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	352-405	2.3(+10)	0	3370	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2$ ETHÈNE + ETHYL, 1,1-DIMÉTHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	300-650	2.8(+10)	0	3575	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH}(\text{CH}_2)_3\text{CH}_2$ ETHÈNE + 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	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}=\text{CH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}$ ETHYL FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2.	373-473	5.0(+10)	0	3500	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}$ ETHYL FREE RADICAL + ETHÈNE 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	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_2=\text{CHCH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{OH}$ + . $\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{OH}$ ETHYL FREE RADICAL + 2-PROPEN-1-OL 72 KER/PAR REACTION ORDER: 2.	323-415	1.9(+11)	0	3901	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_2=\text{CHCN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CN} + .\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ 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	
$\text{CH}_3\text{CH}_2 \cdot + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4265	
$\text{CH}_3\text{CH}_2 \cdot + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4350	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{COOCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_3)\text{CH}_2$ . ETHYL FREE RADICAL + ACETIC ACID ETHENYL ESTER 72 KER/PAR REACTION ORDER: 2.	303-417	7.8(+10)	0	3475	
$\text{CH}_3\text{CH}_2 \cdot + \text{cis}-\text{CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ + $\text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + cis-2-BUTENENITRILE 72 KER/PAR REACTION ORDER: 2.	323-454	1.5(+10)	0	2500	
$\text{CH}_3\text{CH}_2 \cdot + \text{trans}-\text{CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ + $\text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ 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
$\text{CH}_3\text{CH}_2\cdot + \text{cis}-\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4300	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ ETHYL FREE RADICAL + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2.	298	-	-	3620	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{COOCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + ACETIC ACID 2-PROPYENYL ESTER 72 KER/PAR REACTION ORDER: 2.	308-448	2.5(+11)	0	3900	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{COCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3$ ETHYL FREE RADICAL + 3-PENTANONE 72 KON REACTION ORDER: 2.	300-520	2.8(+11)	0	3986+100	0.4 2.2
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ + $\text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ ETHYL FREE RADICAL + 1,3-BUTADIENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.	318-414	1.6(+11)	0	2265	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-HEXENE 72 KER/PAR REACTION ORDER: 2.	338-435	3.9(+10)	0	3400	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}=\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + PROPANOIC ACID 2-PROPYENYL ESTER 72 KER/PAR REACTION ORDER: 2.	352-435	2.5(+11)	0	3875	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{O}(\text{CH}_2)_3\text{CH}_3$ + $\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{O}(\text{CH}_2)_3\text{CH}_3$ ETHYL FREE RADICAL + BUTANE, 1-ETHENOXY- 72 KER/PAR REACTION ORDER: 2.	303-435	2.5(+10)	0	3070	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_4\text{C}=\text{CH} \rightarrow \text{CH}_3((\text{CH}_2)_4\text{C}(\cdot)=\text{CH}\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH}$ ETHYL FREE RADICAL + 1-HEPTYNE 72 KER/PAR REACTION ORDER: 2.	300-455	3.9(+11)	0	4430	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ 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	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}=\text{C}(\text{CH}_3)_2 \rightarrow$ $(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}=\text{C}(\text{CH}_3)_2$ + $(\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}=\text{C}(\text{CH}_3)_2$ ETHYL FREE RADICAL + 2,4-HEXADIENE, 2,5-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.	328-420	6.2(+10)	0	3300	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ 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
$\text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\cdot + \text{CH}_3$ ETHANE 70 BEN/0'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.	300–1000	1.0(+12)	0	7000 0.1 10.
NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS $k_{\text{ref}}$ FOR $\text{HO}_2 + \text{CO} \rightarrow \text{HO} + \text{CO}_2$					
$\text{CH}_3\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{CH}_4$ 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 <sub>3</sub> 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 <sub>3</sub> + METHYL-d <sub>3</sub> 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 <sub>3</sub> + METHYL-d <sub>3</sub> 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 <sub>6</sub> + 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 <sub>6</sub> + METHYL-d <sub>3</sub> FREE RADICAL 72 KON	REACTION ORDER: 2.		4.6(+11)	0	6405
$\text{CH}_2=\text{C=O} + \text{O} \rightarrow \text{products}$ ETHENONE + OXYGEN ATOM 73 HER/HUI	REACTION ORDER: 2.	298	5.3(+11)	-	- 0.7 1.3
$\text{HOOC-COOH} \rightarrow \text{HCOOH} + \text{CO}_2$ ETHANEDIOIC ACID 70 BEN/0'N	REACTION ORDER: 1.	390–420	7.9(+11)	0	15100
$\text{CH}_3\text{C(O)}\cdot \rightarrow \text{CH}_3\cdot + \text{CO}$ ETHYL, 1-OXO-, FREE RADICAL 72 KON	REACTION ORDER: 1.	273–413	1.5(+10)	0	6790±115 0.7 1.4
$\text{CH}_3\text{C(O)}\cdot \rightarrow \text{CH}_3\cdot + \text{CO}$ ETHYL, 1-OXO-, FREE RADICAL 70 BEN/0'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
$\text{CH}_3\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C(O)}\cdot + \text{CH}_4$ ACETALDEHYDE + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	300–525	8.5(+10)	0	3000±250 0.4 1.6
$\text{CH}_3\text{CDO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C(O)}\cdot + \text{CH}_3\text{D}$ 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
cy-CH <sub>2</sub> CH <sub>2</sub> O + O → products OXIRANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	7.0(+ 8)	-	-	0.6 1.5
cy-CH <sub>2</sub> CH <sub>2</sub> O + CH <sub>3</sub> · → cy-CH <sub>2</sub> CH(·)O + CH <sub>4</sub> OXIRANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.5(+11)	0	5435±750	0.5 2.0
HCOOCH <sub>3</sub> + CH <sub>3</sub> · → .COOCH <sub>3</sub> + CH <sub>4</sub> 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
HCOOCH <sub>3</sub> + CH <sub>3</sub> · → HCOOCH <sub>2</sub> · + CH <sub>4</sub> 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
HCOOCH <sub>3</sub> + CH <sub>3</sub> · → .COOCH <sub>3</sub> + HCOOCH <sub>3</sub> · + CH <sub>4</sub> 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
DCOOCH <sub>3</sub> + CH <sub>3</sub> · → .COOCH <sub>3</sub> + CH <sub>3</sub> 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
DCOOCH <sub>3</sub> + CH <sub>3</sub> · → DCOOCH <sub>2</sub> · + CH <sub>4</sub> FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.		1.6(+11)	0	5635±500	0.5 1.5
NOTE: TENTATIVE k VALUE.					
CH <sub>3</sub> COOH → CH <sub>2</sub> =C=O + H <sub>2</sub> O ACETIC ACID 70 BEN/O'N REACTION ORDER: 1.	773-973	8.9(+12)	0	33970	
NOTE: SUSPECT VALUE.					
CH <sub>3</sub> COOD + CH <sub>3</sub> · → .CH <sub>2</sub> COOD + CH <sub>4</sub> ACETIC ACID-d + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-600	1.6(+11)	0	5135±500	0.6 1.4
CH <sub>3</sub> CH <sub>2</sub> O · → CH <sub>3</sub> · + HCHO ETHOXY FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	488-468	2.5(+13)	0	8805	
CH <sub>3</sub> CH <sub>2</sub> OH + O → products ETHANOL + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	8.7(+10)	-	-	0.6 1.5
CH <sub>3</sub> CH <sub>2</sub> OH + CH <sub>3</sub> · → CH <sub>3</sub> CH <sub>2</sub> O · + CH <sub>4</sub> ETHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-625	7.9(+10)	0	4730±500	0.6 1.4
CH <sub>3</sub> CH <sub>2</sub> OH + CH <sub>3</sub> · → CH <sub>3</sub> CH(·)OH + CH <sub>4</sub> ETHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-625	4.0(+11)	0	4900±500	0.6 1.4
CH <sub>3</sub> CH <sub>2</sub> OH + CH <sub>3</sub> · → CH <sub>3</sub> CH <sub>2</sub> O · + CH <sub>3</sub> CH(·)OH + .CH <sub>2</sub> CH <sub>2</sub> OH + CH <sub>4</sub> ETHANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-625	5.1(+11)	0	4900±500	0.6 1.4
CH <sub>3</sub> CD <sub>2</sub> OH + CH <sub>3</sub> · → CH <sub>3</sub> CD(·)OH + CH <sub>3</sub> D ETHAN-1,1-d <sub>2</sub> -OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-550	4.1(+11)	0	5735±500	0.6 1.4
CH <sub>3</sub> CD <sub>2</sub> OH + CH <sub>3</sub> · → CH <sub>3</sub> CD <sub>2</sub> O · + .CH <sub>2</sub> CD <sub>2</sub> OH + CH <sub>4</sub> ETHAN-1,1-d <sub>2</sub> -OL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-550	7.1(+10)	0	4530±500	0.6 1.4
CH <sub>3</sub> CH <sub>2</sub> OD + CD <sub>3</sub> · → CH <sub>3</sub> CH <sub>2</sub> O · + CD <sub>4</sub> ETHANOL-d + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-525	6.2(+10)	0	5135±500	0.5 2.0
CH <sub>3</sub> CH <sub>2</sub> OD + CD <sub>3</sub> · → CH <sub>3</sub> CH(·)OD + .CH <sub>2</sub> CH <sub>2</sub> OD + CD <sub>3</sub> H ETHANOL-d + METHYL-d <sub>3</sub> 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.	350–500	4.2(+11)	0	5000±1000	0.3	3.0
NOTE: TENTATIVE k VALUE.							
$\text{CH}_3\text{CH}_2\text{OOH} \rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{OH}$ HYDROPEROXYDE, ETHYL- 70 BEN/O'N	REACTION ORDER: 1.	553–653	2.2(+15)	0	21640		
NOTE: k PROBABLY RELIABLE.							
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CD}_3\cdot \rightarrow \text{cy-CH}_2\text{CH}(\cdot)\text{S} + \text{CD}_3\text{H}$ THYRANE + MÉTHYL-d <sub>3</sub> 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		
$\text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_3\text{CH}_2\cdot + \cdot\text{SH}$ ETHANETHIOL 70 BEN/O'N	REACTION ORDER: 1.	785–938	6.3(+15)	0	36336		
$\text{CH}_3\text{CH}_2\text{SH} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{S} + \text{CH}_3\text{CH}(\cdot)\text{SH}$ + .CH <sub>2</sub> CH <sub>2</sub> SH + CH <sub>4</sub> ETHANETHIOL + MÉTHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	303	3.5(+ 7)	-	-	0.5	2.0
NOTE: TENTATIVE k VALUE.							
$\text{CH}_3\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{CH}_3$ 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		
$\text{CH}_3\text{CN} + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{CH} + \text{CH}_4$ ACETONITRILE + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	350–600	5.4(+11)	0	5100±500	0.7	1.5
$\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{NH} + \text{CH}_3\text{CH}(\cdot)\text{NH}_2$ + .CH <sub>2</sub> CH <sub>2</sub> NH <sub>2</sub> + CH <sub>4</sub> ETHANAMINE + MÉTHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	350–500	2.9(+11)	0	4200±500	0.5	2.0
$\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{NH} + \text{CH}_4$ ETHANAMINE + MÉTHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	350–500	2.0(+11)	0	4600±500	0.5	2.0
NOTE: TENTATIVE k VALUE.							
$\text{CD}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_4 + \text{CH}_3\text{D} + \text{CD}_3\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CD}_2\text{CH}_2\text{NH}_2$ ETHAN-2,2,2-d <sub>3</sub> -AMINE + MÉTHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	350–500	2.9(+11)	0	4200±500	0.5	2.0
$\text{CD}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\cdot \rightarrow \text{CD}_3\text{CH}_2\text{NH} + \text{CH}_4$ ETHAN-2,2,2-d <sub>3</sub> -AMINE + MÉTHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2.	423	4.0(+ 5)	-	-		
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
$(\text{CH}_3)_2\text{NH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} \cdot + \text{CH}_2\text{NH}(\text{CH}_3) + \text{CH}_4$ METHANAMINE, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	1.6(+11)	0	3500±500	0.5 2.0
$(\text{CH}_3)_2\text{NH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} \cdot + \text{CH}_4$ 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
$(\text{CH}_3)_2\text{ND} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} \cdot + \text{CH}_3\text{D}$ 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
$\text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_3 \cdot + \text{CH}_3\text{N}=\text{N}$ . 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	
$\text{CD}_3\text{N}=\text{NCD}_3 + \text{CD}_3 \rightarrow \text{CD}_2\text{N}=\text{NCD}_3 + \text{CD}_4$ DIAZENE, DI(METHYL-d <sub>3</sub> )-, + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	6.6(+10)	0	4125±500	
$\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{NHCH}_2\text{CH}_2\text{NH}_2$ + $\text{NH}_2\text{CH}(\cdot)\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANEDIAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.8(+11)	0	4200±500	
$\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{NHCH}_2\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANEDIAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	4430±500	
NOTE: TENTATIVE k VALUE.					
$\text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3 \rightarrow \text{ND}_2\text{CH}(\cdot)\text{CH}_2\text{ND}_2 + \text{CH}_4$ ETHANDI(AMINE-d <sub>2</sub> ) + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.2(+11)	0	5100±500	
NOTE: TENTATIVE k VALUE.					
$\text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3 \rightarrow \text{ND}_2\text{CH}(\cdot)\text{CH}_2\text{ND}_2 + \text{CH}_4$ ETHANDI(AMINE-d <sub>2</sub> ) + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	4025±500	
$(\text{CH}_3)_2\text{NNH}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NNH} \cdot + \text{CH}_4$ 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	
$(\text{CH}_3)_2\text{NND}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NND} \cdot + \text{CH}_3\text{D}$ HYDRAZINE-d <sub>2</sub> , 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 <sub>2</sub> , 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.2(+11)	0	4125±750	
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\text{NNHCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{N}(\cdot)\text{NHCH}_3 + \text{CH}_2\text{NNHCH}_3 + \text{CH}_4$ HYDRAZINE, 1,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.5(+11)	0	2400±250	
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
$\text{CH}_3\text{NDNDCH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{N}(\cdot)\text{NDCH}_3 + \text{CH}_3\text{D}$ HYDRAZINE-d <sub>2</sub> , 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	
$\text{HCONHCH}_3 + \text{CH}_3 \cdot \rightarrow \text{CONHCH}_3 + \text{HCON}(\cdot)\text{CH}_3$ + HCONHCH <sub>2</sub> · + CH <sub>4</sub> FORMAMIDE, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–600	7.9(+10)	0	3800±500	
$\text{CH}_3\text{CONH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CONH} \cdot + \text{CH}_2\text{CONH}_2 + \text{CH}_4$ ACETAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–600	2.1(+11)	0	5235±500	
$\text{CH}_3\text{CONH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_2\text{CONH}_2 + \text{CH}_4$ ACETAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–600	1.0(+11)	0	5200±500	
$\text{CD}_3\text{CONH}_2 + \text{CD}_3 \cdot \rightarrow \text{CD}_2\text{CONH}_2 + \text{CD}_4$ ACETAMIDE-2,2,2-d <sub>3</sub> + METHYL-d <sub>3</sub> 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 <sub>3</sub> + METHYL-d <sub>3</sub> 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
$\text{CH}_3\text{C}\equiv\text{CH} + \text{H} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{C}(\cdot)=\text{CH}_2$ 1-PROPYNE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	298	2.5(+11)	-	-	
NOTE: k TAKEN AS LOWER LIMIT.					
$\text{CH}_3\text{C}\equiv\text{CH} + \text{S} \rightarrow \text{cy-CH}_3\text{C}-\text{CHS}$ 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.	435	-	-	-	
NOTE: k <sub>ref</sub> : CHCH + 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
$\text{CH}_3\text{C}\equiv\text{CH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}\equiv\text{CH}_2 + \text{CH}_3\text{C}(\cdot)=\text{CHCH}_3$ 1-PROPYNE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. $\text{CH}_3$ ADDITION OCCURS PREDOMINANTLY AT TERMINAL C ATOM.	379-465	5.0(+11)	0	4400	
$\text{CH}_3\text{C}\equiv\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\cdot)\text{CH}_3$ 1-PROPYNE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.	360-439	1.9(+9)	0	2870	
$\text{CH}_3\text{C}\equiv\text{CH} + (\text{CH}_3)_2\text{C} \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2$ + $(\text{CH}_3)_3\text{CCH}=\text{C}(\cdot)\text{CH}_3$ 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	
$\text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	373-483	2.0(+11)	0	4100	
$\text{CH}_3=\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	379-465	3.2(+11)	0	4630	
$\text{CH}_2=\text{C}=\text{CH}_2 + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)=\text{CH}_2$ 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	
$\text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{H}$ 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
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2$ 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	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{OH} + \text{CH}_3\text{CH(OH)}\text{CH}_2$ 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. $k/k_{ref}$ : 6.9 NOTE: $k_{ref}$ : $\text{CH}_2=\text{CH}_2 + \text{S}$	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. $k/k_{ref}$ : 1.7 NOTE: $k_{ref}$ : $\text{CH}_2=\text{CH}_2 + \text{S}^*(^1\text{D})$	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. $k/k_{\text{ref}}$ : 2.8 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{N}$	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. $k/k_{\text{ref}}$ : 1.27 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$	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. $k/k_{\text{ref}}$ : 1.0 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$	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	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow [\text{C}_3\text{H}_5] + \text{CH}_4$ 1-PROPENE + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	350-580	3.2(+10)	0	3775±300	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2$ 1-PROPENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	353-453	1.7(+11)	0	3770	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2$ 1-PROPENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.72 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$	453	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CCO} \rightarrow \text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}$ 1-PROPENE + CARBON OXIDE( $\text{C}_2\ddot{\text{O}}$ ) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 5.7 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	297	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2 \cdot$ + $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ 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	9100	
$\text{CH}_3\text{CH}_2\text{CH}_2 \cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ 1-PROPYL FREE RADICAL + ETHÈNE 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	
$\text{CH}_3\text{CH}_2\text{CH}_2 \cdot + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ 1-PROPYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	4370	
$\text{CH}_3\text{CH}_2\text{CH}_2 \cdot + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ 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
$\text{CH}_3\text{CH}_2\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ 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	
$(\text{CH}_3)_2\text{CD}\cdot \rightarrow \text{CH}_3\text{CD}=\text{CH}_2 + \text{H}$ ETHYL-1-d, 1-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	673-777	2.00(+14)	0	20800	
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}=\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{CH}$ ETHYL, 1-METHYL, FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2.	363-577	5.0(+10)	0	3475	
NOTE: TENTATIVE k VALUE.					
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ 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.	360-439	1.90(+9)	0	2870	
NOTE: SUSPECT k VALUE.					
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)=\text{CH}_2$ ETHYL, 1-METHYL-, FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2.	366-473	3.6(+10)	0	3600	
NOTE: TENTATIVE k VALUE.					
$(\text{CH}_3)_2\text{CH}\cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ ETHYL, 1-METHYL-, FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	3480	
$(\text{CH}_3)_2\text{CH}\cdot + \text{cis}-\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}[\text{CH}(\text{CH}_3)_2]\text{CH}(\cdot)\text{CH}_3$ ETHYL, 1-METHYL-, FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2.	298	-	-	3950	
$(\text{CH}_3)_2\text{CH}\cdot + \text{trans}-\text{CH}_3\text{CH}=\text{CHCH} \rightarrow \text{CH}_3\text{CH}[\text{CH}(\text{CH}_3)_2]\text{CH}(\cdot)\text{CH}_3$ 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.	300-1000	2.0(+11)	0	5300	
NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS $k_{ref}$ FOR $\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$					
$\text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CH}\cdot + \text{CH}_4$ 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 <sub>2</sub> + METHYL-d <sub>3</sub> 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 <sub>2</sub> + METHYL-d <sub>3</sub> 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
$\text{CH}_3\text{COCH}_2 \cdot \rightarrow \text{CH}_3 \cdot + \text{CH}_2=\text{C=O}$ PROPYL, 2-OXO-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	365–435	3.2(+12)	0	20130	
$\text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{C(O)} \cdot + \text{CH}_4$ PROPANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350–500	1.0(+11)	0	2970±500	
$(\text{CH}_3)_2\text{CO} \rightarrow \text{CH}_3\text{C(O)} \cdot + \text{CH}_3$ 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	
$(\text{CD}_3)_2\text{CO} + \text{CD}_3 \cdot \rightarrow \text{CD}_3\text{COCD}_2 \cdot + \text{CD}_4$ 2-PROPANONE-1,1,1,3,3-d <sub>6</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–800	4.8(+11)	0	5735±250	
$\text{CH}_2=\text{CHCH}_2\text{OH} + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{OH}$ + .CH <sub>2</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )CH <sub>2</sub> 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	
$\text{HCOOCH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{COOCH}_2\text{CH}_2 \cdot + \text{HCOOCH}(\cdot)\text{CH}_3 + \text{CH}_4$ 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	
$\text{CH}_3\text{COOCH}_3 + \text{CH}_3 \cdot \rightarrow .\text{CH}_2\text{COOCH}_3 + \text{CH}_3\text{COOCH}_2 \cdot + \text{CH}_4$ ACETIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350–600	2.1(+11)	0	5035±500	
$\text{CH}_3\text{COOCd}_3 + \text{CH}_3 \cdot \rightarrow .\text{CH}_2\text{COOCd}_3 + \text{CH}_4$ ACETIC ACID METHYL-d <sub>3</sub> 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 <sub>3</sub> ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–600	1.7(+11)	0	5990±500	
$\text{CH}_3\text{OCOOCH}_3 + \text{CH}_3 \cdot \rightarrow .\text{CH}_2\text{OCOOCH}_3 + \text{CH}_4$ 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	
$(\text{CH}_3)_2\text{CHOD} + \text{CD}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OD} + .\text{CH}_2\text{CH}(\text{CH}_3)\text{OD} + \text{CD}_3\text{H}$ 2-PROPAN-d + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400–525	1.5(+11)	0	3975±500	
$(\text{CH}_3)_2\text{CHOH} \rightarrow (\text{CH}_3)_2\text{CHO} \cdot + \text{OH}$ 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
cy-CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> S + CH <sub>3</sub> → cy-CH <sub>2</sub> CH(.)CH <sub>2</sub> S + CH <sub>4</sub> THIETANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	300-450	3.2(+11)	0	4630±750	
(CH <sub>3</sub> ) <sub>2</sub> CHSH + CH <sub>3</sub> . → (CH <sub>3</sub> ) <sub>2</sub> CHS. + (CH <sub>3</sub> ) <sub>2</sub> C(.)SH + .CH <sub>2</sub> CH(CH <sub>3</sub> )SH + CH <sub>4</sub> 2-PROPANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	303	4.1(+ 7)	-	-	
CH <sub>2</sub> =CHCN + CH <sub>3</sub> CH <sub>2</sub> . → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(.)CN + .CH <sub>2</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )CN 2-PROPENENITRILE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	323-454	6.2(+10)	0	1700	
CH <sub>3</sub> CH <sub>2</sub> CN → CH <sub>3</sub> . + .CH <sub>2</sub> CN PROPANENITRILE 70 BEN/O'N REACTION ORDER: 1.	958-1038	1.3(+14)	0	36600	
CH <sub>3</sub> CH <sub>2</sub> CN + CD <sub>3</sub> . → CH <sub>3</sub> CH(.)CN + .CH <sub>2</sub> CH <sub>2</sub> CN + CD <sub>3</sub> H PROPANENITRILE + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	3.6(+11)-	0	4330±500	
(CH <sub>3</sub> ) <sub>3</sub> N + CH <sub>3</sub> . → .CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>4</sub> METHANAMINE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	4.7(+11)	0	4600±500	
O <sub>2</sub> NOCH <sub>2</sub> CH(ONO <sub>2</sub> )CH <sub>2</sub> ONO <sub>2</sub> → products 1,2,3-PROPANETRIOL, TRINITRATE 70 BEN/O'N REACTION ORDER: 1.	348-378	1.3(+17)	0	20300	
O <sub>2</sub> NOCH <sub>2</sub> CH(ONO <sub>2</sub> )CH <sub>3</sub> → products 1,2-PROPANEDIOL, DINITRATE 70 BEN/O'N REACTION ORDER: 1.	353-373	1.6(+15)	0	18800	
O <sub>2</sub> NOCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ONO <sub>2</sub> → products 1,3-PROPANEDIOL, DINITRATE 70 BEN/O'N REACTION ORDER: 1.	358-383	1.6(+15)	0	19175	
HCON(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> . → CON(CH <sub>3</sub> ) <sub>2</sub> + HCO-(CH <sub>3</sub> )NCH <sub>3</sub> . + CH <sub>4</sub> 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	
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> NO <sub>2</sub> → CH <sub>3</sub> CH=CH <sub>2</sub> + HONO PROPANE, 1-NITRO- 70 BEN/O'N REACTION ORDER: 1.	687-733	2.50(+13)	0	24005	
CH <sub>3</sub> CH(NO <sub>2</sub> )CH <sub>3</sub> → CH <sub>3</sub> CH=CH <sub>2</sub> + HONO PROPANE, 2-NITRO- 70 BEN/O'N REACTION ORDER: 1.	800-1000	2.0(+11)	0	20130	
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> ONO → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> O. + NO NITROUS ACID PROPYL ESTER 70 BEN/O'N REACTION ORDER: 1.	443-483	1.6(+16)	0	20230	
(CH <sub>3</sub> ) <sub>2</sub> CHONO → (CH <sub>3</sub> ) <sub>2</sub> CHO. + NO NITROUS ACID 1-METHYL ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	443-483	3.2(+16)	0	18600	
CH≡CC≡CH + O → products 1,3-BUTADIYNE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	300	9.0(+11)	-	-	0.7 1.4
CH <sub>3</sub> CH <sub>2</sub> C≡CH + N → products 1-BUTYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 13.0	320-550 435	3.5(+11) -	0 -	1125 -	
NOTE: k <sub>ref</sub> : 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	
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{S} \rightarrow \text{cy-(CH}_3\text{)C=C(CH}_3\text{)S}$ 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 <sub>ref</sub> : 12.0 NOTE: k <sub>ref</sub> : CH≡CH + N	320-550 435	1.9(+11)	0	926	
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}\equiv\text{CH}_2\cdot + \text{CH}_4$ 2-BUTYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	486-619	1.1(+12)	0	4900±500	
$\text{CH}_3\text{C}\equiv\text{CCH}_3 + \text{CCO} \rightarrow \text{products}$ 2-BUTYNE + CARBON OXIDE(C <sub>2</sub> O) 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 8.5 NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CCO	304	-	-	-	
$\text{CH}_2=\text{CHCH=CH}_2 + \text{O} \rightarrow \text{products}$ 1,3-BUTADIENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-400	3.4(+12)	0	- 380	0.7 1.3
$\text{CH}_2=\text{CHCH=CH}_2 + \text{H} \rightarrow \text{CH}_2=\text{CHCH}(\cdot)\text{CH}_3 + \text{CH}_2=\text{CHCH}_2\text{CH}_2$ 1,3-BUTADIENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGED k. k/k <sub>ref</sub> : 4.9 NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H	298 300	4.10(+13)	0	655	
$\text{CH}_2=\text{CHCH=CH}_2 + \text{S} \rightarrow \text{cy-(CH}_2=\text{CH)CHCH}_2\text{S}$ 1,3-BUTADIENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	6.0(+13)	-	-	
$\text{CH}_2=\text{CHCH=CH}_2 + \text{N} \rightarrow \text{products}$ 1,3-BUTADIENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2.	340	3.5(+10)	-	-	
$\text{CH}_2=\text{CHCH=CH}_2 + ^1\text{CH}_2 \rightarrow \text{products}$ 1,3-BUTADIENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.2 NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + <sup>1</sup> CH <sub>2</sub> ASSUMING 10% <sup>3</sup> CH <sub>2</sub>	297	-	-	-	
$\text{CH}_2=\text{CHCH=CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH=CH}_2$ 1,3-BUTADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	353-453	8.1(+10)	0	2065	
$\text{CH}_2=\text{CHCH=CH}_2 + \text{CH}_3\cdot + \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH=CH}_2$ 1,3-BUTADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 12.0 NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CH <sub>3</sub> .	435	-	-	-	
$\text{CH}_2=\text{CHCH=CH}_2 + \text{CCO} \rightarrow \text{CH}_2=\text{C=CHCH=CH}_2 + \text{CO}$ 1,3-BUTADIENE + CARBON OXIDE(C <sub>2</sub> O) 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 210. NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CCO	298	-	-	-	
$\text{CH}_3\text{CH}_2\text{CH=CH}_2 + \text{O} \rightarrow \text{cy-(CH}_3\text{CH}_2\text{)CHCH}_2\text{O}$ 1-BUTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	2.3(+12)	-	-	0.8 1.2
$\text{CH}_3\text{CH}_2\text{CH=CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ 1-BUTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.03 NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H	298 300	8.7(+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
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ . 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)	-	-	
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy-(CH}_3\text{CH}_2\text{)CHCH}_2\text{S}$ . 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: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + {}^3\text{CH}_2 \cdot \rightarrow \text{products}$ . 1-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.6$	297	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}=\text{CH}_2 + \text{CH}_4$ . 1-BUTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	350-650	2.5(+11)	0	4200±500	0.6 1.4
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ . + $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ . 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: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CH}_3$ .					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}=\text{CH}_2 + \text{CO}$ . 1-BUTENE + CARBON OXIDE ( $\text{CO}$ ) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 7.0$	298	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CO}$					
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ . 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.	900-1051	1.00(+16)	0	36900	
NOTE: k ESTIMATED.					
$\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{S} \cdot \rightarrow \text{CH}_3\text{CH}(\text{SCH}_3)\text{CH}(\cdot)\text{CH}_3$ . 2-BUTENE + METHYLIOTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298-333	1.6(+ 9)	-	-	
NOTE: cis-trans EQUILIBRIUM - WEIGHTED k.					

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
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> cis-2-BUTENE 70 BEN/0'N REACTION ORDER: 1.	686-742	6.00(+13)	0	31600	
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + O → products cis-2-BUTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	250-500	5.9(+12)	0	- 165	0.8 1.2
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + H → CH <sub>3</sub> CH <sub>2</sub> CH(.)CH <sub>3</sub> cis-2-BUTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION. k/k <sub>ref</sub> : 0.47	208 300	4.6(+11) -	-	-	
NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + S → cy-(CH <sub>3</sub> CH)CH(CH <sub>3</sub> )S cis-2-BUTENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 16.0	298 298	1.4(+13) -	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + S					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + N → products cis-2-BUTENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 2.4	320-550 435	2.3(+11) -	0	995	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + N					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + <sup>1</sup> CH <sub>2</sub> : → products cis-2-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.37	297	-	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + <sup>1</sup> CH <sub>2</sub>					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + <sup>3</sup> CH <sub>2</sub> : → products cis-2-BUTENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.94	297	-	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + <sup>3</sup> CH <sub>2</sub>					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> . → CH <sub>3</sub> CH=CHCH <sub>2</sub> . + CH <sub>4</sub> cis-2-BUTENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-650	1.8(+11)	0	4100±500	
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> . → (CH <sub>3</sub> ) <sub>2</sub> CHCH(.)CH <sub>3</sub> cis-2-BUTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.2	353-453 453	4.5(+10)	0	3675	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CH <sub>3</sub> .					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + CCO → cis-CH <sub>3</sub> CH=C=CHCH <sub>3</sub> + CO cis-2-BUTENE + CARBON OXIDE(C <sub>2</sub> O) 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 9.1	297	-	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CCO					
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> . → CH <sub>3</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )CH(.)CH <sub>3</sub> cis-2-BUTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4265	
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> . → CH <sub>3</sub> CH(CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> )CH(.)CH <sub>3</sub> cis-2-BUTENE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4370	
cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> + (CH <sub>3</sub> ) <sub>2</sub> CH. → CH <sub>3</sub> CH[CH(CH <sub>3</sub> ) <sub>2</sub> ]CH(.)CH <sub>3</sub> cis-2-BUTENE + ETHYL-, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3950	
trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> + O → products trans-2-BUTENE + 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
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $\text{trans-2-BUTENE} + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. NOTE: AVERAGE k. k/k <sub>ref</sub> : 0.59	298	5.6(+11)	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_3\text{CH=CH}_2 + \text{H}$	300	-	-	-	
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{S} \rightarrow \text{cy-(CH}_3\text{CH)}\text{CH(CH}_3\text{)S}$ $\text{trans-2-BUTENE} + \text{SULFUR ATOM}$ 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 20.0	298	1.4(+13)	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + \text{S}$	298	-	-	-	
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{N} \rightarrow \text{products}$ $\text{trans-2-BUTENE} + \text{NITROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.0	320-550	3.4(+11)	0	1055	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + \text{N}$	435	-	-	-	
$\text{trans-CH}_3\text{CH=CHCH}_3 + {}^1\text{CH}_2 \rightarrow \text{products}$ $\text{trans-2-BUTENE} + \text{METHYLENE FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.39	297	-	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$					
$\text{trans-CH}_3\text{CH=CHCH}_3 + {}^3\text{CH}_2 \rightarrow \text{products}$ $\text{trans-2-BUTENE} + \text{METHYLENE FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.89	297	-	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$					
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH=CHCH}_2\cdot + \text{CH}_4$ $\text{trans-2-BUTENE} + \text{METHYL FREE RADICAL}$ 76 KER/PAR REACTION ORDER: 2.	350-500	1.0(+12)	0	4830±500	
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ $\text{trans-2-BUTENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	353-453	1.4(+11)	0	4075	
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ $\text{trans-2-BUTENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.4	453	-	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$					
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{CO} \rightarrow \text{CH}_3\text{CH=C=CHCH}_3 + \text{CO}$ $\text{trans-2-BUTENE} + \text{CARBON OXIDE(C}_2\text{O)}$ 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 10.6	297	-	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + \text{CO}$					
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{trans-2-BUTENE} + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4350	
$\text{trans-CH}_3\text{CH=CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow$ $\text{CH}_3\text{CH}(\text{CH}_2\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{trans-2-BUTENE} + \text{PROPYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4515	
$\text{trans-CH}_3\text{CH=CHCH}_3 + (\text{CH}_3)_2\text{CH}\cdot \rightarrow \text{CH}_3\text{CH}[\text{CH}(\text{CH}_3)_2]\text{CH}(\cdot)\text{CH}_3$ $\text{trans-2-BUTENE} + \text{ETHYL, 1-METHYL-, FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	4065	
$(\text{CH}_3)_2\text{C=CH}_2 \rightarrow \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{H}$ 1-PROPENE, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	930-1082	1.0(+17)	0	44400	
$(\text{CH}_3)_2\text{C=CH}_2 + \text{O} \rightarrow \text{cy-[}(\text{CH}_3)_2\text{]CCH}_2\text{O}$ 1-PROPENE, 2-METHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	1.2(+13)	-	-	0.7 1.3
$(\text{CH}_3)_2\text{C=CH}_2 + \text{H} \rightarrow (\text{CH}_3)_3\text{C}$ 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
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHCH}_2$ . 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)	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_2\text{CHCH}_2$ . 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 2.52 NOTE: $k_{\text{ref}}$ : $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$	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. $k/k_{\text{ref}}$ : 50.0 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{S}$	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. $k/k_{\text{ref}}$ : 3.5 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{S}^*(^1\text{D})$	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. $k/k_{\text{ref}}$ : 4.1 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{N}$	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. $k/k_{\text{ref}}$ : 1.96 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$	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. $k/k_{\text{ref}}$ : 2.86 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$	297	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_4$ . 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. $k/k_{\text{ref}}$ : 1.1 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$	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( $\text{C}_2\text{O}$ ) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 50.0 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{CCO}$	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	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2$ . 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
$\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2$ . + $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ PROPYL, 1-METHYL-, FREE RADICAL + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	381-412	6.3(+10)	0	3725	
$(\text{CH}_3)_2\text{CHCH}_2 \rightarrow \text{CH}_3 \cdot + \text{CH}_3\text{CH}=\text{CH}_2$ PROPYL, 2-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	299-691	1.6(+14)	0	16455	
$(\text{CH}_3)_2\text{CHCH}_2 \rightarrow (\text{CH}_3)_3\text{C}=\text{CH}_2 + \text{H}$ 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
$(\text{CH}_3)_3\text{C} \cdot + \text{CH}=\text{CH} \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2$ . ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	363-577	1.0(+11)	0	3875	
$(\text{CH}_3)_3\text{C} \cdot + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2$ . ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	300-650	2.8(+10)	0	3575	
$(\text{CH}_3)_3\text{C} \cdot + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 + (\text{CH}_3)_3\text{CCH}=\text{C}(\cdot)\text{CH}_3$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + 1-PROPYNE 72 KER/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.	360-439	5.0(+8)	0	2770	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2$ . BUTANE 70 BEN/O'N REACTION ORDER: 1. NOTE: k ESTIMATED.	693-803	4.0(+17)	0	43230	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{CH}_2$ . 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 <sub>4</sub> + METHYL-d <sub>3</sub> 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
$\text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 + \text{CD}_3 \rightarrow \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_2\cdot + \text{CD}_3\text{H}$ BUTANE-2,2,3,3-d <sub>4</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	600-750	4.8(+11)	0	5735±250	0.7	1.3
$(\text{CH}_3)_3\text{CH} + \text{H} \rightarrow (\text{CH}_3)_3\text{C}\cdot + (\text{CH}_3)_2\text{CHCH}_2\cdot + \text{H}_2$ PROPANE, 2-METHYL-, + HYDROGEN ATOM 72 KON REACTION ORDER: 2.	300-800	1.9(+13)	0	2680±85	0.8	1.2
$(\text{CH}_3)_3\text{CH} + \text{HO}_2 \rightarrow (\text{CH}_3)_3\text{C}\cdot + \text{H}_2\text{O}_2$ PROPANE, 2-METHYL-, + HYDROPEROXYL FREE RADICAL 74 LLO REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k <sub>ref</sub> 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.
$(\text{CH}_3)_3\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{C}\cdot + \text{CH}_4$ PROPANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	9.6(+10)	0	3975±250	0.7	1.3
$(\text{CH}_3)_3\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{C}\cdot + (\text{CH}_3)_2\text{CHCH}_2\cdot + \text{CH}_4$ PROPANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	8.3(+10)	0	4000±500	0.5	2.0
$(\text{CH}_3)_3\text{CD} + \text{CD}_3 \rightarrow (\text{CH}_3)_3\text{C}\cdot + \text{CD}_4$ PROPANE-2-d, 2-METHYL, + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	1.2(+11)	0	4800±250	0.7	1.3
$(\text{CH}_3)_3\text{CD} + \text{CD}_3 \rightarrow (\text{CH}_3)_2\text{CDCH}_2\cdot + \text{CD}_3\text{H}$ PROPANE-2-d, 2-METHYL-, + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	550-750	6.0(+11)	0	5735±250	0.7	1.3
$\text{CH}_3\text{CH}=\text{CHCHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}=\text{CHC}(0)\cdot + \text{CH}_4$ 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		
$\text{CH}_3\text{COOCH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{COOCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + CH <sub>3</sub> COOCH(CH <sub>2</sub> CH <sub>3</sub> )CH <sub>2</sub> ACETIC ACID ETHENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	303-417	7.8(+10)	0	3475		
$\text{CH}_3\text{COCOCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{COCOCH}_2\cdot + \text{CH}_4$ 2,3-BUTANEDIONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-800	2.2(+11)	0	4300±500	0.5	1.5
$\text{CH}_3\text{COCOCH}_3 \rightarrow \text{CH}_3\text{C}(0)\cdot + \text{CH}_3\text{C}(0)\cdot$ 2,3-BUTANEDIONE 70 BEN/O'N REACTION ORDER: 1.	626-698	1.6(+16)	0	33970		
$(\text{CH}_3\text{CO})_2\text{O} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}=0$ ACETIC ACID ANHYDRIDE 70 BEN/O'N REACTION ORDER: 1.	553-646	1.0(+12)	0	17365		
$(\text{CH}_3\text{CO})_2\text{O} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{COOCOCH}_2\cdot + \text{CH}_4$ ACETIC ACID ANHYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300-500	1.8(+11)	0	4830±500	0.6	1.4
$\text{CH}_3\text{C}(0)\text{OOC}(0)\text{CH}_3 \rightarrow \text{CH}_3\text{C}(0)\text{O} + \text{CH}_3\text{C}(0)\text{O}$ PEROXIDE, DIACETYL 70 BEN/O'N REACTION ORDER: 1.	363-463	1.8(+14)	0	14845		
$\text{CH}_3\text{CH}_2\text{COCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{COCH}_3 + \text{CH}_2\text{CH}_2\text{COCH}_3$ + CH <sub>3</sub> CH <sub>2</sub> COCH <sub>2</sub> <sub>·</sub> + CH <sub>4</sub> 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
HCOOCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> . → COOCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>4</sub> FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	347-455	1.3(+10)	0	3675	
HCOOCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> . → COOCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + HCOOCH(.)CH <sub>2</sub> CH <sub>3</sub> + HCOOCH <sub>2</sub> CH(.)CH <sub>3</sub> + HCOOCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> . + CH <sub>4</sub> 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
HCOOCH(CH <sub>3</sub> ) <sub>2</sub> → HCOOH + CH <sub>3</sub> CH=CH <sub>2</sub> FORMIC ACID 1-METHYLETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	721-811	4.0(+12)	0	22145	
HCOOCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> . → COOCH(CH <sub>3</sub> ) <sub>2</sub> + HCOOC(.)CH <sub>3</sub> ) <sub>2</sub> + HCOOCH(CH <sub>3</sub> )CH <sub>2</sub> . + CH <sub>4</sub> 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
CH <sub>3</sub> COOCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> COOH + CH <sub>2</sub> =CH <sub>2</sub> ACETIC ACID ETHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	725-883	3.9(+12)	0	24155	
CH <sub>3</sub> OOCCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> OH + CO <sub>2</sub> + CH <sub>2</sub> =CH <sub>2</sub> CARBONIC ACID ETHYL METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	573-648	4.0(+12)	0	21640	
CH <sub>3</sub> CH(.)OCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CHO + CH <sub>3</sub> CH <sub>2</sub> . ETHYL, 1-ETHOXO-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. NOTE: logA PROBABLY LOW.	418-453	8.1(+10)	0	11825	
CH <sub>3</sub> CH(O.)CH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CHO + CH <sub>3</sub> CH <sub>2</sub> . ETHOXO, 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	
(CH <sub>3</sub> ) <sub>3</sub> CO. → (CH <sub>3</sub> ) <sub>2</sub> CO + CH <sub>3</sub> . ETHOXO, 1,1-DIMETHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1. NOTE: TENTATIVE k.	393-453	3.2(+13)	0	8300	
(CH <sub>3</sub> ) <sub>3</sub> COH → (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> + H <sub>2</sub> O 2-PROPANOL, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	1050-1300	2.5(+13)	0	31001	
CH <sub>3</sub> CH <sub>2</sub> OCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> . + CH <sub>3</sub> CH <sub>2</sub> O. ETHANE, 1,1'-OXYBIS- 70 BEN/O'N REACTION ORDER: 1. NOTE: k PROBABLY RELIABLE.	833-913	1.0(+18)	0	42275	
CH <sub>3</sub> CH <sub>2</sub> OCH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> . → CH <sub>3</sub> CH <sub>2</sub> OCH(.)CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> OCH <sub>2</sub> CH <sub>2</sub> . + CH <sub>4</sub> 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
CH <sub>3</sub> CH <sub>2</sub> OOCCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> O. + CH <sub>3</sub> CH <sub>2</sub> O. PEROXIDE, DIETHYL 70 BEN/O'N REACTION ORDER: 1.	413-518	4.0(+15)	0	18770	
(CH <sub>3</sub> ) <sub>3</sub> COOH → (CH <sub>3</sub> ) <sub>3</sub> CO. + OH HYDROPEROXIDE, 1,1-DIMETHYLETHYL 70 BEN/O'N REACTION ORDER: 1.	553-653	4.0(+15)	0	21640	
(CH <sub>3</sub> ) <sub>3</sub> CSH → (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> + H <sub>2</sub> S 2-PROPANETHIOL, 2-METHYL- 70 BEN/O'N REACTION ORDER: 1.	950-1230	2.5(+13)	0	27830	
(CH <sub>3</sub> ) <sub>3</sub> CSH + CH <sub>3</sub> . → (CH <sub>3</sub> ) <sub>3</sub> CS. + .CH <sub>2</sub> C(CH <sub>3</sub> ) <sub>2</sub> SH + CH <sub>4</sub> 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
$\text{CH}_2=\text{CHCH}_2\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\cdot + \text{CH}_3\text{SO}_2$ . 1-PROPENE, 3-METHYLSULFONYL- 70 BEN/0'N REACTION ORDER: 1.	633-733	1.3(+14)	0	24006	
$\text{cis}-\text{CH}_3\text{CH}=\text{CHCN} \rightarrow \text{trans}-\text{CH}_3\text{CH}=\text{CHCN}$ $\text{cis}-2\text{-BUTENENITRILE}$ 70 BEN/0'N REACTION ORDER: 1.	573-633	5.0(+12)	0	28030	
$\text{cis}-\text{CH}_3\text{CH}=\text{CHCN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ + $\text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ $\text{cis}-2\text{-BUTENENITRILE} + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	323-454	1.5(+10)	0	2500	
$\text{trans}-\text{CH}_3\text{CH}=\text{CHCN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ + $\text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ $\text{trans}-2\text{-BUTENENITRILE} + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	323-754	3.1(+10)	0	2600	
$\text{CH}_2=\text{C}(\text{CH}_3)\text{CN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CN}$ + $\text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CN}$ $2\text{-PROPENENITRILE}, 2\text{-METHYL-}, + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	312-400	2.5(+11)	0	2300	
$\text{CH}_3\text{CH}=\text{NN}=\text{CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\cdot)=\text{NN}=\text{CHCH}_3$ + $\text{CH}_3\text{CH}=\text{NN}=\text{CHCH}_3 + \text{CH}_4$ $\text{ACETALDEHYDE ETHYLIDENEHYDRAZONE} + \text{METHYL FREE RADICAL}$ 76 KER/PAR REACTION ORDER: 2.	350-600	2.5(+11)	0	3975±500	0.5 2.0
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{N}=\text{N} + \text{CH}_3\text{CH}_2$ . DIAZENE, DIETHYL- 70 BEN/0'N REACTION ORDER 1.		2.0(+16)	0	25165	
$\text{CH}_3\text{N}=\text{NCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{N}=\text{N} + (\text{CH}_3)_2\text{CH}$ . DIAZENE, METHYL(1-METHYLETHYL)- 70 BEN/0'N REACTION ORDER 1.	543-605	2.5(+16)	0	23900	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}$ . + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{NH}_2$ $1\text{-BUTANAMINE} + \text{METHYL FREE RADICAL}$ 76 KER/PAR REACTION ORDER: 2.	426	3.2(+7)	-	-	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$(\text{CH}_3\text{CH}_2)_2\text{NH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3\text{CH}_2)_2\text{N} + \text{CH}_3\text{CH}(\cdot)\text{NHCH}_2\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{NHCH}_2\text{CH}_3 + \text{CH}_4$ $\text{ETHANAMINE}, \text{N-ETHYL-}, + \text{METHYL FREE RADICAL}$ 76 KER/PAR REACTION ORDER: 2.	350-500	2.2(+11)	0	3550±500	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_3)_2 + \text{CH}_2\text{CH}_2\text{N}(\text{CH}_3)_2$ + $\text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)\text{CH}_2\cdot + \text{CH}_4$ $\text{ETHANAMINE}, \text{N,N-DIMETHYL-}, + \text{METHYL FREE RADICAL}$ 76 KER/PAR REACTION ORDER: 2.	420	2.6(+7)	-	-	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$(\text{CH}_3)_2\text{NN}=\text{NN}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{NN}=\text{N} + (\text{CH}_3)_2\text{N}$ . 2-TETRAZENE, 1,1,4,4-TETRAMETHYL- 70 BEN/0'N REACTION ORDER: 1.	466-539	2.5(+14)	0	18170	
$\text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CHO} + \text{CH}_2=\text{CH}_2$ . ETHENE, ETHOXY- 70 BEN/0'N REACTION ORDER: 1.	640-859	4.0(+11)	0	22345	
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HCHO}$ . 3-BUTEN-1-OL 70 BEN/0'N REACTION ORDER: 1.	643-685	4.5(+11)	0	20635	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\cdot + \text{CH}_4$ $\text{BUTANAL} + \text{METHYL FREE RADICAL}$ 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
$(\text{CH}_3)_2\text{CHCHO} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHC(O)} + \text{CH}_4$ PRÖPANAL, 2-MÉTHYL-, + MÉTHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-500	1.0(+11)	0	2970±500	0.4 1.6
$\text{CH}_3\text{CON}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2 + \text{CH}_4$ 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
$\text{CH}_3\text{CON}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \text{CH}_2\text{CON}(\text{CH}_3)_2$ + $\text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2 + \text{CH}_4$ 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
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} + \text{NO}$ 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 <sub>ref</sub> : 14.0	320-550 435	3.0(+11) -	0 -	1047	
NOTE: k <sub>ref</sub> : CHCH + N					
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{O} \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2)\text{CHCH}_2\text{O}$ 1-PENTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	2.8(+12)	-	-	0.7 1.3
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_2$ 1-PENTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.89	298 300	8.3(+11) -	-	-	
NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H					
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3(\text{CH}_2)_2)\text{CHCH}_2\text{S}$ 1-PENTENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	8.1(+12)	-	-	
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2 + \text{CH}_4$ 1-PENTENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	450-650	4.5(+11)	0	4500±500	0.6 1.4
$\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{CHCH}_2\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)\text{CH}_2(\text{CH}_2)_2\text{CH}_3$ 1-PENTENE + PROPYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3410	
cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + O → products cis-2-PENTENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	1.1(+13)	-	-	0.7 1.3
cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + H → CH <sub>3</sub> CH <sub>2</sub> CH(·)CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(·)CH <sub>3</sub> cis-2-PENTENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.39	298 300	3.8(+11) -	-	-	
NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H					
cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> → CH <sub>2</sub> CH <sub>2</sub> CH(·)CH(CH <sub>3</sub> ) <sub>2</sub> cis-2-PENTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> → CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(·)CH <sub>3</sub> cis-2-PENTENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4125	
cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )CH(·)CH <sub>3</sub> 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
$\text{trans}-\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $\text{trans}-2\text{-PENTENE} + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.44$ NOTE: $k_{\text{ref}}: \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$	300 298	- 4.1(+11)	- -	- -	
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$ + $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ . $1\text{-BUTENE}, 2\text{-METHYL-}, + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	9.1(+11)	-	-	
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{D} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{D}$ + $\text{CH}_3\text{CH}_2\text{CD}(\text{CH}_3)\text{CH}_2$ . $1\text{-BUTENE}, 2\text{-METHYL-}, + \text{DEUTERIUM ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	2.0(+12)	-	-	
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{S} \rightarrow \text{cy}-[\text{CH}_3\text{CH}_2]\text{C}(\text{CH}_3)\text{CH}_2\text{S}$ $1\text{-BUTENE}, 2\text{-METHYL-}, + \text{SULFUR ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	7.4(+13)	-	-	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ . $1\text{-BUTENE}, 3\text{-METHYL-}, + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	7.4(+11)	-	-	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{D} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{D} + (\text{CH}_3)_2\text{CHCHDCH}_2$ . $1\text{-BUTENE}, 3\text{-METHYL-}, + \text{DEUTERIUM ATOM}$ 72 KER/PAR REACTION ORDER: 2.	298	7.6(+11)	-	-	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_3$ $1\text{-BUTENE}, 3\text{-METHYL-}, + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	3500	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}=\text{CH}_2 + \text{CH}_4$ $1\text{-BUTENE}, 3\text{-METHYL-}, + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	450-600	4.4(+11)	0	4225±750	0.5 1.5
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $1\text{-BUTENE}, 3\text{-METHYL-}, + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2.	298	-	-	3620	
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{O} \rightarrow \text{products}$ $2\text{-BUTENE}, 2\text{-METHYL-}, + \text{OXYGEN ATOM}$ 73 HER/HUI REACTION ORDER: 2.	298-400	3.9(+12)	0	- 680	0.8 1.2
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHC}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ $2\text{-BUTENE}, 2\text{-METHYL-}, + \text{HYDROGEN ATOM}$ 73 HER/HUI REACTION ORDER: 2. $k/k_{\text{ref}}: 1.03$	298 300	9.1(+11) -	- -	- -	
NOTE: $k_{\text{ref}}: \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$					
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{S} \rightarrow \text{cy}-[(\text{CH}_3)_2]\text{CCH}(\text{CH}_3)\text{S}$ $2\text{-BUTENE}, 2\text{-METHYL-}, + \text{SULFUR ATOM}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 56.0$	298 298	6.5(+13) -	- -	- -	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S}$					
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{N} \rightarrow \text{products}$ $2\text{-BUTENE}, 2\text{-METHYL-}, + \text{NITROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 3.5$	320-550 435	9.3(+10) -	0 -	433 -	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{N}$					
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + {}^1\text{CH}_2 \rightarrow \text{products}$ $2\text{-BUTENE}, 2\text{-METHYL-}, + \text{METHYLENE FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 2.12$	297	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$					
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + {}^3\text{CH}_2 \rightarrow \text{products}$ $2\text{-BUTENE}, 2\text{-METHYL-}, + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 1.83$		-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$					

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
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_2$ + . $\text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3 + \text{CH}_4$ 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
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}_3$ + $(\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ 2-BUTENE, 2-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	403-455	1.4(+10)	0	3070	
NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CH}_3$ $k/k_{\text{ref}}: 0.4$	453	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CO} \rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{CO}$ 2-BUTENE, 2-METHYL-, + CARBON OXIDE( $\text{C}_2\text{O}$ ) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 100$ . NOTE: $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CO}$	298	-	-	-	
$(\text{CH}_3)_3\text{CCH}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3$ . PROPYL, 2,2-DIMETHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	762	1.0(+14)	0	18875	
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH}(\text{CH}_2)_3\text{CH}_2$ . BUTYL, 3-METHYL-, FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	340-413	1.2(+10)	0	3235	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{OH}$ PENTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{OH}$ PENTANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	8.0(+13)	0	2320	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{CH}_4$ 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
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4$ 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
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_4$ 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
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3 + \text{CH}_4$ 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
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ . + . $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 + \text{CH}_4$ 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
$(\text{CH}_3)_4\text{C} \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3$ 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	
$\text{cis}-\text{CH}_3\text{CH}=\text{CHCOOCH}_3 \rightarrow \text{trans}-\text{CH}_3\text{CH}=\text{CHCOOCH}_3$ cis-2-BUTENOIC ACID METHYL ESTER 70 BEN/O'N REACTION ORDER: 1.	673–833	1.6(+11)	0	29090	
$\text{trans}-\text{CH}_3\text{CH}=\text{CHCOOCH}_3 \rightarrow \text{cis}-\text{CH}_3\text{CH}=\text{CHCOOCH}_3$ 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-PROPYNYL 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	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(0)\cdot + \text{CH}_4$ 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
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(0)\cdot + \text{CH}_4$ 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
$(\text{CH}_3)_2\text{CHCH}_2\text{CHO} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(0)\cdot + \text{CH}_4$ 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
$(\text{CH}_3)_3\text{CCHO} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{C}(0)\cdot + \text{CH}_4$ 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
$(\text{CH}_3\text{CH}_2)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{COCH}_2\text{CH}_3$ + $\text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3 + \text{CH}_4$ 3-PENTANONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	300–450	1.9(+11)	0	3675±500	0.5 1.5
$(\text{CH}_3\text{CD}_2)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{COCD}_2\text{CH}_2\cdot + \text{CH}_4$ 3-PENTANONE-2,2,4,4-d <sub>4</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	500–600	2.0(+11)	0	5535±500	0.5 2.0
$(\text{CH}_3\text{CD}_2)_2\text{CO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{COCD}(\cdot)\text{CH}_3 + \text{CH}_4$ 3-PENTANONE-2,2,4,4-d <sub>4</sub> + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	500–600	1.3(+11)	0	4200±500	0.5 2.0
$(\text{CH}_3\text{CH}_2)_2\text{CO} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3 + \text{CH}_3\text{CH}_3$ 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
$\text{HC}(\text{OOCCH}_2)_3\text{CH}_3 + \text{CH}_3 \rightarrow \text{COO}(\text{CH}_2)_3\text{CH}_3 + \text{HC}(\text{OOCH})_2\text{CH}_3$ $+ \text{HC}(\text{OOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{HC}(\text{OOCH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{HC}(\text{OOCCH}_2)_3\text{CH}_2 + \text{CH}_4$ <b>FORMIC ACID BUTYL ESTER + METHYL FREE RADICAL</b> <b>76 KER/PAR</b> <b>REACTION ORDER: 2.</b> <b>NOTE: TENTATIVE k VALUE.</b>	350–500	2.5(+11)	0	4980±500	0.5 2.0
$\text{HC}(\text{OOCCH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HCOOH}$ <b>FORMIC ACID 1,1-DIMETHYLETHYL ESTER</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	503–573	7.9(+12)	0	19730	
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ <b>ACETIC ACID PROPYL ESTER</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b> <b>NOTE: RELIABILITY NO BETTER THAN AN ORDER OF MAGNITUDE.</b>	725–810	2.5(+12)	0	24006	
$\text{CH}_3\text{COOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ <b>ACETIC ACID 1-METHYLETHYL ESTER</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	586–801	1.0(+13)	0	22645	
$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{COOH} + \text{CH}_2=\text{CH}_2$ <b>PROPANOIC ACID ETHYL ESTER</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	778–875	5.6(+12)	0	24400	
$\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{COOCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}(\cdot)\text{CH}_3 + \text{CH}_2\text{CH}_2\text{COOCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_2 + \text{CH}_4$ <b>PROPANOIC ACID ETHYL ESTER + METHYL FREE RADICAL</b> <b>76 KER/PAR</b> <b>REACTION ORDER: 2.</b>	300–650	2.5(+11)	0	4125±500	0.5 1.5
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_2=\text{CHOCH}_3 + \text{CH}_3\text{COOH}$ <b>ACETIC ACID (2-METHOXYETHYL) ESTER</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	725–810	1.6(+12)	0	24460	
$\text{CH}_3\text{CH}_2\text{OCOOCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ <b>CARBONIC ACID DIETHYL ESTER</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	573–648	7.9(+12)	0	21800	
$(\text{CH}_3\text{CH}_2)\text{C}(\text{CH}_3)_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $+ \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 + \text{H}_2\text{O}$ <b>2-BUTANOL, 2-METHYL-</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	757–799	3.2(+13)	0	30200	
$(\text{CH}_3)_3\text{CCN} \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CN} + \text{CH}_3$ <b>PROPANENITRILE, 2,2-DIMETHYL-</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	875–925	1.4(+15)	0	35330	
$(\text{CH}_3\text{CH}_2)_2\text{NCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3\text{CH}_3$ $+ \text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3\text{CH}_3) + (\text{CH}_3\text{CH}_2)_2\text{NCH}_2 + \text{CH}_4$ <b>ETHANAMINE, N-ETHYL-N-METHYL-, + METHYL FREE RADICAL</b> <b>76 KER/PAR</b> <b>REACTION ORDER: 2.</b> <b>NOTE: TENTATIVE k VALUE.</b>	420	3.0(+7)	-	-	0.5 2.0
$(\text{CH}_3)_2\text{NCON}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \text{CH}_2(\text{CH}_3)\text{NCON}(\text{CH}_3)_2 + \text{CH}_4$ <b>UREA, TETRAMETHYL-, + METHYL FREE RADICAL</b> <b>76 KER/PAR</b> <b>REACTION ORDER: 2.</b>	350–550	2.0(+11)	0	3975±500	0.5 1.5
$\text{CH}_2=\text{CHCH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{cy-CH}_2\text{CH}=\text{CHCH}=\text{CHCH}_2$ <b>cis-1,3,5-HEXATRIENE</b> <b>70 BEN/O'N</b> <b>REACTION ORDER: 1.</b>	390–463	7.1(+11)	0	15050	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}=\text{CH} + \text{N} \rightarrow \text{products}$ <b>1-HEXYNE + NITROGEN ATOM</b> <b>72 KER/PAR</b> <b>REACTION ORDER: 2.</b> <b>k/k<sub>ref</sub>: 14.0</b>	320–550 435	4.6(+11) -	0 -	1233 -	
<b>NOTE: k<sub>ref</sub>: CHCH + N.</b>					
$\text{CH}_3\text{CH}_2\text{C}=\text{CCH}_2\text{CH}_3 + \text{N} \rightarrow \text{products}$ <b>3-HEXYNE + NITROGEN ATOM</b> <b>72 KER/PAR</b> <b>REACTION ORDER: 2.</b> <b>k/k<sub>ref</sub>: 14.0</b>	320–550 435	3.4(+11) -	0 -	1102 -	
<b>NOTE: k<sub>ref</sub>: CH=CH + N</b>					

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
cis-CH <sub>2</sub> =CHCH=CHCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CH=CHCH=CHCH <sub>3</sub> cis-1,3-HEXADIENE 70 BEN/0'N REACTION ORDER: 1.	474-518	6.3(+10)	0	16355	
CD <sub>2</sub> =CHCH <sub>2</sub> CH <sub>2</sub> CH=CD <sub>2</sub> → CH <sub>2</sub> =CHCD <sub>2</sub> CD <sub>2</sub> CH=CH <sub>2</sub> 1,5-HEXADIENE-1,1,6,6-D <sub>4</sub> 70 BEN/0'N REACTION ORDER: 1.	530	1.3(+11)	0	17865	
(CH <sub>3</sub> ) <sub>2</sub> C=CHCH=CH <sub>2</sub> → CH <sub>2</sub> =C(CH <sub>3</sub> )CH=CHCH <sub>3</sub> 1,3-PENTADIENE, 4-METHYL- 70 BEN/0'N REACTION ORDER: 1.	473-510	5.2(+11)	0	18199	
CH <sub>2</sub> =C(CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub> + CH <sub>3</sub> CH <sub>2</sub> · → + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C(·)(CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub> + CH <sub>2</sub> C(CH <sub>3</sub> )(CH <sub>2</sub> CH <sub>3</sub> )C(CH <sub>3</sub> )=CH <sub>2</sub> 1,3-BUTADIENE, 2,3-DIMETHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	318-414	1.6(+11)	0	2265	
cis-CH <sub>2</sub> =C(CH <sub>3</sub> )CH=CHCH <sub>3</sub> → (CH <sub>3</sub> ) <sub>2</sub> C=CHCH=CH <sub>2</sub> cis-1,3-PENTADIENE, 2-METHYL- 70 BEN/0'N REACTION ORDER: 1.	473	1.7(+11)	0	16485	
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH=CH <sub>2</sub> + O → cy-[CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> ]CHCH <sub>2</sub> O 1-HEXENE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298	3.1(+12)	-	-	0.7 1.3
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH=CH <sub>2</sub> + CH <sub>3</sub> CH <sub>2</sub> · → CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH(·)CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )CH <sub>2</sub> · 1-HEXENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	338-435	3.9(+10)	0	3400	
cis-CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> · → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(·)CH(CH <sub>3</sub> ) <sub>2</sub> cis-2-HEXENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4060	
cis-CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> · → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(·)CH <sub>3</sub> cis-2-HEXENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4150	
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> + CH <sub>3</sub> · → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C(·)(CH <sub>3</sub> )CH <sub>2</sub> CH <sub>3</sub> 1-PENTENE, 2-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	3450	
cis-(CH <sub>3</sub> ) <sub>2</sub> CHCH=CHCH <sub>3</sub> + CH <sub>3</sub> · → (CH <sub>3</sub> ) <sub>2</sub> CHCH(·)CH(CH <sub>3</sub> ) <sub>2</sub> cis-2-PENTENE, 4-METHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	298	-	-	4390	
(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> + O → products 2-BUTENE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-400	3.4(+12)	0	-790	0.8 1.2
(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> + H → (CH <sub>3</sub> ) <sub>2</sub> C(·)CH(CH <sub>3</sub> ) <sub>2</sub> 2-BUTENE, 2,3-DIMETHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.84	298 300	7.8(+11) -	-	-	
NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H					
(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> + S → cy-[ (CH <sub>3</sub> ) <sub>2</sub> CC(CH <sub>3</sub> ) <sub>2</sub> S 2-BUTENE, 2,3-DIMETHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2.	298	8.5(+13)	-	-	
(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> + N → products 2-BUTENE, 2,3-DIMETHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5	320-550 435	1.7(+11)	0	690	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + N					
(CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> + <sup>1</sup> CH <sub>2</sub> → products 2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 2.16	297	-	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + <sup>1</sup> CH <sub>2</sub>					

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
$(CH_3)_2C=C(CH_3)_2 + ^3CH_2 \rightarrow$ products 2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 2.74 NOTE: $k_{ref}$ : $CH_2=CH_2 + ^3CH_2$	297	-	-	-	
$(CH_3)_2C=C(CH_3)_2 + CH_3 \cdot \rightarrow (CH_3)_2C=(CH_3)CCH_2 \cdot + CH_4$ 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
$(CH_3)_2C=C(CH_3)_2 + CH_3 \cdot \rightarrow (CH_3)_3CC( \cdot )(CH_3)_2$ 2-BUTENE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. $k/k_{ref}$ : 0.2	403-453	1.0(+10)	0	3400	
NOTE: $k_{ref}$ : $CH_2=CH_2 + CH_3$	453	-	-	-	
$(CH_3)_2C=C(CH_3)_2 + CO \rightarrow (CH_3)_2C=C(CH_3)_2 + CO$ 2-BUTENE, 2,3-DIMETHYL-, + CARBON OXIDE( $C_2O$ ) 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 250. NOTE: $k_{ref}$ : $CH_2=CH_2 + CO$	298	-	-	-	
$CH_3CH( \cdot )CH_2CH_2CH_2CH_3 \rightarrow CH_3CH=CH_2 + CH_3CH_2CH_2$ PENTYL, 1-METHYL-, FREE RADICAL 70 BEN/O'N REACTION ORDER: 1.	822	2.0(+14)	0	13800	
$CH_3(CH_2)_4CH_3 + O \rightarrow CH_3(CH_2)_4CH_2 \cdot + OH$ HEXANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$CH_3(CH_2)_4CH_3 + O \rightarrow CH_3CH( \cdot )CH_2CH_2CH_2CH_3$ $+ CH_3CH_2CH( \cdot )CH_2CH_2CH_3 + OH$ HEXANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	1.1(+14)	0	2250	0.7 1.3
$CH_3(CH_2)_4CH_3 + CH_3 \cdot \rightarrow CH_3(CH_2)_4CH_2 \cdot + CH_4$ 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
$CH_3(CH_2)_4CH_3 + CH_3 \cdot \rightarrow CH_3CH_2CH( \cdot )CH_2CH_2CH_3$ $+ CH_3CH_2CH_2CH_2CH( \cdot )CH_3 + CH_4$ 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
$(CH_3)_2CHCH(CH_3)_2 \rightarrow (CH_3)_2CH \cdot + (CH_3)_2CH$ BUTANE, 2,3-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	1000-1200	3.2(+16)	0	39250	
$(CH_3)_2CHCH(CH_3)_2 \rightarrow (CH_3)_2CH( \cdot )CH(CH_3)_2 + CH_3$ BUTANE, 2,3-DIMETHYL- 70 BEN/O'N REACTION ORDER: 1.	1000-1200	1.0(+17)	0	41800	
$(CH_3)_2CHCH(CH_3)_2 + O \rightarrow .CH_2CH(CH_3)CH(CH_3)_2 + OH$ BUTANE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.3
$(CH_3)_2CHCH(CH_3)_2 + O \rightarrow (CH_3)_2C( \cdot )CH(CH_3)_2 + OH$ BUTANE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2.	298-650	3.1(+13)	0	1650	0.7 1.3
$(CH_3)_2CHCH(CH_3)_2 + CH_3 \cdot \rightarrow .CH_2CH(CH_3)CH(CH_3)_2 + CH_4$ 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
$(CH_3)_2CHCH(CH_3)_2 + CH_3 \cdot \rightarrow (CH_3)_2C( \cdot )CH(CH_3)_2 + CH_4$ 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
$(CH_3)_2CHCH(CH_3)_2 + CH_3 \rightarrow (CH_3)_2CHC(\cdot)(CH_3)_2$ + $CH_2CH(CH_3)CH(CH_3)_2 + CH_4$ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 72 KON REACTION ORDER: 2.	300-500	5.0(+10)	0	3445	
$(CH_3)_2CHCH(CH_3)_2 + CD_3 \rightarrow (CH_3)_2C(\cdot)CH(CH_3)_2$ + $CH_2CH(CH_3)CH(CH_3)_2 + CD_3H$ BUTANE, 2,3-DIMETHYL-, + METHYL-d <sub>3</sub> FREE RADICAL 72 KON REACTION ORDER: 2.	439-566	4.7(+11)	0	4525	
$CH_2=C(CH_3)OCH_2CH=CH_2 \rightarrow CH_2C(O)CH_2CH_2CH=CH_2$ 1-PROPENE, 3-(1-METHYLETHENYLOXY)- 70 BEN/0'N REACTION ORDER: 1.	416-467	5.4(+11)	0	14745	
$CH_2=C(CH_3)CH_2OCH=CH_2 \rightarrow CH_2=C(CH_3)CH_2CH_2CHO$ 1-PROPENE, 2-METHYL-3(ETHENYLOXY)- 70 BEN/0'N REACTION ORDER: 1.	423-461	1.4(+11)	0	14645	
$CH_2=CHCH(CH_3)OCH=CH_2 \rightarrow CH_3CH=CHCH_2CH_2CHO$ 1-PROPENE, 3-METHYL-3(ETHENYLOXY)- 70 BEN/0'N REACTION ORDER: 1.	423-461	2.1(+11)	0	14025	
$CH_2=CHC(CH_3)_2COOH \rightarrow CH_3CH=C(CH_3)_2 + CO_2$ 3-BUTENOIC ACID, 2,2-DIMETHYL- 70 BEN/0'N REACTION ORDER: 1.	511-548	1.4(+11)	0	18400	
$CH_3CH_2COOCH_2CH=CH_2 + CH_3CH_2 \rightarrow CH_3CH_2COOCH_2CH(CH_2CH_3)CH_2$ PROPANOIC ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	352-453	2.5(+11)	0	3875	
$(CH_3COO)_2CHCH_3 \rightarrow CH_3COOCOCH_3 + CH_3CHO$ 1,1-ETHANEDIOL, DIACETATE 70 BEN/0'N REACTION ORDER: 1.	493-541	1.9(+10)	0	16560	
$CH_3CH_2C(O)OOC(O)CH_2CH_3 \rightarrow CH_3CH_2C(O)O + CH_3CH_2C(O)O$ PEROXIDE, BIS(1-OXOPROPYL)- 70 BEN/0'N REACTION ORDER: 1.	373-464	2.5(+14)	0	15100	
$CH_2=CHCH_2C(OH)(CH_3)_2 \rightarrow CH_3CH=CH_2 + (CH_3)_2CO$ 4-PENTEN-2-OL, 2-METHYL- 70 BEN/0'N REACTION ORDER: 1.	607-643	1.4(+12)	0	20500	
$CH_2=CHO(CH_2)_3CH_3 \rightarrow CH_3CH_2CH=CH_2 + CH_3CHO$ BUTANE, 1-(ETHENYLOXY)- 70 BEN/0'N REACTION ORDER: 1.	590-650	1.4(+11)	0	21330	
$CH_2=CHO(CH_2)_3CH_3 + CH_3CH_2 \rightarrow CH_3CH_2CH_2CH(\cdot)O(CH_3)_3CH_3$ + $CH_2CH(CH_2CH_3)O(CH_2)_3CH_3$ BUTANE, 1-ETHENYLOXY-, + ETHYL FREE RADICAL 70 BEN/0'N REACTION ORDER: 2.	303-435	2.5(+10)	0	3070	
$CH_3COO(CH_2)_3CH_3 \rightarrow CH_3CH_2CH=CH_2 + CH_3COOH$ ACETIC ACID BUTYL ESTER 72 KER/PAR REACTION ORDER: 1.	725-810	1.6(+12)	0	23150	
$CH_3COOCH(CH_3)CH_2CH_3 \rightarrow CH_3COOH + cis-CH_3CH=CHCH_3$ + trans- $CH_3CH=CHCH_3 + CH_3CH_2CH=CH_2$ ACETIC ACID 1-METHYLPEROPYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 57% 1-BUTENE: trans/cis-2-BUTENE = 0.64.	576-710	2.0(+13)	0	23450	
$CH_3COOCH_2CH(CH_3)_2 \rightarrow (CH_3)_2C=CH_2 + CH_3COOH$ ACETIC ACID 2-METHYLPROPYL ESTER 70 BEN/0'N REACTION ORDER: 1.	725-810	7.9(+11)	0	23800	
$CH_3COOC(CH_3)_3 \rightarrow (CH_3)_2C=CH_3 + CH_3COOH$ ACETIC ACID 1,1-DIMETHYLETHYL ESTER 70 BEN/0'N REACTION ORDER: 1.	514-564	1.4(+13)	0	20130	
$(CH_3)_2C(OH)CH_2COCH_3 \rightarrow (CH_3)_2CO + (CH_3)_2CO$ 2-PENTANONE, 4-HYDROXY-4-METHYL- 70 BEN/0'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/0'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/0'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/0'N REACTION ORDER: 1. NOTE: SUSPECT RATE CONSTANT.	696-760	4.2(+14)	0	31960	
$(\text{CH}_3)_2\text{CHOCH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OCH}(\text{CH}_3)_2$ + $\text{CH}_2\text{CH}(\text{CH}_3)\text{OCH}(\text{CH}_3)_2 + \text{CH}_4$ 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/0'N REACTION ORDER: 1.	420-428	4.0(+15)	0	18700	
$(\text{CH}_3)_2\text{CHOOCH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OOCH}(\text{CH}_3)_2$ + $\text{CH}_2\text{CH}(\text{CH}_3)\text{OOC}(\text{CH}_3)_2 + \text{CH}_2 \cdot + \text{CH}_4$ 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
$\text{CH}_3\text{CH}=\text{NC}(\text{CH}_3)_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{C}(\cdot)\text{NC}(\text{CH}_3)_3$ + $\text{CH}_2\text{CH}=\text{NC}(\text{CH}_3)_3 + \text{CH}_3\text{CH}=\text{NC}(\text{CH}_3)_2\text{CH}_2 \cdot + \text{CH}_4$ 2-PROPANIMINE, N-ETHYLDENE-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/0'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.	350-500	2.0(+11)	0	3370±750	
NOTE: TENTATIVE k VALUE.					
$(\text{CH}_3\text{CH}_2)_3\text{N} + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$ + $\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2 + \text{CH}_4$ ETHANAMINE, N,N-DIETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	5.0(+11)	0	4000±500	0 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHC}(\text{=CH}_2)\text{CH}_2\text{CH}=\text{CH}_2$ 1,2,6-HEPTATRIENE 70 BEN/0'N REACTION ORDER: 1.	445-491	9.3(+ 9)	0	14330	
$\text{CH}_3(\text{CH}_2)_4\text{CCH} + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{C}(\cdot)=\text{CHCH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH}$ 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/0'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/0'N REACTION ORDER: 1.	451-523	7.1(+10)	0	17590	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CCO} \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}$ 2,3-PENTADIENE, 2,4-DIMETHYL-, + CARBON OXIDE(C <sub>2</sub> O) 70 BEN/0'N REACTION ORDER: 2. k/k <sub>ref</sub> : 113.	304	-	-	-	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 + \text{CCO}$					

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
$\text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2$ . 1-HEPTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	359-439	6.2(+10)	0	3500	
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2$ . + $(\text{CH}_3)_3\text{C}(\cdot)(\text{CH}_3)_2$ . 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)	-	-	
$\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2$ . 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
$(\text{CH}_3\text{CH}_2)_3\text{CH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3\text{CH}_2)_3\text{C} + \text{CH}_4$ PENTANE, 3-ETHYL-, + MÉTHYL 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-, + MÉTHYL 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-, + MÉTHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_2\text{CH}$ . 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	
$\text{trans}-\text{CH}_3\text{CH}=\text{CHC}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ $\text{trans}-3\text{-PENTENOIC ACID}, 2,2\text{-DIMETHYL-}$ 70 BEN/O'N REACTION ORDER: 1.	526-564	5.5(+11)	0	20300	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ + cis-, and trans $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ 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-ACETOXY- 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/0'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/0'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/0'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/0'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/0'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/0'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/0'N REACTION ORDER: 1.	725-810	1.6(+12)	0	23350	
$(\text{CH}_3)_3\text{CCOOCH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_3\text{COOH} + \text{CH}_2=\text{CH}_2$ PRÓPANOIC ACID, 2,2-DIMÉTHYL-, ETHYL ESTER 70 BEN/0'N REACTION ORDER: 1.	635-694	4.0(+12)	0	24200	
$\text{CH}_3\text{CH}_2\text{COOC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{COOH}$ PRÓPANOIC ACID, 1,1-DIMÉTHYLETHYL ESTER 70 BEN/0'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/0'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	
$\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2$ 1-OCTENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	339-425	1.2(+11)	0	3825	
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_2\text{CH}_2$ + $(\text{CH}_3)_3\text{CCH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ + $(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2$ 1-PENTENE, 2,4,4-TRIMETHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	309-364	1.9(+10)	0	2870	
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{O} \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_2 + \text{OH}$ 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
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow$ . $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ 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
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_2\text{C}(\text{CH}_3)_2\text{CC}(\text{CH}_3)_2 + \text{CH}_4$ 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
$(\text{CH}_3\text{COO})_2\text{CHCH}=\text{CHCH}_3 \rightarrow (\text{CH}_3\text{CO})_2\text{O} + \text{cis}-\text{CH}_3\text{CH}=\text{CHCHO}$ 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/0'N REACTION ORDER: 1.	484–538	2.5(+10)	0	16560	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(0)\text{OOC}(0)\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(0)\text{O}$ . + $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(0)\text{O}$ . PEROXIDE, BIS(1-OXOBUTYL) 70 BEN/0'N REACTION ORDER: 1.	370–452	2.0(+14)	0	14900	
$\text{CH}_3\text{COOC}(\text{CH}_2\text{CH}_3)_2\text{CH}_3 \rightarrow \text{cis}-\text{, and trans-CH}_3\text{CH=C(CH}_3\text{)CH}_2\text{CH}_3$ + $\text{CH}_2=\text{C}(\text{CH}_2\text{CH}_3)_2$ + $\text{CH}_3\text{COOH}$ ACETIC ACID 1-ETHYL-1-METHYLPROPYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 65% 1-BUTENE, 2-ETHYL-.	560–610	1.4(+13)	0	19400	
$\text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{C=CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 2-ETHYLBUTYL ESTER 70 BEN/0'N REACTION ORDER: 1.	725–810	7.9(+11)	0	23050	
$\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ + $\text{cis-}$ , and $\text{trans-CH}_3\text{CH=C(CH}_3\text{)CH}_2\text{CH}_3$ + $\text{CH}_3\text{COOH}$ ACETIC ACID 1,2-DIMETHYLBUTYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 76% 1-PENTENE, 3-METHYL-.	650–710	4.0(+12)	0	21740	
$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ + $(\text{CH}_3)_2\text{C=CHCH}_2\text{CH}_3$ + $\text{CH}_3\text{COOH}$ ACETIC ACID 1,1-DIMETHYLBUTYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 72% 1-PENTENE, 2-METHYL-.	560–610	1.5(+13)	0	19525	
$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C=C(CH}_3\text{)}_2$ + $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ + $\text{CH}_3\text{COOH}$ ACETIC ACID 1,1,2-TRIMETHYLPROPYL ESTER 70 BEN/0'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/0'N REACTION ORDER: 1.	403–443	4.0(+15)	0	18800	
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 + \text{CH}_3\cdot \rightarrow \text{CH}_2\text{C}(\text{CH}_3)_2\text{OOOC}(\text{CH}_3)_3 + \text{CH}_4$ . 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
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N=NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N=N}$ . + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ . DIAZENE, DIBUTYL- 70 BEN/0'N REACTION ORDER: 1.	473–673	3.2(+16)	0	25165	
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N=NCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N=N}$ . + $\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ . DIAZENE, BIS(1-METHYLPROPYL)- 70 BEN/0'N REACTION ORDER: 1.	539–618	4.0(+16)	0	23500	
$(\text{CH}_3)_2\text{CHCH}_2\text{N=NCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{N=N}$ . + $(\text{CH}_3)_2\text{CHCH}_2\cdot$ . DIAZENE, BIS(2-METHYLPROPYL)- 70 BEN/0'N REACTION ORDER: 1.	473–673	1.7(+16)	0	24660	
$(\text{CH}_3)_3\text{CN=NC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{CN=N} + (\text{CH}_3)_3\text{C}$ . DIAZENE, BIS(1,1-DIMETHYLETHYL)- 70 BEN/0'N REACTION ORDER: 1.	473–673	1.4(+17)	0	21900	
$(\text{CH}_3\text{CH}_2)_2\text{NN=NN}(\text{CH}_2\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{NN=N} + (\text{CH}_3\text{CH}_2)_2\text{N}$ . 2-TETRAZENE, 1,1,4,4-TETRAETHYL- 70 BEN/0'N REACTION ORDER: 1.	471–508	2.5(+14)	0	17365	
$(\text{CH}_3)_2\text{CHCH}_2\text{N(O)(O)CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{NO}$ . + $(\text{CH}_3)_2\text{CHCH}_2\text{NO}$ . PROPANE, 1-NITROSO-2-METHYL-, DIMERIC 70 BEN/0'N REACTION ORDER: 1.	374–402	2.5(+14)	0	12900	

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
$\text{CH}_3\text{CH}=\text{C}(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)_2\text{COOH} \rightarrow (\text{CH}_3\text{CH}_2)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ PENTANOIC ACID, 2,2-DIMETHYL-3-ETHYLDENE- 70 BEN/0'N REACTION ORDER: 1. NOTE: RELIABLE k.	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/0'N REACTION ORDER: 1.	493-578	5.0(+10)	0	18300	
$\text{CH}_3\text{COOCH}(\text{CH}_3)(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2$ + cis-, and trans- $\text{CH}_2\text{CH}=\text{CH}(\text{CH}_2)_3\text{CH}_3$ ACETIC ACID 1-METHYLHEXYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 58% 1-HEPTENE.	650-710	5.4(+12)	0	21995	
$\text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}(\text{CH}_2)_3\text{CH}_3$ + cis-, and trans- $\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-ETHYL PENTYL ESTER 70 BEN/0'N REACTION ORDER: 1.	650-710	5.6(+12)	0	21740	
$\text{CH}_3\text{COOCH}(\text{CH}_2\text{CH}_2\text{CH}_3)_2 \rightarrow$ + cis-, and trans- $\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-PROPYLBUTYL ESTER 70 BEN/0'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-METHYL PROPYL ESTER 70 BEN/0'N REACTION ORDER: 1.	650-710	6.9(+12)	0	22500	
$(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow$ cy-[ $\text{CH}_2=\text{C}(\text{CH}_3)$ ]CHCH( $\text{CH}_3$ )CH( $\text{CH}_3$ )CH $_2\text{CH}_2$ 1,6-OCTADIENE, 3,7-DIMETHYL- 70 BEN/0'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/0'N REACTION ORDER: 1. NOTE: PROBABLY RELIABLE k.	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/0'N REACTION ORDER: 1. NOTE: PROBABLY RELIABLE k.	473-573	3.0(+10)	0	16600	

### 3. Sources of Recommended Rate Constants

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## Appendix: Conversion Tables

### Equivalent second order rate constants

<i>A</i>	<i>B</i>	$\text{cm}^3\text{mol}^{-1}\text{s}^{-1}$	$\text{dm}^3\text{mol}^{-1}\text{s}^{-1}$	$\text{m}^3\text{mol}^{-1}\text{s}^{-1}$	$\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$	$(\text{mm Hg})^{-1}\text{s}^{-1}$	$\text{atm}^{-1}\text{s}^{-1}$	$\text{ppm}^{-1}\text{min}^{-1}$	$\text{m}^3\text{kN}^{-1}\text{s}^{-1}$
$1 \text{ cm}^3\text{mol}^{-1}\text{s}^{-1}$	1	$10^{-3}$	$10^{-6}$		$1.66 \times 10^{-24}$	$1.604 \times 10^{-5} T^{-1}$	$1.219 \times 10^{-2} T^{-1}$	$2.453 \times 10^{-9}$	$1.203 \times 10^{-4} T^{-1}$
$1 \text{ dm}^3\text{mol}^{-1}\text{s}^{-1} =$	$10^3$	1	$10^{-3}$		$1.66 \times 10^{-21}$	$1.604 \times 10^{-2} T^{-1}$	$12.19 T^{-1}$	$2.453 \times 10^{-6}$	$1.203 \times 10^{-1} T^{-1}$
$1 \text{ m}^3\text{mol}^{-1}\text{s}^{-1}$	$10^6$	$10^3$	1		$1.66 \times 10^{-18}$	$16.04 T^{-1}$	$1.219 \times 10^4 T^{-1}$	$2.453 \times 10^{-3}$	$120.3 T^{-1}$
$1 \text{ cm}^3\text{molecule}^{-1}\text{s}^{-1} =$	$6.023 \times 10^{23}$	$6.023 \times 10^{20}$	$6.023 \times 10^{17}$	1		$9.658 \times 10^{18} T^{-1}$	$7.34 \times 10^{21} T^{-1}$	$1.478 \times 10^{15}$	$7.244 \times 10^{19} T^{-1}$
$1 (\text{mm Hg})^{-1}\text{s}^{-1} =$	$6.236 \times 10^4 T$	$62.36 T$	$6.236 \times 10^{-2} T$		$1.035 \times 10^{-19} T$	1	760	$4.56 \times 10^{-2}$	7.500
$1 \text{ atm}^{-1}\text{s}^{-1} =$	$82.06 T$	$8.206 \times 10^{-2} T$	$8.206 \times 10^{-5} T$		$1.362 \times 10^{-22} T$	$1.316 \times 10^{-3}$	1	$6 \times 10^{-5}$	$9.969 \times 10^{-3}$
$1 \text{ ppm}^{-1}\text{min}^{-1} =$ at 298 K, 1 atm total pressure	$4.077 \times 10^8$	$4.077 \times 10^6$	407.7		$6.76 \times 10^{-16}$	21.93	$1.667 \times 10^4$	1	164.5
$1 \text{ m}^3\text{kN}^{-1}\text{s}^{-1} =$	$8.314 T$	$8.314 T$	$8.314 \times 10^{-3} T$		$1.38 \times 10^{-20} T$	0.1333	101.325	$6.079 \times 10^{-3}$	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  $\text{cm}^3\text{molecule}^{-1}\text{s}^{-1}$  to  $\text{m}^3\text{mol}^{-1}\text{s}^{-1}$  multiply by  $6.023 \times 10^{23}$ .

Table adapted from Evaluated Kinetic Data for High Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the H<sub>2</sub>-O<sub>2</sub> System, Butterworths, London, 1972.

### Equivalent third order rate constants

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

See note to Table for second order rate constants.

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