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Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion

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Washington, D.C. 20234

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Prepared for
Department of Energy
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U.S. DEPARTMENT OF COMMERCE

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Table of Recommended Rate Constants for Chemical
Reactions Occurring in Combustion

by

Francis Westley

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National Bureau of Standards
Washington, DC 20234

Sponsored by the

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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_1 to C_{10} hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides and their free radicals, as well as the reactions of O, O_2 , H, H_2 , OH, H_2O , H_2O_2 , N, N_2 , NO, N_2O , NO_2 , N_2O_4 , N_2O_5 , S, S_2 , SH, SO, SO_2 , SOH, NS, with each other. The table includes 169 first order reactions 782 second order reactions and 57 third order reactions. There are 1770 entries covering 1008 distinct chemical reactions. These recommendations have been taken from eleven evaluations and critical reviews published between 1970 and 1976. The papers examined by the evaluators extend from the nineteen fifties up to - and including - 1975.

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

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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.

<u>SOURCE</u>	<u># RECOMMENDED RATE CONSTANTS</u>
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 - respectively - third order rate constant units are appended at the end of this publication.

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.

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 can not 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.

Beside 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:

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

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 $\log_{10} k_0$; and c). Uncertainty expressed as a percentage of k_0 . With respect to the type a) uncertainties, the B factor uncertainties have been eliminated as being unimportant, while the uncertainties for the E/R factor may be omitted because they are of secondary importance and are included in the k factors. Therefore, the only uncertainty of type a) considered below is the one appended to the coefficient of the A factor.

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

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

where a is a numerical coefficient less than 10 and n is the power of 10.

If an uncertainty $\pm a'$ is appended to the coefficient a , the A factor takes the form:

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

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

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

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

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

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

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

Formulas (8) and (9) are the relationships needed to transform an uncertainty appended to the coefficient of the A factor into one using a k factor. A numerical example follows:

$$A = (2.0 \pm 0.5) \times 10^{14} \quad \text{therefore: } a = 2.0 \quad \text{and } a' = 0.5$$

$$a'/a = 0.5/2.0 = 0.25 \quad \text{and the k factors are: } f = 1 - 0.25 = 0.75$$

$$\text{and } F = 1 + 0.25 = 1.25$$

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:

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

or

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

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:

$$\log_{10} k = 14.23 \pm 0.3 \quad \text{therefore: } f = 10^{-0.3} = 0.5 \text{ and } F = 10^{0.3} = 2.0$$

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

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

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

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

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

$$\begin{aligned} f &= 1 - r & (18) \\ \text{and} \quad F &= 1 + r & (19) \end{aligned}$$

which are the relationships needed to transform the type c uncertainties into reliability limits expressed by k factors. A numerical example follows:

$$k = 3.7 \times 10^{12} \pm 20\% \quad \text{therefore } p = 20\% \text{ and } r = 0.2$$

$$\text{Thus: } f = 1 - 0.2 = 0.8$$

$$\text{and } F = 1 + 0.2 = 1.2$$

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 each 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 the factors are 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

This publication is in two parts:

Part I. The table, 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 .

Part II. The bibliography of part I, including 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 - respectively - 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 neames 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 reactionss⁻¹
- 2 for second order reactionscm³mol⁻¹s⁻¹
- 3 for third order reactionscm⁶mol⁻²s⁻¹

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

For 124 reactions, no Arrhenius parameters are indicated. Instead, for each of these 124 reactions, the ratio of the rate constant with

respect to the rate of a reference reaction - taken as unity - is given. This information follows the reaction order information, on the same line, and is indicated by the symbol k/k_{ref} : followed by a number.

E.g.: k/k_{ref} : 0.59.

The last line of column 1, placed under the line including the short reference and reaction order information, begins with the heading NOTE:. It is given only when necessary and might include information about the dependence of k factors on temperature range, or the reaction taken as reference when the ratio k/k_{ref} is given in the previous line, or other information pertinent to the reaction indicated above. The rate constant, k_{ref} , for the reference reaction indicated in the note (by the same author) can be found in the table in the proper place. For a certain number of reactions taken from Baulch, et al. (1972, 1973, and 1976) the relationship $k_1 = K k_{-1}$ 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 degrees Kelvin 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 on page 11 of this introduction. For those cases when the recommended value is only for one temperature, the entry under this column is in fact the value of the rate constant k at this temperature. As for the temperatures, the data for the A factor are aligned with the short reference and reaction order information. If a dash appears in this column, it means that no A factor value was reported by the evaluator for the corresponding reaction.

Column 4, with the heading B, gives the value of B for the equation $k = AT^B \exp(-E/RT)$. The value of B is usually low and varies from 0 to about 3 or 4. It may be negative, or positive. The negative values of B are preceded by the sign -, while the positive values are without sign. No more than one digit is given after the decimal dot. If in this column

a dash appears instead of a figure, it means that no B value was reported by the evaluator for the corresponding reaction. As for the temperature and A factor, the data for B are aligned with the short reference and reaction order information.

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

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

Ordering of chemical reactions.

The general rule for ordering the chemical equations of the reactions listed in column 1 of the table is the standard order of arrangement as described in NBS Technical Note 270-3 pp. 5, 6, and 22*). 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

*) . 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 pgs. 5, 16, 22 (1968).

the fact that all the compounds containing the atoms of a system with the exception of the underlined atom, are already listed in the previous systems. In each of these five chemical systems, the order of the compounds listed in the table as first reactants is as follows:

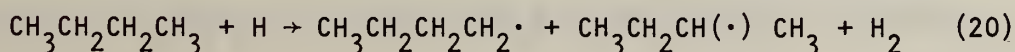
- 1). O system: O, O₂, O₃.
- 2). H-O system: H, H₂, OH, HO₂, H₂O, H₂O₂.
- 3). S-O-H system: S, S₂, SO, SO₂, SO₃, SH, SH₂, SOH.
- 4). N-O-H-S system: N, N₂, NO, NO₂, NO₃, N₂O, N₂O₄, N₂O₅, NH, NH₂,
NH₃, N₂H₄, HN₃, HNO, HNO₃, NS.
- 5). C-O-H-S-N system: C₁ compounds: C, CO, CO₂, CH, CH₂, CH₃, CH₄, CHO, HCHO, CH₃O., CH₃OH, CH₃OOH, CS, CS₂, COS, CH₃S, CH₃SH, CN, C(NO₂)₄, CHN, CH₃NH₂, CH=N=N, CH₃NHNH₂, CH₃NO, CH₃NO₂, CH₃NO₃, CH₃ONH₂.
C₂ compounds: C₂, C₂O, CH≡CH, CH₂=CH₂, CH₃CH₂., CH₃CH₃, CH₂=C=O, etc.
C₃ compounds, etc., up to C₁₀ compounds follow, being ordered according to the same pattern.

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

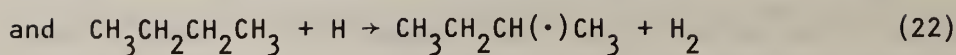
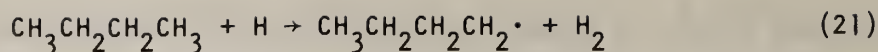
The standard order is applied in the same way for the second, or third reactants of chemical reactions. Since the reactants of a chemical equation

can be switched around, a number of bimolecular and termolecular reactions are inserted in the table in two - and respectively - three places. E.g.: Reaction $\text{CH}_4 + \text{O} \rightarrow \text{CH}_3\cdot + \text{OH}$, is inserted in the C-O-H-S-N system. This reaction may also be written as $\text{O} + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3\cdot$ 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_4 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 $\text{NO} + \text{NO}_2 + \text{O}_2 \rightarrow \text{N}_2\text{O}_5$. This reaction will also be inserted under the forms: $\text{NO}_2 + \text{NO} + \text{O}_2 \rightarrow \text{N}_2\text{O}_5$ and $\text{O}_2 + \text{NO} + \text{NO}_2 \rightarrow \text{N}_2\text{O}_5$. A number of second and third order reactions includes a second and - respectively - third body M . 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 $\text{O}_3 + \text{M} \rightarrow \text{O} + \text{O}_2 + \text{M}$ is inserted in the table only once, while reaction $\text{NO} + \text{O} + \text{M} \rightarrow \text{NO}_2 + \text{M}$ is inserted as such, and also under the form $\text{O} + \text{NO} + \text{M} \rightarrow \text{NO}_2 + \text{M}$.

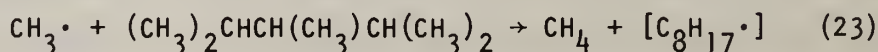
Most of the chemical reactions included in the table are balanced. A number of reactions are only apparently unbalanced. For instance, reaction



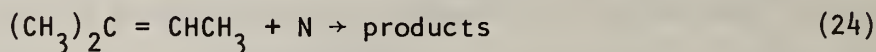
has a rate constant which in fact the sum of the rate constants for the two reactions



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



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-Tri-methyl-pentane. There are a number of reactions with the products totally unspecified. In such a case, the word "products" appears after the arrow:



Display of Chemical Reactions and Formulae

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

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

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

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

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

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

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

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

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

Oxy free radicals. If the oxygen atom of an oxy radical is attached to the terminal carbon atom, the radical is written in the usual manner: $\text{CH}_3\text{O}\cdot$.

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

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

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

Sources of Recommended Rate Constants

- Baulch, D. L., Drysdale, D. D., Horne, D. G., and Lloyd, A. C., "Evaluated Kinetics Data for High Temperature Reactions, Vol. 1: Homogeneous Gas Phase Reactions of the H_2-O_2 System," (Butterworths, London, 1972).
- Baulch, D. L., Drysdale, D. D., and Horne, D. G., "Evaluated Kinetic Data for high Temperature Reactions, Vol. 2: Homogeneous Gas Phase Reactions of the $H_2-N_2-O_2$ System," (Butterworths, London, 1973).
- Baulch, D. L., Drysdale, D. D., Duxbury, J., and Grant, S. J., "Evaluated Kinetic Data for High Temperature Reactions, Vol. 3: Homogeneous Gas Phase Reactions of the O_2-O_3 System, the $CO-O_2-H_2$ System, and of Sulphur-Containing Species," (Butterworths, London, 1976).
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- Benson, S. W., and O'Neal, H. E., "Kinetic Data on Gas Phase Unimolecular Reactions," NBS-NSRDS-21 (1970). (Supt. Doc., U.S. Govt. Printing Office, Washington, D.C. 20402).
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- Lloyd, A. C., "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical," Int. J. Chem. Kinet. 6, 169-228 (1974).

CHEMICAL REACTIONS

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f F
$\text{O} \cdot \text{O} \cdot \text{M} \rightarrow \text{O}_2 \cdot \text{M}$ OXYGEN ATOM 76 HAU/DRY REACTION ORDER: 3. M: Ar NOTE: k FACTORS CHANGING TO: f = 0.4; F = 1.6 AT 4000K. M: N ₂ M: O ₂	150-4000	1.9(+13)	0	-900±175	0.8 1.2
NOTE: k ₁ = k ₂ -1.0 k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 8000K. ----- $\text{O} \cdot \text{O}_2 \rightarrow \text{O}_2 \cdot \text{O}$ OXYGEN ATOM + OXYGEN MOLECULE 76 HEN/GEL REACTION ORDER: 2.	190-400 2000-1000 AT 8000K	1.0(+14) 4.7(+23)	0 -2.5	-720 0	0.5 1.5 0.4 2.5
$\text{O} \cdot \text{O}_2 \cdot \text{M} \rightarrow \text{O}_3 \cdot \text{M}$ OXYGEN ATOM + OXYGEN MOLECULE 76 HAU/DRY NOTE: M eff: O ₂ (1.5) NOTE: M eff: Ar(1.0) NOTE: M eff: N ₂ (1.4) -----	300 300 300	6.3(+11) 2.2(+14) 1.5(+14) 2.1(+14)	0.5 - - -	0 - - -	0.8 1.2 0.8 1.3 0.8 1.2
$\text{O} \cdot \text{O}_3 \rightarrow \text{O}_2 \cdot \text{O}_2$ OXYGEN ATOM + OZONE 76 HAU/DRY 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
$\text{O} \cdot \text{H} \cdot \text{M} \rightarrow \text{OH} \cdot \text{M}$ OXYGEN + HYDROGEN ATOMS 76 ENG REACTION ORDER: 3.	1500-2500	7.9(+15)	0	0	0.1 10.
$\text{O} \cdot \text{H}_2 \rightarrow \text{OH} \cdot \text{H}$ OXYGEN ATOM + HYDROGEN MOLECULE 72 HAU/DRY REACTION ORDER: 2.	400-2000	1.8(+10)	1.0	4480±150	0.7 1.3
$\text{O} \cdot \text{D}_2 \rightarrow \text{OD} \cdot \text{D}$ OXYGEN ATOM + DEUTERIUM MOLECULE 72 HAU/DRY REACTION ORDER: 2.	416-968	2.0(+13)	0	5500	0.5 2.0
$\text{O} \cdot \text{OH} \rightarrow \text{O}_2 \cdot \text{H}$ OXYGEN ATOM + HYDROXYL FREE RADICAL 72 HAU/DRY 76 ENG REACTION ORDER: 2.	300 1500-2500	2.3(+13) 2.5(+13)	- 0	- 0	0.6 1.4 0.5 2.0
$\text{O} \cdot \text{OH} \rightarrow \text{O}_2 \cdot \text{H}$ OXYGEN ATOM + HYDROXYL FREE RADICAL 75 HEN/GEL REACTION ORDER: 2.		6.3(+11)	0.5	0	
$\text{O} \cdot \text{OH} \cdot \text{M} \rightarrow \text{HO}_2 \cdot \text{M}$ OXYGEN ATOM + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+17)	0	0	0.01 100.
$\text{O} \cdot \text{OH} \rightarrow \text{OH} \cdot \text{O}$ OXYGEN ATOM + HYDROXYL FREE RADICAL					

CHEMICAL REACTIONS

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
75 BEN/GOL	REACTION ORDER: 2. -----					
6 * H ₂ O - CH * CH OXYGEN ATOM * WATER 72 BAU/DRY	REACTION ORDER: 2. -----	300-2000	6.3(+11)	0.5	4000	
6 * S ₂ - SO * S OXYGEN ATOM * SULFUR DIMER 75 BEN/GOL	REACTION ORDER: 2. -----		6.8(+13)	0	9240±200	0.7 1.5
6 * SO - O ₂ * S OXYGEN ATOM * SULFUR MONOXIDE 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
6 * SO - SO * O OXYGEN ATOM * SULFUR MONOXIDE 75 BEN/GOL	REACTION ORDER: 2. -----		2.0(+11)	0.5	2770	
6 * SO * M - SO ₂ * M OXYGEN ATOM * SULFUR MONOXIDE 76 BAU/DRY	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
6 * SO * M - SO ₂ * M OXYGEN ATOM * SULFUR MONOXIDE 76 BAU/DRY	REACTION ORDER: 3. M: Ar -----	298	6.7(+16)	-	-	0.7 1.3
6 * SO ₂ - O ₂ * SO OXYGEN ATOM * SULFUR DIOXIDE 76 BAU/DRY	REACTION ORDER: 2. -----	440-2100	1.3(+14)	-0.5	5980	0.3 1.7
NOTE: k ₁ = k ₋₁	-----					
6 * SH - H * SO OXYGEN ATOM * MERCAPTO FREE RADICAL 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
6 * SH - CH * S OXYGEN ATOM * MERCAPTO FREE RADICAL 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0	4000	
6 * N * M - NO * M OXYGEN ATOM * NITROGEN ATOM 73 BAU/DRY	REACTION ORDER: 3. M: N ₂ -----	200-400	6.4(+16)	-0.5	0	
6 * N ₂ - NO * N OXYGEN ATOM * NITROGEN MOLECULE 73 BAU/DRY	REACTION ORDER: 2. -----	2000-5000	7.6(+13)	0	38000±150	0.5 2.0
NOTE: k ₁ = k ₋₁	-----					
6 * N ₂ * M - N ₂ O * M OXYGEN ATOM * NITROGEN MOLECULE 73 BAU/DRY	REACTION ORDER: 3. M: Ar -----	1300-2500	1.4(+13)	0	10400±1500	0.7 1.5
6 * NO - O ₂ * N OXYGEN ATOM * NITROGEN OXIDE(NO) 73 BAU/DRY	REACTION ORDER: 2. -----	1000-3000	1.5(+9)	1.0	19500±150	0.7 1.3
NOTE: k ₁ = k ₋₁ k FACTORS CHANGING 10: f = 0.5; F = 2.0 AT 3000K						

CHEMICAL REACTIONS					T/K	A	B	E/R (in °K)	k factors f
----- O + NO → NO + O OXYGEN ATOM + NITROGEN OXIDE(NO) 75 BEN/GOL REACTION ORDER: 2. -----						6.3(+11)	0.5	0	
O + NO + M → NO ₂ + M OXYGEN ATOM + NITROGEN OXIDE(NO) 73 BAU/DRY NOTE: M eff: O ₂ (1.0) AT 297K					200-500	1.1(+15)	0	-940±50	0.8 1.2
Ar(0.1) AT 297K					200-500	1.1(+14)	0	-940±50	0.8 1.2
H ₂ O(6.1) AT 297K					200-500	6.7(+15)	0	-940±15	0.8 1.2
D ₂ O(5.0) AT 297K					200-500	5.5(+15)	0	-940±50	0.8 1.2
SF ₆ (2.6) AT 297K					200-500	2.9(+15)	0	-940±50	0.8 1.2
N ₂ (1.4) AT 297K					200-500	1.5(+15)	0	-940±50	0.8 1.2
N ₂ O(2.1) AT 297K					200-500	2.3(+15)	0	-940±50	0.8 1.2
CO ₂ (2.1) AT 297K					200-500	2.3(+15)	0	-940±50	0.8 1.2
CH ₄ (2.2) AT 297K					200-500	2.4(+15)	0	-940±50	0.8 1.2
CF ₄ (2.2) AT 297K -----					200-500	2.4(+15)	0	-940±50	0.8 1.2
O + NO ₂ → O ₂ + NO OXYGEN ATOM + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 2. -----					300-550	1.0(+13)	0	300±100	0.8 1.3
O + NO ₂ → O ₂ + NO OXYGEN ATOM + NITROGEN OXIDE(NO ₂) 76 ENG REACTION ORDER: 2. -----					1500-2500	1.0(+13)	0	500±250	0.5 2.0
O + NO ₂ + M → NO ₃ + M OXYGEN ATOM + NITROGEN OXIDE(NO ₂) 73 BAU/DRY NOTE: k ₀ (LOW PRESSURE). NOTE: LIMITING HIGH PRESSURE k _∞ -----					295	2.3(+16)	-	-	0.4 2.5
O + N ₂ O → O ₂ + N ₂ OXYGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2. -----					295	1.1(+13)	-	-	0.4 2.5
O + N ₂ O → O ₂ + N ₂ OXYGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2. -----					1200-2000	1.0(+14)	0	1±100±2000	0.4 2.5
O + N ₂ O → NO + NO OXYGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2. -----					1200-2000	1.0(+14)	0	1±100±1500	0.5 2.0
O + NH → OH + N OXYGEN ATOM + IMIDGEN FREE RADICAL -----									

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
75 BEN/G6L	REACTION ORDER: 2. -----					
$\phi + NH \rightarrow NO + H$			6.3(+11)	0.5	4000	
OXYGEN ATOM + IMIDGEN FREE RADICAL						
75 BEN/G6L	REACTION ORDER: 2. -----					
$\phi + NH + M \rightarrow HNO + M$			6.3(+11)	0.5	0	
OXYGEN ATOM + IMIDGEN FREE RADICAL						
76 ENG	REACTION ORDER: 3. -----	1500-2500	1.0(+16)	-0.5	0+2500	0.3 3.2
$\phi + NH_3 \rightarrow \phi H + NH_2$						
OXYGEN ATOM + AMMONIA						
73 BAU/DRY	REACTION ORDER: 2. -----	300-1000	1.5(+12)	0	3000+300	0.5 1.5
$\phi + HNO \rightarrow \phi H + NO$						
OXYGEN ATOM + NITROSYL HYDRIDE						
76 ENG	REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	0+2500	0.3 3.2
$\phi + HNO \rightarrow \phi_2 + NH$						
OXYGEN ATOM + NITROSYL HYDRIDE						
76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.5	3500+2500	0.3 3.2
$\phi + HNO \rightarrow NO_2 + H$						
OXYGEN ATOM + NITROSYL HYDRIDE						
76 ENG	REACTION ORDER: 2. -----	1500-2500	5.0(+10)	0.5	0+2500	0.3 3.2
$\phi + NS \rightarrow SO + N$						
OXYGEN ATOM + NITROGEN SULFIDE(NS)						
75 BEN/G6L	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
$\phi + NS \rightarrow NO + S$						
OXYGEN ATOM + NITROGEN SULFIDE(NS)						
75 BEN/G6L	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$\phi + C + M \rightarrow CO + M$						
OXYGEN ATOM + CARBON ATOM						
76 BAU/DRY	REACTION ORDER: 3. -----	7000-15000	3.3(+26)	-3.1	2114	0.3 1.8
NOTE: M = Ar, Br, Cl, K ₁ = K ₁₋₁						
$\phi + CO \rightarrow \phi_2 + C$						
OXYGEN ATOM + CARBON MONOXIDE						
75 BEN/G6L	REACTION ORDER: 2. -----		1.0(+12)	0.5	69300	
$\phi + CO \rightarrow CO + \phi$						
OXYGEN ATOM + CARBON MONOXIDE						
75 BEN/G6L	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$\phi + CO + M \rightarrow CO_2 + M$						
OXYGEN ATOM + CARBON MONOXIDE						
76 BAU/DRY	REACTION ORDER: 3. M: CO 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
$\phi + CO_2 \rightarrow \phi_2 + CO$						

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
OXYGEN ATOM + FORMALDEHYDE-d 73 BEN/HUI REACTION ORDER: 2. ----- $O + CH_3O \rightarrow OH + ECHO$ OXYGEN ATOM + METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. ----- NOTE: k ESTIMATED	300	4.9(+10)	-	-	
$O + CS \rightarrow C + S$ OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----	1500-2500	1.0(+14)	0	0±1500	
$O + CS \rightarrow C + S$ OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 76 EAU/DRY REACTION ORDER: 2. -----	300	1.6(+12)	0.5	28940	
$O + CS_2 \rightarrow S + COS$ OXYGEN ATOM + CARBON DISULFIDE 76 EAU/DRY REACTION ORDER: 2. -----	302	1.3(+13) 6.3(+11)	-	-	0.5 1.5
$O + CS_2 \rightarrow S + COS$ OXYGEN ATOM + CARBON DISULFIDE 76 EAU/DRY REACTION ORDER: 2. -----	302	2.2(+11)	-	-	0.5 1.5
$O + COS \rightarrow SO + CO$ OXYGEN ATOM + CARBON OXIDE SULFIDE 76 EAU/DRY REACTION ORDER: 2. -----	200-1000	2.2(+13)	0	700±150	0.7 1.3
$O + COS \rightarrow SO + CO$ OXYGEN ATOM + CARBON OXIDE SULFIDE 76 EAU/DRY REACTION ORDER: 2. -----	190-1200	1.6(+13)	0	2250±250	0.5 1.5
NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 ABOVE 600K. -----					
$O + CN \rightarrow C + N$ OXYGEN ATOM + CYANOGEN FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----		1.3(+12)	0.5	14545	
$O + CN \rightarrow C + N$ OXYGEN ATOM + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	0±2500	0.3 3.2
$O + C_2 \rightarrow C + C$ OXYGEN ATOM + CARBON DIMER 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$O + CH_3CE \rightarrow Products$ OXYGEN ATOM + ETHYLENE 73 BEN/HUI REACTION ORDER: 2. -----	200-700	1.4(+13)	0	1500	0.8 1.2
$O + CH_2=CH_2 \rightarrow cy-CH_2CH_2O$ OXYGEN ATOM + ETHYLENE 73 BEN/HUI REACTION ORDER: 2. -----	200-500	3.3(+12)	0	565	0.8 1.2
$O + CH_3CH_3 \rightarrow OE + CH_2CH_2O$ OXYGEN ATOM + ETHANE 73 BEN/HUI REACTION ORDER: 2. -----	298-650	2.5(+13)	0	3200	0.7 1.3

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
----- 0 + CH₂=C=O → products OXYGEN ATOM + ETHENE 73 HRR/HUI REACTION ORDER: 2. -----	5.3(+11)	-	-	0.7 1.3
0 + CH₃CHO → products OXYGEN ATOM + ACETALDEHYDE 73 HRR/HUI REACTION ORDER: 2. -----	1.4(+13)	0	1140	0.5 2.0
0 + cy-CH₂CH₂δ → products OXYGEN ATOM + OXIRANE 73 HRR/HUI REACTION ORDER: 2. -----	7.0(+8)	-	-	0.6 1.5
0 + CH₃CH₂δB → products OXYGEN ATOM + ETHANOL 73 HRR/HUI REACTION ORDER: 2. -----	8.7(+10)	-	-	0.6 1.5
0 + CH₃δCH₃ → products OXYGEN ATOM + METHANE, OXYEIS- 73 HRR/HUI REACTION ORDER: 2. -----	5.9(+12)	0	1520	0.7 1.3
0 + CH₃C≡CH → products OXYGEN ATOM + PROPENE 73 HRR/HUI REACTION ORDER: 2. -----	4.0(+11)	-	-	0.5 2.0
0 + CH₃CH=CH₂ → cy-(CH₃)CHCH₂δ OXYGEN ATOM + 1-PROPENE 73 HRR/HUI REACTION ORDER: 2. -----	2.5(+12)	0	38	0.8 1.2
0 + CH₃CH₂CH₃ → δH + CH₃CH₂CH₂δ + (CH₃)₂CH. OXYGEN ATOM + PROPANE 73 HRR/HUI REACTION ORDER: 2. -----	9.0(+9)	-	-	0.7 2
0 + (CH₃)₂CHOH → products OXYGEN ATOM + 2-PROPANOL 73 HRR/HUI REACTION ORDER: 2. -----	1.3(+11)	-	-	0.6 1.5
0 + (CH₃)₂C=CH₂ → cy-(CH₃)₂CCCH₂δ OXYGEN ATOM + 1-PROPENE, 2-METHYL- 73 HRR/HUI REACTION ORDER: 2. -----	1.2(+13)	-	-	0.7 1.3
0 + CH₃CC=CH → products OXYGEN ATOM + 1,3-BUTADIENE 73 HRR/HUI REACTION ORDER: 2. -----	9.0(+11)	-	-	0.7 1.4
0 + CH₂=C(CH₃)CH₂ → products OXYGEN ATOM + 1,3-BUTADIENE 73 HRR/HUI REACTION ORDER: 2. -----	3.4(+12)	0	-380	0.7 1.3
0 + CH₃CH₂CH=CH₂ → cy-(CH₃CH₂)CHCH₂δ OXYGEN ATOM + 1-BUTENE 73 HRR/HUI REACTION ORDER: 2. -----	2.3(+12)	-	-	0.8 1.2

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
6	$\text{cis-CH}_3\text{CH=CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + cis-2-BUTENE 73 HRR/HUI REACTION ORDER: 2. -----	250-500	5.9(+12)	0	-165	0.8 1.2
6	$\text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + trans-2-BUTENE 73 HRR/HUI REACTION ORDER: 2. -----	298	1.4(+13)	-	-	0.7 1.3
6	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O}$ OXYGEN ATOM + BUTANE 73 HRR/HUI REACTION ORDER: 2. -----	298-650	3.0(+13)	0	2920	0.7 1.3
6	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH} + \text{CH}_3\text{CH}_2\text{CH}(\text{O})\text{CH}_3$ OXYGEN ATOM + BUTANE 73 HRR/HUI REACTION ORDER: 2. -----	298-650	4.3(+13)	0	2410	0.7 1.3
6	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH})\text{CH}_2\text{O}$ OXYGEN ATOM + 1-PENTENE 73 HRR/HUI REACTION ORDER: 2. -----	298	2.8(+12)	-	-	0.7 1.3
6	$\text{cis-CH}_3\text{CH}_2\text{CH=CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + cis-2-PENTENE 73 HRR/HUI REACTION ORDER: 2. -----	298	1.1(+13)	-	-	0.7 1.3
6	$(\text{CH}_3)_2\text{C=CHCH}_3 \rightarrow \text{products}$ OXYGEN ATOM + 2-BUTENE, 2-METHYL- 73 HRR/HUI REACTION ORDER: 2. -----	298-400	3.9(+12)	0	-680	0.8 1.2
6	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{O}$ OXYGEN ATOM + PENTANE 73 HRR/HUI REACTION ORDER: 2. -----	298-650	2.9(+13)	0	2920	0.7 1.3
6	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{O})\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}(\text{O})\text{CH}_2\text{CH}_3$ OXYGEN ATOM + PENTANE 73 HRR/HUI REACTION ORDER: 2. -----	298-650	8.0(+13)	0	2320	0.7 1.3
6	$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{OH} + (\text{CH}_3)_2\text{C}(\text{O})\text{CH}_2\text{CH}_3$ $+ (\text{CH}_3)_2\text{CHCH}(\text{O})\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{O} + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ OXYGEN ATOM + BUTANE, 2-METHYL- 73 HRR/HUI REACTION ORDER: 2. -----	307	8.0(+10)	-	-	0.7 1.4
6	$(\text{CH}_3)_4\text{C} \rightarrow \text{OH} + (\text{CH}_3)_3\text{COCH}_3$ OXYGEN ATOM + PROPANE, 2,2-DIMETHYL- 73 HRR/HUI REACTION ORDER: 2. -----	298-650	5.9(+13)	0	2920	0.7 1.4
6	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH=CH}_2 \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH})\text{CH}_2\text{O}$ OXYGEN ATOM + 1-HEXENE 73 HRR/HUI REACTION ORDER: 2. -----	298	3.1(+12)	-	-	0.7 1.3
6	$(\text{CH}_3)_2\text{C=C}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 73 HRR/HUI REACTION ORDER: 2. -----	298-400	3.4(+12)	0	-790	0.8 1.2

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
$\phi + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \phi\text{H} + \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ OXYGEN ATOM + HEXANE 73 HBR/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\phi + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \phi\text{H} + \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\phi + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ OXYGEN ATOM + HEXANE 73 HBR/HUI REACTION ORDER: 2.	298-650	1.1(+14)	0	2250	0.8 1.3
$\phi + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \phi\text{H} + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ OXYGEN ATOM + BUTANE, 2,3-DIMETHYL- 73 HBR/HUI REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.3
$\phi + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \phi\text{H} + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$ OXYGEN ATOM + BUTANE, 2,3-DIMETHYL- 73 HBR/HUI REACTION ORDER: 2.	298-650	3.1(+13)	0	1650	0.7 1.3
$\phi + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \phi\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_2\cdot$ OXYGEN ATOM + HEPTANE 73 HBR/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\phi + \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \phi\text{H} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_3$ $\phi + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ OXYGEN ATOM + HEPTANE 73 HBR/HUI REACTION ORDER: 2.	298-650	1.2(+14)	0	2190	0.7 1.3
$\phi + (\text{CH}_3)_3\text{C}(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,2-DIMETHYL- 73 HBR/HUI REACTION ORDER: 2.	307	6.5(+10)	-	-	0.7 1.4
$\phi + (\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,4-DIMETHYL- 73 HBR/HUI REACTION ORDER: 2.	307	1.0(+11)	-	-	0.7 1.4
$\phi + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \phi\text{H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot$ OXYGEN ATOM + OCTANE 73 HBR/HUI REACTION ORDER: 2.	298-650	2.9(+13)	0	2920	0.7 1.3
$\phi + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \phi\text{H} + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3$ $\phi + \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ OXYGEN ATOM + OCTANE 73 HBR/HUI REACTION ORDER: 2.	298-650	9.3(+13)	0	2030	0.7 1.3
$\phi + (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,2,4-TRIMETHYL- 73 HBR/HUI REACTION ORDER: 2.	307	5.5(+10)	-	-	0.6 1.5
$\phi + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$ OXYGEN ATOM + PENTANE, 2,3,4-TRIMETHYL- 73 HBR/HUI REACTION ORDER: 2.	307	3.0(+10)	-	-	0.6 1.5
$\phi + (\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow \text{products}$					

CHEMICAL REACTIONS	T/K	A	B	E/R (in OK)	k factors f
OXYGEN ATOM + BUTANE, 2,2,3,3-TETRAMETHYL- 73 HBR/HUI REACTION ORDER: 2. -----	307	8.0(+9)	-	-	0.6 1.5
O ₂ + C → C + O ₂ OXYGEN MOLECULE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
O ₂ + C + M → C ₃ + M OXYGEN MOLECULE + OXYGEN ATOM 76 HAV/DRY REACTION ORDER: 3. M: O ₂ NOTE: M eff: O ₂ (1.5) Ar(1.0) N ₂ (1.4) -----	300	2.2(+14)	-	-	0.8 1.2
	300	1.5(+14)	-	-	0.8 1.3
	300	2.1(+14)	-	-	0.8 1.2
O ₂ + H → C + OH OXYGEN MOLECULE + HYDROGEN ATOM 72 HAV/DRY REACTION ORDER: 2. -----	700-2500 310-2050	2.2(+14) 1.5(+14)	0 0	8450±250 8420±125	0.7 1.3 0.9 1.2
O ₂ + D → C + OD OXYGEN MOLECULE + DEUTERIUM ATOM 72 HAV/DRY REACTION ORDER: 2. -----	800-1000	8.9(+13)	-	7500	
O ₂ + H + M → HO ₂ + M OXYGEN MOLECULE + HYDROGEN ATOM 72 HAV/DRY REACTION ORDER: 3. M: H ₂ NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = KK-1 Ar(0.3). K ₁ = KK-1 N ₂ (0.4) CO ₂ (1.5) -----	300-2000 300-2000 300-2000 300-2000 300-2000 300-2000 300-2000	1.5(+15) 5.9(+14) 9.5(+15) 4.4(+14) 4.4(+14) 5.9(+14) 2.2(+15)	0 0 0 0 0 0 0	-500±250 -500±250 -500±250 -500±250 -500±250 -500±250 -500±250	0.5 1.5 0.5 1.5 0.5 1.5 0.5 1.5 0.5 1.5 0.5 1.5 0.5 1.5
O ₂ + H ₂ → OH + OH OXYGEN MOLECULE + HYDROGEN MOLECULE 76 HNG REACTION ORDER: 2. -----	1500-2500	2.5(+12)	0	19630±5000	0.1 10.
O ₂ + H ₂ → HO ₂ + H OXYGEN MOLECULE + HYDROGEN MOLECULE 72 HAV/DRY REACTION ORDER: 2. -----	290-800	5.5(+13)	0	29100±350	0.4 2.5
O ₂ + S → C + SO OXYGEN MOLECULE + SULFUR ATOM 76 HAV/DRY REACTION ORDER: 2. -----	250-450	1.4(+12)	0	0±50	0.3 1.7

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f F
$O_2 + SO \rightarrow O + SO_2$ OXYGEN MOLECULE + SULFUR MONOXIDE 76 BAU/DRY REACTION ORDER: 2. -----		440-2100	4.5(+11)	0	3250±590	0.3 1.7
$O_2 + N \rightarrow O + NO$ OXYGEN MOLECULE + NITROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 3000K. -----		300-3000	6.4(+9)	1.0	3150±150	0.7 1.3
$O_2 + N_2 \rightarrow O + N_2O$ OXYGEN MOLECULE + NITROGEN MOLECULE 73 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = k_{-1}$ -----		1200-2000	6.3(+13)	0	55200±2000	0.4 2.5
$O_2 + NO \rightarrow O + NO_2$ OXYGEN MOLECULE + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 2. NOTE: $k_1 = k_{-1}$ -----		300-550	1.7(+12)	0	23400	0.8 1.3
$O_2 + NO + NO \rightarrow NO_2 + NO_2$ OXYGEN MOLECULE + NITROGEN OXIDE(NO) 73 BAU/DRY REACTION ORDER: 3. -----		273-660	1.2(+9)	0	-530±100	0.5 1.5
$O_2 + NO + NO_2 \rightarrow NO_2 + NO_3$ OXYGEN MOLECULE + NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO ₂) 73 BAU/DRY REACTION ORDER: 3. -----		300-500	2.9(+7)	0	-400±500	0.4 2.5
$O_2 + C \rightarrow O + CO$ OXYGEN MOLECULE + CARBON ATOM 75 BEN/GOEL REACTION ORDER: 2. -----			6.3(+11)	0.5	0	
$O_2 + CO \rightarrow O + CO_2$ OXYGEN MOLECULE + CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K. -----		1500-3000	2.5(+12)	0	24000±2500	0.5 2.0
$O_2 + CH \rightarrow O + \cdot CH_3$ OXYGEN MOLECULE + METHYLDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+11)	0.5	3000±2500	0.3 3.2
$O_2 + CH_2 \rightarrow O + HCHO$ OXYGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+11)	0.5	3500±2500	0.3 3.2
$O_2 + CH_3 \rightarrow O + CH_3O$ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----		1500-2500	3.2(+12)	0	15100±1500	
$O_2 + CH_3 \rightarrow OH + HCHO$ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.		1500-2500	3.2(+13)	0	10000±5000	0.3 3.2

CHEMICAL REACTIONS				T/K	A	B	E/R (in °K)	k factors f
$\phi_2 + CH_3 \rightarrow H\phi_2 + \cdot CH_3$ OXYGEN MOLECULE + METHYL FREE RADICAL 76 ENG NOTE: k ESTIMATED	----- REACTION ORDER: 2. -----	0	34975±1500		3.2(+12)			
$\phi_2 + \cdot C_2H_5 \rightarrow H\phi_2 + C_2H_5$ OXYGEN MOLECULE + METHYL, ETHYL, FREE RADICAL 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2. -----	0	3500±1500		1.6(+12)			
$\phi_2 + CH_3\phi \rightarrow H\phi_2 + HCH\phi$ OXYGEN MOLECULE + METHOXY FREE RADICAL 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2. -----	0	3000±1500		1.0(+12)			
$\phi_2 + CN \rightarrow C\phi + N\phi$ OXYGEN MOLECULE + CYANOGEN FREE RADICAL 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2. -----	0	0±5000		3.2(+11)			0.3 3.2
$\phi_2 + M \rightarrow \phi + \phi + M$ OXYGEN MOLECULE 76 BAU/DRY NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 8000K M: O ₂ M: Ar	----- REACTION ORDER: 2. -----	-2.5 -2.5 -1.0	59380 59380 59380±4900		3.5(+25) 9.8(+24) 1.8(+18)			0.5 2.0 0.4 2.5 0.5 2.0
$\phi_3 + \phi \rightarrow \phi_2 + \phi_2$ OZONE + OXYGEN ATOM 76 BAU/DRY NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 AT 1000K	----- REACTION ORDER: 2. -----	0	2090±260		5.2(+12)			0.5 1.5
$\phi_3 + H \rightarrow \phi_2 + \phi H$ OZONE + HYDROGEN ATOM 76 BAU/DRY	----- REACTION ORDER: 2. -----	-	-		1.6(+13)			0.5 2.0
$\phi_3 + \phi H \rightarrow \phi_2 + H\phi_2$ OZONE + HYDROXYL FREE RADICAL 76 BAU/DRY	----- REACTION ORDER: 2. -----	-	-		3.9(+10)			0.5 1.5
$\phi_3 + H\phi_2 \rightarrow \phi_2 + \phi_2 + \phi H$ OZONE + HYDROPEROXYL FREE RADICAL 76 BAU/DRY	----- REACTION ORDER: 2. -----	-	-		9.1(+ 8)			0.5 1.5
$\phi_3 + H_2S \rightarrow S\phi_2 + H_2\phi$ OZONE + HYDROGEN SULFIDE 76 BAU/DRY	----- REACTION ORDER: 2. -----	-	-		4.0(+ 2)			0.1 10.
$\phi_3 + N\phi \rightarrow \phi_2 + N\phi_2$ OZONE + NITROGEN OXIDE(NO) 73 BAU/DRY	----- REACTION ORDER: 2. -----	0	1230±130		8.9(+11)			0.5 1.5
$\phi_3 + N\phi_2 \rightarrow \phi_2 + N\phi_3$	-----							

CHEMICAL REACTIONS

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
OZONE + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2. ----- O ₃ + N ₂ O → O + O ₂ + N OZONE 76 BAU/DRY REACTION ORDER: 2. ----- M: Ar	286-302	5.9(+12)	0	3500	0.5 2.0
H + O + N → OH + N HYDROGEN ATOM + OXYGEN ATOM 76 ENG REACTION ORDER: 3. -----	200-1000	2.48(+14)	0	11430±120	0.8 1.3
H + O ₂ → OH + O HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2. -----	1500-2500	7.9(+15)	0	0	0.1 10.
D + O ₂ → OD + O DEUTERIUM ATOM + OXYGEN MOLECULE 72 BAU/DRY REACTION ORDER: 2. -----	700-2500	2.2(+14)	0	8450±250	0.7 1.3
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 2. -----	800-1000	8.9(+13)	0	7500	
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	1.5(+15)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	5.9(+14)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	5.5(+15)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	4.4(+14)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	4.4(+14)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	5.9(+14)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300-2000	2.2(+15)	0	-500±250	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300	1.6(+13)	-	-	0.5 2.0
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	300	3.0(+15)	-	-	0.5 1.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	2500-5000	2.6(+15)	-1.0	0	0.4 2.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	2500-5000	6.4(+17)	-1.0	0	0.4 2.5
H + O ₂ + N → HO ₂ + N HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H ₂ (1.0) O ₂ (0.4) H ₂ O(6.4) He(0.3). K ₁ = K _{K-1} Ar(0.3). K ₁ = K _{K-1} N ₂ (0.4) CO ₂ (1.5) ----- REACTION ORDER: 3. -----	4000	6.3(+11)	0.5		

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
HYDROGEN ATOM + DEUTERIUM MOLECULE 72 KGN REACTION ORDER: 2. -----		368-1000	3.1(+13)	0	4485±250	0.6 1.6
D + H ₂ → DH + H DEUTERIUM ATOM + HYDROGEN MOLECULE 72 KGN REACTION ORDER: 2. -----		400-1000	5.0(+13)	0	3890±40	0.9 1.1
H + CH → H ₂ + C HYDROGEN ATOM + HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. -----		400-2000	8.3(+9)	1.0	3500±150	0.7 1.3
H + CH → CH + H HYDROGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----			6.3(+11)	0.5	0	
H + CH + M → H ₂ + M HYDROGEN ATOM + HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 3. NOTE: M eff: H ₂ O(1.0). k ₁ = k _{k-1} Ar(0.06) N ₂ (0.16) -----		1000-3000	1.4(+23)	-2.0	0	0.7 1.5
		1000-3000	8.4(+21)	-2.0	0	0.5 2.0
		1000-3000	2.2(+22)	-2.0	0	0.5 2.0
H + H ₂ → C + H ₂ HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 74 IIC REACTION ORDER: 2. NOTE: E ESTIMATED. 76 ENG -----		300-1000	5. (+13)	0	500	0.3 3.2
		1500-2500	1.0(+13)	0	500±500	0.1 1.0
H + H ₂ → H ₂ + O ₂ HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. -----		290-800	2.5(+13)	0	350±350	0.4 2.5
		1500-2500	2.5(+13)	0	350±350	0.5 2.0
H + H ₂ → CH + CH HYDROGEN ATOM + HYDROPEROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. -----		290-800	2.5(+14)	0	950±350	0.5 2.0
		1500-2500	2.5(+14)	0	950±500	0.5 2.0
H + H ₂ → CH + H ₂ HYDROGEN ATOM + WATER 72 HAU/DRY REACTION ORDER: 2. NOTE: ERROR LIMITS ARE 50% FOR UPPER 1'S. -----		300-2500	9.3(+13)	0	10250±100	0.5 1.5
H + H ₂ O ₂ → H ₂ + H ₂ O HYDROGEN ATOM + HYDROGEN PEROXIDE 72 HAU/DRY REACTION ORDER: 2. -----		300-800	1.7(+12)	0	1900±250	0.5 2.0
H + S ₂ → SH + S HYDROGEN ATOM + SULFUR DIMER 75 BEN/GGL REACTION ORDER: 2. -----			7.9(+12)	0.5	8355	

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
H • S ₈ → CH • S						
HYDROGEN ATOM • SULFUR MONOXIDE 75 BEN/GOL	REACTION ORDER: 2. -----		4.0(•12)	0.5	11200	
H • S ₈ → SH • S						
HYDROGEN ATOM • SULFUR MONOXIDE 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(•11)	0.5	19930	
H • S ₈ → M → HS ₂ • M						
HYDROGEN ATOM • SULFUR DIOXIDE 76 HAU/DRY	REACTION ORDER: 3. -----	1660-2120	5.1(•15)	-	-	0.5 1.5
H • SH → H ₂ • S						
HYDROGEN ATOM • MERCAPTO FREE RADICAL 76 HAU/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 ₂ S → H ₂ • SH						
HYDROGEN ATOM • HYDROGEN SULFIDE 76 HAU/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 ₂ → NH • N						
HYDROGEN ATOM • NITROGEN MOLECULE 75 BEN/GOL	REACTION ORDER: 2. -----		2.0(•13)	0.5	75945	
H • NO → CH • 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 HAU/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 ₂ -----	1500-2500	5.0(•15)	0	-300±150	0.5 2.0
H • NO ₂ → CH • NO						
HYDROGEN ATOM • NITROGEN OXIDE(NO ₂) 73 HAU/DRY	REACTION ORDER: 2. -----	298-630	3.5(•14)	0	740±500	0.5 1.5

NOTE: k FACTORS CHANGING 16: f = 0.5; F = 2.0 AT T = 633K

CHEMICAL REACTIONS				T/K	A	B	E/R (in °K)	k factors f
H + NO ₂ → OH + NO HYDROGEN ATOM + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2. -----				1500-2500	3.2(+14)	0	750±500	0.5 2.0
H + N ₂ O → OH + N ₂ HYDROGEN ATOM + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2. -----				700-2500	7.6(+13)	0	7600±500	0.5 1.5
H + N ₂ O → NH + NO HYDROGEN ATOM + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2. -----				1500-2500	1.0(+11)	0.5	15100±2500	0.3 3.2
H + NH → H ₂ + N HYDROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	4000	
H + NH → NH + H HYDROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	0	
H + NH ₂ + M → NH ₃ + M HYDROGEN ATOM + AMIDGEN FREE RADICAL 73 BAU/DRY NOTE: K ₁ = K ₂ -1 REACTION ORDER: 3. M: Ar -----				2000-3000	4.8(+14)	0	-8300±2500	0.5 2.0
H + NH ₂ NH ₂ → H ₂ + NH ₂ NH. HYDROGEN ATOM + HYDRAZINE 73 BAU/DRY REACTION ORDER: 2. -----				250-500	1.3(+13)	0	1250±100	0.5 2.0
H + HNO → H ₂ + NO HYDROGEN ATOM + NITROSYL HYDRIDE 73 BAU/DRY REACTION ORDER: 2. -----				2000	4.8(+12)	-	-	0.5 1.5
H + HNO → CH + 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/GGL REACTION ORDER: 2. -----					2.5(+12)	0.5	15700	
H + NS → NH + S HYDROGEN ATOM + NITROGEN SULFIDE(NO) 75 BEN/GGL REACTION ORDER: 2. -----					2.5(+12)	0.5	20735	
H + CO → CH + C HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GGL REACTION ORDER: 2. -----					2.0(+13)	0.5	77755	
H + CO → CH + d HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GGL REACTION ORDER: 2. -----					2.5(+13)	0.5	88020	

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f	k factors F
H + C6 + M → •CH6 + M HYDROGEN ATOM + CARBON MONOXIDE 76 BAU/DRY NOTE: k FACTORS CHANGING 16: f = 0.5; F = 2.0 AT 773K. 76 ENG	----- REACTION ORDER: 3. M: H2 -----	298-773	6.9(+14)	0	850±500	0.7	1.3
		1500-2500	1.6(+20)	-1.5	0	0.3	3.2
H + C62 → 6H + C6 HYDROGEN ATOM + CARBON DIOXIDE 76 BAU/DRY	----- REACTION ORDER: 2. -----	1000-3000	1.5(+14)	0	13300±150	0.8	1.2
H + CH → H2 + C HYDROGEN ATOM + METHYLIDINE FREE RADICAL 75 BEN/GOL	----- REACTION ORDER: 2. -----		6.3(+11)	0.5	4000		
H + CH → CH + H HYDROGEN ATOM + METHYLIDINE FREE RADICAL 75 BEN/GOL	----- REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
H + CH + M → CH2 + M HYDROGEN ATOM + METHYLIDINE FREE RADICAL 76 ENG	----- REACTION ORDER: 3. -----	1500-2500	1.0(+19)	-1.0	0	0.3	3.2
H + CH2 → H2 + 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 + CH4 → H2 + CH3• HYDROGEN ATOM + METHANE 76 ENG	----- REACTION ORDER: 2. -----	1500-2500	6.3(+13)	0	5990±150	0.5	2.0
D + CH4 → DH + CH3• DEUTERIUM ATOM + METHANE 72 KON	----- REACTION ORDER: 2. -----	523-673	8.3(+12)	0	5100		
H + •CH6 → H2 + C6 HYDROGEN ATOM + METHYL, 6X6-, FREE RADICAL 76 ENG	----- REACTION ORDER: 2. -----	1500-2500	1.6(+12)	0.5	0±2500	0.3	3.2
H + HCH6 → H2 + •CH6 HYDROGEN ATOM + FORMALDEHYDE 76 ENG	----- REACTION ORDER: 2. -----	1500-2500	1.3(+10)	1.0	1600	0.3	3.2
H + CH36 → H2 + HCH6 HYDROGEN ATOM + METHOXY FREE RADICAL 76 ENG	----- REACTION ORDER: 2. -----	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	----- REACTION ORDER: 2. -----						

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
75 BEN/GOL	REACTION ORDER: 2. -----		1.3(+13)	0.5	50930	
H + C6S → HS + C6						
HYDROGEN ATOM + CARBON OXIDE SULFIDE						
76 HAU/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 → CN + 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 + C2 → C2 + C						
HYDROGEN ATOM + CARBON DIMER						
75 BEN/GOL	REACTION ORDER: 2. -----		1.6(+13)	0.5	30450	
H + CH2=CH2 → CH3CH2•						
HYDROGEN ATOM + ETHENE						
72 IER/PAR	REACTION ORDER: 2. -----	298	9.3(+13)	0	1410	
H + CH2=CH2 + M → CH3CH2• + M						
HYDROGEN ATOM + ETHENE						
72 ION	REACTION ORDER: 3. -----	298-813	5.6(+17)	0.5	495	
H + CH3CH3 → H2 + CH3CH2•						
HYDROGEN ATOM + ETHANE						
72 ION	REACTION ORDER: 2. -----	285-1440	1.0(+14)	0	4815+70	0.8 1.2
H + CH3C≡CH → CH3CH=CH + CH3C(•)=CH2						
HYDROGEN ATOM + 1-PROPENE						
72 IER/PAR	REACTION ORDER: 2. -----	298	0.5(+11)	-	-	
NOTE: K TAKEN AS LOWER LIMIT.						
H + CH3CH=CH2 → CH3CH2CH2•						
HYDROGEN ATOM + 1-PROPENE						
72 IER/PAR	REACTION ORDER: 2. -----	298	7.2(+12)	0	1460	
NOTE: TENTATIVE K VALUE.						
H + CH3CH=CH2 → CH3CH(•)CH3						
HYDROGEN ATOM + 1-PROPENE						
72 IER/PAR	REACTION ORDER: 2. -----	298	7.2(+12)	0	605	
NOTE: ARRHENIUS PARAMETERS ARE MINIMUM VALUES OF THEIR HIGH-PRESSURE LIMITS.						
H + CH3CH2CH3 → H2 + (CH3)2CH• + CH3CH2CH2•						
HYDROGEN ATOM + PROPANE						
72 ION	REACTION ORDER: 2. -----	333-933	1.0(+13)	0	3130+180	0.7 1.4

CHEMICAL REACTIONS

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f F
----- H • (CH₃)₂CO → H₂ • CH₃C(•)CH₂• HYDROGEN ATOM • 2-PYRACETONE 72 KJN REACTION ORDER: 2. ----- H • CH₂-CHCH-CH₂ → CH₂-CHCH(•)CH₃ • CH₂-CHCH₂CH₂• HYDROGEN ATOM • 1,3-BUTADIENE 72 KJN/PAW REACTION ORDER: 2. NOTE: AVERAGED RATE CONSTANT.	298-873	4.6(•13)	0	4220±20	
----- H • CH₂-CHCH-CH₂ → CH₂-CHCH(•)CH₃ • CH₂-CHCH₂CH₂• HYDROGEN ATOM • 1,3-BUTADIENE 72 KJN/PAW REACTION ORDER: 2. NOTE: AVERAGED RATE CONSTANT.	298	4.10(•13)	0	655	
----- H • CH₂-CHCH-CH₂ → CH₂-CHCH(•)CH₃ • CH₂-CHCH₂CH₂• HYDROGEN ATOM • 1,3-BUTADIENE 72 KJN/PAW REACTION ORDER: 2. k/k_{ref}: 4.9 NOTE: k_{ref}: H • CH₃CH-CH₂	300	-	-	-	
----- H • CH₃CH₂CH-CH₂ → CH₃CH₂CH(•)CH₃ • CH₃CH₂CH₂CH₂• HYDROGEN ATOM • 1-BUTENE 72 KJN/PAW REACTION ORDER: 2. k/k_{ref}: 1.03 NOTE: k_{ref}: H • CH₃CH-CH₂	300	-	-	-	
----- H • CH₃CH₂CH-CH₂ → CH₃CH₂CH(•)CH₃ • CH₃CH₂CH₂CH₂• HYDROGEN ATOM • 1-BUTENE 72 KJN/PAW REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	8.7(•11)	-	-	
----- H • CH₃CH₂CH-CH₂ → CH₃CH₂CH(•)CH₃ • CH₃CH₂CH₂CH₂• HYDROGEN ATOM • 1-BUTENE 72 KJN/PAW REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	5.0(•10)	-	-	
----- H • CH₃CH₂CH-CH₂ → CH₃CH₂CH(•)CH₃ • CH₃CH₂CH₂CH₂• HYDROGEN ATOM • 1-BUTENE 72 KJN/PAW REACTION ORDER: 2. NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	8.1(•11)	-	-	
----- H • cis-CH₃CH-CHCH₃ → CH₃CH₂CH(•)CH₃ • CH₃CH₂CH₂CH₂• HYDROGEN ATOM • cis-2-BUTENE 72 KJN/PAW REACTION ORDER: 2. NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION. k/k_{ref}: 0.47	298	4.6(•11)	-	-	
----- NOTE: k_{ref}: H • CH₃CH-CH₂	300	-	-	-	
----- H • trans-CH₃CH-CHCH₃ → CH₃CH₂CH(•)CH₃ • CH₃CH₂CH₂CH₂• HYDROGEN ATOM • trans-2-BUTENE 72 KJN/PAW REACTION ORDER: 2. NOTE: AVERAGE k	298	5.6(•11)	-	-	
----- NOTE: k_{ref}: H • CH₃CH-CH₂	300	-	-	-	
----- H • (CH₃)₂C-CH₂ → (CH₃)₃C• HYDROGEN ATOM • 1-PROPENE, 2-METHYL- 72 KJN/PAW REACTION ORDER: 2.	298	3.10(•13)	0	755	
----- H • (CH₃)₂C-CH₂ → (CH₃)₂CHCH₂• HYDROGEN ATOM • 1-PROPENE, 2-METHYL- 72 KJN/PAW REACTION ORDER: 2.	298	-	-	-	

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
298	1.3(+11)	-	-	
300	-	-	-	
320-930	4.1(+12)	0	2637±320	0.5 2.0
300-800	1.9(+13)	0	2680±85	0.8 1.2
298	8.3(+11)	-	-	
300	-	-	-	
298	3.8(+11)	-	-	
300	-	-	-	
298	4.1(+11)	-	-	
300	-	-	-	
298	9.1(+11)	-	-	
298	2.0(+12)	-	-	
298	7.4(+11)	-	-	

72 KER/PAR
NOTE: CALCULATED ON THE BASIS OF 0.5% NON-TERMINAL
ADDITION OF H TO $(CH_3)_2C=CH_2$.

H + $(CH_3)_2C=CH_2 \rightarrow (CH_3)_3C \cdot + (CH_3)_2CHCH_2 \cdot$
HYDROGEN ATOM + 1-PENTENE, 2-METHYL-
72 KER/PAR
NOTE: k_{ref} : H + $CH_3CH=CH_2$

H + $CH_3CH_2CH_2CH_2CH_3 \rightarrow H_2 + CH_3CH_2CH_2CH_2CH_2CH_2 \cdot$
HYDROGEN ATOM + BUTANE
72 KER

H + $(CH_3)_3C \cdot \rightarrow H_2 + (CH_3)_3C \cdot + (CH_3)_2CHCH_2 \cdot$
HYDROGEN ATOM + PROPANE, 2-METHYL-
72 KER

H + $CH_3CH_2CH_2CH_2CH_2CH_2 \cdot \rightarrow CH_3CH_2CH_2CH_2CH_2CH_2CH_2 \cdot$
+ $CH_3CH_2CH_2CH_2CH_2CH_2 \cdot$
HYDROGEN ATOM + 1-PENTENE
72 KER/PAR

NOTE: k_{ref} : H + $CH_3CH=CH_2$.
 k/k_{ref} : 0.89

H + $cis-CH_3CH_2CH_2CH_2CH=CHCH_3 \rightarrow CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
+ $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
HYDROGEN ATOM + cis-2-PENTENE
72 KER/PAR

NOTE: k_{ref} : H + $CH_3CH=CH_2$.
 k/k_{ref} : 0.39

H + $trans-CH_3CH_2CH_2CH=CHCH_3 \rightarrow CH_3CH_2CH_2CH_2CH_2CH_2CH_3$
+ $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$
HYDROGEN ATOM + trans-2-PENTENE
72 KER/PAR

NOTE: k_{ref} : H + $CH_3CH=CH_2$.
 k/k_{ref} : 0.44

H + $CH_3CH_2C(CH_3)=CH_2 \rightarrow CH_3CH_2C(CH_3)_2CH_2 \cdot$
+ $CH_3CH_2CH_2C(CH_3)_2CH_2 \cdot$
HYDROGEN ATOM + 1-BUTENE, 2-METHYL-
72 KER/PAR

D + $CH_3CH_2C(CH_3)=CH_2 \rightarrow CH_3CH_2C(CH_3)_2CH_2 \cdot$
+ $CH_3CH_2CH_2C(CH_3)_2CH_2 \cdot$
DEUTERIUM ATOM + 1-BUTENE, 2-METHYL-
72 KER/PAR

H + $(CH_3)_2CHCH=CH_2 \rightarrow (CH_3)_2CHCH_2CH_2 \cdot$
+ $(CH_3)_2CHCH_2CH_2 \cdot$
HYDROGEN ATOM + 1-BUTENE, 3-METHYL-
72 KER/PAR

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$D + (CH_3)_2CHCH=CH_2 \rightarrow (CH_3)_2CHCH(\cdot)(CH_3)_2$ $\cdot (CH_3)_2CHCHDCH_2$ DEUTERIUM ATOM + 1-HUTENE, 3-METHYL- 72 KER/PAR	298	7.6(+11)	-	-	
$H + (CH_3)_2C=CHCH_3 \rightarrow (CH_3)_2CHCH(\cdot)(CH_3)_3$ $\cdot (CH_3)_2C(\cdot)CH_2CH_3$ HYDROGEN ATOM + 2-HUTENH, 2-METHYL- 72 KER/PAR	298 300	9.1(+11)	-	-	
NOTE: $k_{ref}: H + CH_3CH=CH_2$					
$H + (CH_3)_2C=C(CH_3)_2 \rightarrow (CH_3)_2CHC(\cdot)(CH_3)_2$ HYDROGEN ATOM + 2-EUTENH, 2,3-DIMETHYL- 72 KER/PAR	298 300	7.8(+11)	-	-	
NOTE: $k_{ref}: H + CH_3CH=CH_2$					
$H + (CH_3)_3CC(CH_3)=CH_2 \rightarrow (CH_3)_3CCH(\cdot)(CH_3)_2$ $\cdot (CH_3)_3CC(\cdot)(CH_3)_2$ HYDROGEN ATOM + 1-HUTENB, 2,3,3-TRIMETHYL- 72 KER/PAR	298	1.6(+12)	-	-	
NOTE: TENTATIVE VALUE BASED ON REACTION:					
$H + (CH_3)_2C=CH_2$					
$H_2 + \phi \rightarrow H + \phi H$					
H_2 HYDROGEN MOLECULE + OXYGEN ATOM 72 BAU/DRY	400-2000	1.8(+10)	1.0	4480±150	0.7 1.3
D_2 DEUTERIUM MOLECULE + OXYGEN ATOM 72 BAU/DRY	416-968	2.0(+13)	0	5500	0.5 2.0
$H_2 + \phi_2 \rightarrow H + H\phi_2$ HYDROGEN MOLECULE + OXYGEN MOLECULE 72 BAU/DRY	290-800	5.5(+13)	0	29100±350	0.4 2.5
$H_2 + \phi_2 \rightarrow \phi H + \phi H$ HYDROGEN MOLECULE + OXYGEN MOLECULE 76 ENG	1500-2500	2.5(+12)	0	19630±5000	0.1 10.
$H_2 + H \rightarrow H + H_2$ HYDROGEN MOLECULE + HYDROGEN ATOM 75 HEN/GOL		6.3(+11)	0.5	4000	
$H_2 + D \rightarrow H + HD$ HYDROGEN MOLECULE + DEUTERIUM ATOM 72 KON	400-1000	5.0(+13)	0	3890±40	0.9 1.1
$D_2 + H \rightarrow D + DH$ DEUTERIUM MOLECULE + HYDROGEN ATOM 72 KON	1000	3.1(+13)	0	4485±250	0.6 1.6

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$H_2 + OH \rightarrow H + H_2O$ HYDROGEN MOLECULE + HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING 10: f = 0.5; F = 1.5 FOR T : 300K T > 300K	300-2500	2.2(+13)	0	2590±100	0.8 1.2
$D_2 + OH \rightarrow D + DHO$ DEUTERIUM MOLECULE + HYDROXYL FREE RADICAL 72 KGN REACTION ORDER: 2.	300-623	1.9(+13)	0	2904±280	0.5 2.0
$H_2 + HO_2 \rightarrow H + H_2O_2$ HYDROGEN MOLECULE + HYDROPEROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2.	300-800	7.3(+11)	0	9400±250	0.5 2.0
$H_2 + S \rightarrow H + SH$ HYDROGEN MOLECULE + SULFUR ATOM 76 HAU/DRY REACTION ORDER: 2. NOTE: k ₁ = k _{k-1} 75 BEN/GOL	298	1.3(-1)	-	13640	0.5 1.5
$H_2 + N \rightarrow H + NH$ HYDROGEN MOLECULE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.		2.5(+12)	0.5	18700	
$H_2 + C \rightarrow H + CH$ HYDROGEN MOLECULE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.		1.6(+12)	0.5	15700	
$H_2 + CO_2 \rightarrow H_2O + CO$ HYDROGEN MOLECULE + CARBON DIOXIDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+9)	0.5	7550±2500	0.3 3.2
$H_2 + CH_2 \rightarrow H + CH_3$ HYDROGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	3525±1500	
$H_2 + CH_3 \rightarrow H + CH_4$ HYDROGEN MOLECULE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	370-700	8.5(+11)	0	5500±500	0.7 1.3
$H_2 + CD_3 \rightarrow H + CD_3$ HYDROGEN MOLECULE + METHYL-D ₃ -FREE RADICAL 72 KGN REACTION ORDER: 2.	400-570	7.4(+11)	0	5250±235	0.6 1.7
$DH + CH_3 \rightarrow D + CH_3D$ DEUTERIUM HYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-700	2.4(+11)	0	5635±500	0.5 1.5
$DH + CH_3 \rightarrow D + CH_4$ DEUTERIUM HYDRIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-700	2.1(+11)	0	5300±500	0.5 1.5

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f F
300-700	7.1(+11)	0	5990±250	0.7 1.3
1500-2500	3.2(+12)	0	2500±1500	
473-823	3.0(+11)	0	5435	
2500-5000	2.2(+14)	0	48300±2000	0.5 2.0
	6.3(+11)	0.5	4000	
300	2.3(+13)	-	-	0.6 1.4
1500-2500	2.5(+13)	0	0	0.5 2.0
1500-2500	1.0(+17)	0	0	0.01 100.
300	3.9(+10)	-	-	0.5 1.5
400-2000	8.3(+9)	1.0	3500±150	0.7 1.3
	6.3(+11)	0.5	0	
1000-3000	1.4(+23)	-2.0	0	0.7 1.5
1000-3000	8.4(+21)	-2.0	0	0.5 2.0

$D_2 + CH_3 \rightarrow D + CH_3D$
 DEUTERIUM MOLECULE + METHYL FREE RADICAL
 76 KEV/PAR
 REACTION ORDER: 2.

$H_2 + CN \rightarrow H + HCN$
 HYDROGEN MOLECULE + CYANOGEN FREE RADICAL
 76 ENG
 REACTION ORDER: 2.
 NOTE: k ESTIMATED.

$H_2 + CH_3CH_2 \rightarrow H + CH_3CH_3$
 HYDROGEN MOLECULE + ETHYL FREE RADICAL
 72 ION
 REACTION ORDER: 2.

$H_2 + M \rightarrow H + H + M$
 HYDROGEN MOLECULE
 72 BAU/DRY
 NOTE: $k_1 = k_{k-1}$

$CH + O \rightarrow C + OH$
 HYDROXYL FREE RADICAL + OXYGEN ATOM
 75 BEN/GGL
 REACTION ORDER: 2.

$CH + O \rightarrow H + C_2$
 HYDROXYL FREE RADICAL + OXYGEN ATOM
 72 BAU/DRY
 NOTE: k_1 CALCULATED FROM k_{-1} IS: $1.3 \times 10^{13} \text{ cc.mole}^{-1} \text{ s}^{-1}$

$CH + O \rightarrow H + C_2$
 HYDROXYL FREE RADICAL + OXYGEN ATOM
 76 ENG
 REACTION ORDER: 2.

$CH + O + M \rightarrow H_2O + M$
 HYDROXYL FREE RADICAL + OXYGEN ATOM
 76 ENG
 REACTION ORDER: 3.

$CH + O_3 \rightarrow HO_2 + C_2$
 HYDROXYL FREE RADICAL + OZONE
 76 BAU/DRY
 REACTION ORDER: 2.

$CH + H \rightarrow C + H_2$
 HYDROXYL FREE RADICAL + HYDROGEN ATOM
 72 BAU/DRY
 REACTION ORDER: 2.

$CH + H \rightarrow H + CH$
 HYDROXYL FREE RADICAL + HYDROGEN ATOM
 75 BEN/GGL
 REACTION ORDER: 2.

$CH + H + M \rightarrow H_2O + M$
 HYDROXYL FREE RADICAL + HYDROGEN ATOM
 72 BAU/DRY
 NOTE: M eff: $H_2O(1.0)$, $k_1 = k_{k-1}$
 Ar(0.06)

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f	k factors F
$N_2(0.16)$ $CH + H_2 \rightarrow H_2O + H$ HYDROXYL FREE RADICAL + HYDROGEN MOLECULE 72 HAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING 16: f = 0.5; F = 1.5 FOR T > 300K -----		1000-3000	2.2(+22)	-2.0	0	0.5	2.0
$CH + D_2 \rightarrow DH_2 + D$ HYDROXYL FREE RADICAL + DEUTERIUM MOLECULE 72 HEN REACTION ORDER: 2. -----		300-2500	2.2(+13)	0	2590±100	0.8	1.2
$CH + CH_2 \rightarrow H_2 + H$ HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. -----		300-623	1.9(+13)	0	2904±280	0.5	2.0
$CH + CH_2 \rightarrow H_2 + H$ HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. -----		290-800	1.2(+13)	0	20200±350	0.5	2.0
$CH + CH_2 \rightarrow H_2 + H$ HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 2. -----		300-2000	6.3(+12)	0	550±200	0.7	1.5
$CH + CH_2 \rightarrow H_2 + H$ HYDROXYL FREE RADICAL 72 HAU/DRY REACTION ORDER: 3. M: N_2 NOTE: k FACTORS CHANGING 16: f = 0.5; F = 2.0 AT 1500K. -----		700-1500	9.1(+14)	0	2550±1000	0.8	1.3
$CH + H_2O_2 \rightarrow H_2O + HO_2$ HYDROXYL FREE RADICAL + HYDROGEN PEROXIDE 72 HAU/DRY REACTION ORDER: 2. -----		300-800	1.0(+13)	0	910±150	0.5	1.5
$CH + S \rightarrow SH + S$ HYDROXYL FREE RADICAL + SULFUR ATOM 75 HEN/GOL REACTION ORDER: 2. -----			1.3(+12)	0.5	12700		
$CH + S \rightarrow H + SH$ HYDROXYL FREE RADICAL + SULFUR ATOM 75 HEN/GOL REACTION ORDER: 2. -----			6.3(+11)	0.5	0		
$CH + H_2S \rightarrow H_2 + HS$ HYDROXYL FREE RADICAL + HYDROGEN SULFIDE 76 HAU/DRY REACTION ORDER: 2. NOTE: k FACTORS INCREASING 16: f = 0.5; F = 1.5 AT 900K. -----		258-900	6.3(+12)	0	200±150	0.7	1.3
$CH + N \rightarrow C + NH$ HYDROXYL FREE RADICAL + NITROGEN ATOM 75 HEN/GOL REACTION ORDER: 2. -----			1.3(+12)	0.5	17765		
$CH + N \rightarrow H + NO$ HYDROXYL FREE RADICAL + NITROGEN ATOM 75 HEN/GOL REACTION ORDER: 2. -----			6.3(+11)	0.5	0		
$CH + N + M \rightarrow HNC + M$ HYDROXYL FREE RADICAL + NITROGEN ATOM 75 HEN/GOL REACTION ORDER: 2. -----							

CHEMICAL REACTIONS		T/K	A	B	E/R (ln OK)	k factors f F
76 ENG	REACTION ORDER: 3. -----	1500-2500	1.0(+15)	-0.5	0	
OH + NO ₂ + M → HNO ₃ + M HYDROXYL FREE RADICAL + NITROGEN OXIDE(N ₂ O) 73 BAU/DRY	REACTION ORDER: 3. -----	300	5.0(+17)	-	-	0.4 1.6
OH + N ₂ O → H ₂ O + N ₂ HYDROXYL FREE RADICAL + NITROGEN OXIDE(N ₂ O) 76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+13)	0	7550	
NOTE: k ESTIMATED.	-----					
OH + NH → H ₂ O + N HYDROXYL FREE RADICAL AND IMIDGEN FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	1000±2500	0.3 3.2
OH + HNO → H ₂ O + NO HYDROXYL FREE RADICAL + NITROSYL HYDRIDE 73 BAU/DRY	REACTION ORDER: 2. -----	2000	3.6(+13)	-	-	0.5 1.5
OH + HNO ₃ → H ₂ O + NO ₃ HYDROXYL FREE RADICAL + NITRIC ACID 73 BAU/DRY	REACTION ORDER: 2. -----	300	8.0(+10)	-	-	0.5 2.0
OH + C → C + OH HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL	REACTION ORDER: 2. -----					
OH + C → H + CO HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL	REACTION ORDER: 2. -----					
OH + CO → H + CO ₂ HYDROXYL FREE RADICAL + CARBON MONOXIDE 76 BAU/DRY	REACTION ORDER: 2. -----	250-2000	1.5(+7)	1.3	- 385	0.8 1.2
NOTE: k FACTORS OVER 1000K: f = 0.5; F = 1.5. RECOMMENDED k FOR 250-2500K: log(k)ccmol ⁻¹ s ⁻¹ = 10.83 + 3.94 ⁻⁴ T -----	-----					
OH + CH → H + •CH ₃ HYDROXYL FREE RADICAL AND METHYLIDENE FREE RADICAL 76 ENG	REACTION ORDER: 2. -----					
OH + CH ₂ → H + CH ₃ HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	5000±2500	0.3 3.2
OH + CH ₂ → H + HCHO HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+13)	0	2517	0.3 3.2
NOTE: k ESTIMATED.	-----					
OH + CH ₂ → H ₂ O + CH HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL	-----					

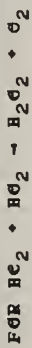
CHEMICAL REACTIONS		T/K	A	B	E/R (in oK)	k factors f	k factors F
76 ENG	REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
6H + CH ₃ • → H + CH ₃ δ.							
76 ENG	HYDROXYL FREE RADICAL AND METHYL FREE RADICAL REACTION ORDER: 2. -----	1500-2500	6.3(+12)	0	0		
6H + CH ₃ • → H ₂ δ + CH ₂							
76 ENG	HYDROXYL FREE RADICAL AND METHYL FREE RADICAL REACTION ORDER: 2. -----	1500-2500	6.3(+10)	0.7	1000±2500	0.3	3.2
6H + CH ₄ → H ₂ δ + CH ₃ •							
76 ENG	HYDROXYL FREE RADICAL + METHANE REACTION ORDER: 2. -----	1500-2500	3.2(+13)	0	2500±250	0.5	2.0
6H + •CHδ → H ₂ δ + Cδ							
76 ENG	HYDROXYL FREE RADICAL + METHYL, δHδ-, FREE RADICAL REACTION ORDER: 2. -----	1500-2500	3.2(+10)	1.0	0±1500		
NOTE: K ESTIMATED.							
6H + CH ₃ δ. → H ₂ δ + HCHδ							
76 ENG	HYDROXYL FREE RADICAL + METHOXY FREE RADICAL REACTION ORDER: 2. -----	1500-2500	3.2(+13)	0	0±1500		
NOTE: K ESTIMATED.							
6H + HCHδ → H ₂ δ + •CHδ							
76 ENG	HYDROXYL FREE RADICAL + FORMALDEHYDE REACTION ORDER: 2. -----	1500-2500	3.2(+10)	1.0	0±1500	0.5	2.0
6H + •CN → δ + HCN							
76 ENG	HYDROXYL FREE RADICAL + CYANOGEN FREE RADICAL REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	1500±1500		
6H + HCN → H ₂ δ + •CN							
76 ENG	HYDROXYL FREE RADICAL + HYDROCYANIC ACID REACTION ORDER: 2. -----	1500-2500	2.0(+11)	0.6	2500±2500	0.3	3.2
6H + CH=CH → H ₂ δ + CH=CH.							
72 KEN	HYDROXYL FREE RADICAL + ETHYNE REACTION ORDER: 2. -----	300-2000	7.6(+12)	0	2335±400	0.5	2.1
6H + CH ₂ =CH ₂ → H ₂ δ + CH ₂ -CH.							
72 KEN	HYDROXYL FREE RADICAL + ETHENE REACTION ORDER: 2. -----	3500-1400	1.6(+14)	0	2831±445	0.4	2.4
6H + CH ₂ =CH ₂ → •CH ₂ CH ₂ δH							
72 KEN/PAR	HYDROXYL FREE RADICAL + ETHENE REACTION ORDER: 2. -----	300	1.1(+12)	-	-	0.8	1.3
6H + CH ₃ CH ₃ → H ₂ δ + CH ₃ CH ₂ •							
72 KEN	HYDROXYL FREE RADICAL + ETHANE REACTION ORDER: 2. -----	302-793	1.3(+14)	0	1998		
6H + CH ₃ CH=CH ₂ → CH ₃ CH(•)CH ₂ δH + CH ₃ CH(δH)CH ₂ •							

CHEMICAL REACTIONS

	T/K	A	B	E/R (in oK)	k factors f F
HYDROXYL FREE RADICAL + 1-PROPENE 72 KEE/PAR REACTION ORDER: 2. NOTE: ADDITION TO TERMINAL CARBON OF DOUBLE BOND IS PREDOMINANTLY 95% $H\dot{O}_2 + \dot{C}_3H_7 \rightarrow CH_3 + \dot{C}_2H_5$ HYDROPEROXYL FREE RADICAL + OZONE 76 BAW/DRY REACTION ORDER: 2. -----	300	6.6(+12)	-	-	
$H\dot{O}_2 + H \rightarrow \dot{O}_2 + H_2$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 72 BAW/DRY 76 ENG REACTION ORDER: 2. -----	298	9.1(+8)	-	-	0.5 1.5
$H\dot{O}_2 + H \rightarrow H_2\dot{O} + \dot{O}$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 74 ILG NOTE: ESTIMATED. -----	290-800 1500-2500	2.5(+13) 2.5(+13)	0 0	350+350 350+500	0.4 2.5 0.5 2.0
$H\dot{O}_2 + H \rightarrow \dot{O}_2 + CH_3$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 72 BAW/DRY 76 ENG REACTION ORDER: 2. -----	300-1000	5. (+13)	0	500	0.3 3.2
$H\dot{O}_2 + H \rightarrow H_2\dot{O} + \dot{O}$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 72 BAW/DRY 76 ENG REACTION ORDER: 2. -----	290-800 1500-2500	2.5(+14) 2.5(+14)	0 0	950+350 956+500	0.5 2.0 0.5 2.0
$H\dot{O}_2 + H \rightarrow H_2\dot{O} + \dot{O}$ HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+13)	0	500+500	0.1 10.
$H\dot{O}_2 + H_2 \rightarrow H_2\dot{O}_2 + H$ HYDROPEROXYL FREE RADICAL + HYDROGEN MOLECULE 72 BAW/DRY REACTION ORDER: 2. -----	300-800	7.3(+11)	0	9400+250	0.5 2.0
$H\dot{O}_2 + H\dot{O}_2 \rightarrow H_2\dot{O}_2 + \dot{O}_2$ HYDROPEROXYL FREE RADICAL 74 ILG NOTE: ESTIMATED. k FACTORS ARE LARGER AT 1-300K. -----	300-1000	1.0(+13)	0	500	0.5 2.0
$H\dot{O}_2 + H_2\dot{O} \rightarrow H_2\dot{O}_2 + \dot{O}H$ HYDROPEROXYL FREE RADICAL + WATER 72 BAW/DRY REACTION ORDER: 2. -----	300-800	2.8(+13)	0	16500+500	0.5 1.5
$H\dot{O}_2 + SO_2 \rightarrow \dot{O}H + SO_3$ HYDROPEROXYL FREE RADICAL + SULFUR DIOXIDE 74 ILG REACTION ORDER: 2. -----	300	5.2(+8)	-	-	0.9 1.2
$H\dot{O}_2 + N \rightarrow \dot{O}_2 + NH$ HYDROPEROXYL FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0	0+2500	0.3 3.2
$H\dot{O}_2 + CO \rightarrow \dot{O}H + CO_2$ HYDROPEROXYL FREE RADICAL + CARBON MONOXIDE 76 BAW/DRY REACTION ORDER: 2. -----	700-1000	1.5(+14)	0	11900+1000	0.3 3.0
$H\dot{O}_2 + CH \rightarrow \dot{O}_2 + CH_2$					

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f F
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
$H\dot{O}_2 + CH \rightarrow \dot{C}H + \cdot CH_3$ 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
$H\dot{O}_2 + CH_3 \rightarrow \dot{C}_2 + CH_4$ 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
$H\dot{O}_2 + \cdot CH_3 \rightarrow \dot{C}_2 + HCHO$ HYDROPEROXYL FREE RADICAL + METHYL, EXG-, FREE RADICAL 76 ENG REACTION ORDER: 2. -----		1500-2500	1.0(+14)	0	1500±1500	
NOTE: k ESTIMATED. -----						
$H\dot{O}_2 + HCHO \rightarrow H_2\dot{O}_2 + \cdot CH_3$ HYDROPEROXYL FREE RADICAL + FORMALDEHYDE 74 IL6 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
$H\dot{O}_2 + CH_2=CH_2 \rightarrow$ products HYDROPEROXYL FREE RADICAL + ETHENE 74 IL6 REACTION ORDER: 2. NOTE: RATIO LATA VERSUS k _{ref} FOR $H\dot{O}_2 + C\dot{C} \rightarrow \dot{C}H + C\dot{O}_2$. k FACTORS MIGHT BE HIGHER. -----		300	1.0(+7)	-	-	0.1 10.
$H\dot{O}_2 + CH_3CH_3 \rightarrow H_2\dot{O}_2 + CH_3CH_2\cdot$ HYDROPEROXYL RADICAL + ETHANE 74 IL6 REACTION ORDER: 2. NOTE: E ESTIMATED. UPPER LIMIT RECOMMENDED. k _{ref} IS FOR $H\dot{O}_2 + C\dot{C} \rightarrow \dot{C}H + C\dot{O}_2$. -----		300-1000	1.0(+12)	0	7000	0.1 10.
$H\dot{O}_2 + CH_3CH_2CH_3 \rightarrow H_2\dot{O}_2 + (CH_3)_2CH\cdot$ HYDROPEROXYL FREE RADICAL + PROPANE 74 IL6 REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO LATA VERSUS k _{ref} FOR $H\dot{O}_2 + H\dot{O}_2 \rightarrow H_2\dot{O}_2 + \dot{O}_2$ -----		300-1000	2.0(+11)	0	5300	0.1 10.
$H\dot{O}_2 + (CH_3)_2C=CH_2 \rightarrow$ products HYDROPEROXYL FREE RADICAL + 1-PROPENE, 2-METHYL- 74 IL6 REACTION ORDER: 2. NOTE: SUGGESTED k VALUE. -----		300	1.0(+8)	-	-	0.1 10.
$H\dot{O}_2 + CH_3CH_2CH_2CH_3 \rightarrow H_2\dot{O}_2 + CH_3CH_2CH(\cdot)CH_3$ HYDROPEROXYL FREE RADICAL + BUTANE 74 IL6 REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO LATA VERSUS k _{ref} FOR $H\dot{O}_2 + H\dot{O}_2 \rightarrow H_2\dot{O}_2 + \dot{O}_2$ -----		300-1000	5.0(+11)	0	5285	0.1 10.
$H\dot{O}_2 + (CH_3)_3CH \rightarrow H_2\dot{O}_2 + (CH_3)_3C\cdot$ HYDROPEROXYL FREE RADICAL + PROPANE, 2-METHYL 74 IL6 REACTION ORDER: 2. -----		300-1000	1.0(+11)	0	3500	0.1 10.

CHEMICAL REACTIONS

NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} 



HYDROPEROXYL FREE RADICAL



REACTION ORDER: 2.

NOTE: $M = Ar, O_2, H_2O$. $k_1 = k_{k-1}$



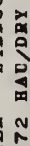
WATER + OXYGEN ATOM



REACTION ORDER: 2.



WATER + HYDROGEN ATOM



REACTION ORDER: 2.

NOTE: GIVEN k FACTORS ARE FOR HIGH T'S.



WATER + HYDROPEROXYL FREE RADICAL



REACTION ORDER: 2.



WATER + IMIDGEN FREE RADICAL



REACTION ORDER: 2.

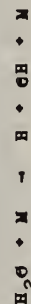


WATER + METHYL FREE RADICAL

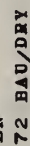


REACTION ORDER: 2.

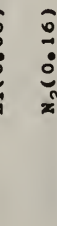
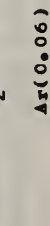
NOTE: TENTATIVE k VALUE.

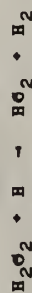


WATER

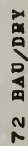


REACTION ORDER: 2.

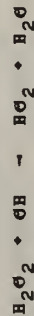
NOTE: $M = Ar$; $H_2O(1.0)$. $k_1 = k_{k-1}$  $M: N_2$



HYDROGEN PEROXIDE + HYDROGEN ATOM



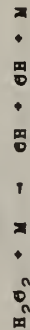
REACTION ORDER: 2.



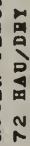
HYDROGEN PEROXIDE + HYDROXYL FREE RADICAL



REACTION ORDER: 2.



HYDROGEN PEROXIDE



REACTION ORDER: 2.

 $M: N_2$ NOTE: k FACTORS CHANGING TO: $f = 0.5$; $F = 2.0$ AT 1500K.



T/K	A	B	E/R (in °K)	k factors f F
300-2000	2.1(+15)	0	23000±250	0.5 1.5
300-2000	6.8(+13)	0	9240±200	0.7 1.5
300-2500	9.3(+13)	0	10250±100	0.5 1.5
300-800	2.8(+13)	0	16500±500	0.5 1.5
1500-2500	1.0(+11)	0.5	1500±2500	0.3 3.2
1273-1773	7.1(+12)	0	12900±1000	0.5 2.0
2000-6000	2.2(+16)	0	52900±2500	0.7 1.5
2000-6000	1.3(+15)	0	52900±2500	0.5 2.0
2000-6000	3.5(+15)	0	52900±2500	0.5 2.0
300-800	1.7(+12)	0	1900±250	0.5 2.0
300-800	1.0(+13)	0	910±150	0.5 1.5
700-1500	1.20(+17)	0	22900±1000	0.8 1.3

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f	F
250-450	1.4(+12)	0	0.0-50	0.5	1.5
298	1.3(-1)	-	-	0.5	1.5
	2.5(+12)	0.5	13640		
	6.3(+11)	0.5	0		
	1.3(+12)	0.5	12700		
	6.3(+11)	0.5	0		
	6.3(+11)	0.5	11500		
	6.3(+11)	0.5	0		
	6.3(+11)	0.5	4000		
	4.0(+12)	0.5	55200		
	4.0(+11)	0.5	17260		
	1.0(+12)	0.5	17465		
	6.3(+11)	0.5	4000		

SULFUR ATOM + OXYGEN MOLECULE
 76 HAU/DRY
 REACTION ORDER: 2.

 S + S₂ → SH + H
 SULFUR ATOM + HYDROGEN MOLECULE
 76 HAU/DRY
 REACTION ORDER: 2.
 NOTE: k₁ = k_{k-1}
 75 BEN/GOL

 S + OH → SO + H
 SULFUR ATOM + HYDROXYL FREE RADICAL
 75 BEN/GOL
 REACTION ORDER: 2.

 S + S₂ → S₂ + S
 SULFUR ATOM + SULFUR DIMER
 75 BEN/GOL
 REACTION ORDER: 2.

 S + SO → S₂ + O
 SULFUR ATOM + SULFUR MONOXIDE
 75 BEN/GOL
 REACTION ORDER: 2.

 S + SO → SO + S
 SULFUR ATOM + SULFUR MONOXIDE
 75 BEN/GOL
 REACTION ORDER: 2.

 S + SH → S₂ + H
 SULFUR ATOM + MERCAPTO FREE RADICAL
 75 BEN/GOL
 REACTION ORDER: 2.

 S + SH → SH + S
 SULFUR ATOM + MERCAPTO FREE RADICAL
 75 BEN/GOL
 REACTION ORDER: 2.

 S + N₂ → NS + N
 SULFUR ATOM + NITROGEN MOLECULE
 75 BEN/GOL
 REACTION ORDER: 2.

 S + NO → SO + N
 SULFUR ATOM + NITROGEN OXIDE (NO)
 75 BEN/GOL
 REACTION ORDER: 2.

 S + NO → NS + O
 SULFUR ATOM + NITROGEN OXIDE (NO)
 75 BEN/GOL
 REACTION ORDER: 2.

 S + NH → SH + N
 SULFUR ATOM + IMIDGEN FREE RADICAL
 75 BEN/GOL
 REACTION ORDER: 2.

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
S + NH → NS + H SULFUR ATOM + NITROGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
S + NS → S ₂ + 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 + Cd → Sc + C SULFUR ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2. -----		4.0(+12)	0.5	66530	
S + Cd → CS + d SULFUR ATOM + CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2. -----		1.3(+12)	0.5	37600	
S + CH → SE + C SULFUR ATOM + METHYLENE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
S + CH → CS + H SULFUR ATOM + METHYLENE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
S + CS → S ₂ + C SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		1.6(+12)	0.5	40463	
S + CS → CS + S SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
S + CS + M → CS ₂ + M SULFUR ATOM + CARBON MONOSULFIDE FREE RADICAL 76 HAU/DRY REACTION ORDER: 3. NOTE: K ₁ = K _{k-1} -----	1800-3700	8.7(+13)	0	4370	0.5 1.5
S + CS ₂ → S ₂ + CS SULFUR ATOM + CARBON DISULFIDE 76 HAU/DRY REACTION ORDER: 2. -----	298	3.9(+11)	-	-	0.5 1.5
S + CdS → S ₂ + Cd SULFUR ATOM + CARBON DIOXIDE SULFIDE 76 HAU/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	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f F
S + CN → CS + N SULFUR ATOM + CYANOGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
S + C₂ → 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 + ETHYLENE 72 KER/PAR REACTION ORDER: 2. -----	298	1.7(+11)	-	-	
S + CH₂=CH₂ → CY-CH₂CH₂S SULFUR ATOM + ETHYLENE 72 KER/PAR REACTION ORDER: 2. -----	298	8.1(+11)	-	-	
S + CH₃C=CH → CY-(CH₃)C=CHS SULFUR ATOM + 1-PROPENE 72 KER/PAR REACTION ORDER: 2. -----	298	1.1(+12)	-	-	
S + CH₃CH=CH₂ → CY-(CH₃)CHCH₂S SULFUR ATOM + 1-PREPENE 72 KER/PAR REACTION ORDER: 2. -----	298	5.8(+12)	-	-	
NOTE: k_{ref}: S + CH₂=CH₂ k/k_{ref}: 6.9	298	-	-	-	
S*(¹D) + CH₃CH=CH₂ → CY-(CH₃)CHCH₂S SULFUR ATOM (¹D) + 1-PREPENE 72 KER/PAR REACTION ORDER: 2. k/k_{ref}: 1.7	300	-	-	-	
NOTE: k_{ref}: S*(¹D) + CH₂=CH₂					
S + CH₃C=CCCH₃ → CY-(CH₃)C=C(CH₃)S SULFUR ATOM + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. -----	298	1.9(+13)	-	-	
S + CH₂=CHCH=CH₂ → CY-(CH₂=CH)CHCH₂S SULFUR ATOM + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. -----	298	6.0(+13)	-	-	
S + CH₃CH₂CH=CH₂ → CY-(CH₃CH₂)CHCH₂S SULFUR ATOM + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. -----	298	9.3(+12)	-	-	
NOTE: k_{ref}: S + CH₂=CH₂ k/k_{ref}: 10.0	298	-	-	-	
S + cis-CH₃CH=CHCH₃ → CY-(CH₃)CHCH(CH₃)S SULFUR ATOM + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. -----	298	1.4(+13)	-	-	
NOTE: k_{ref}: S + CH₂=CH₂ k/k_{ref}: 16.0	298	-	-	-	
S + trans-CH₃CH=CHCH₃ → CY-(CH₃)CHCH(CH₃)S SULFUR ATOM + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. -----	298	-	-	-	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
SULFUR ATOM + trans-2-BUTENE 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 20.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	1.4(+13) -	-	-	.
S + (CH ₃) ₂ C=CH ₂ → cy-(CH ₃) ₂ CCH ₂ S SULFUR ATOM + 1-PENTENE, 2-METHYL- 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 50.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	4.0(+13) -	-	-	
S*(¹ D) + (CH ₃) ₂ C=CH ₂ → cy-(CH ₃) ₂ CCH ₂ S SULFUR ATOM (¹ D) + 1-PENTENE, 2-METHYL- 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 3.5 NOTE: k _{ref} : S*(¹ D) + CH ₂ =CH ₂	300	-	-	-	
S + CH ₃ (CH ₂) ₂ CH=CH ₂ → cy-CH ₃ (CH ₂) ₂ CHCH ₂ S SULFUR ATOM + 1-PENTENE 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	8.1(+12) -	-	-	
S + CH ₃ CH ₂ C(CH ₃)=CH ₂ → cy-CH ₃ CH ₂ C(CH ₃)CH ₂ S SULFUR ATOM + 1-BUTENE, 2-METHYL- 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	7.4(+13) -	-	-	
S + (CH ₃) ₂ C=CHCH ₃ → cy-(CH ₃) ₂ CCH(CH ₃)S SULFUR ATOM + 2-BUTENE, 2-METHYL- 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	6.5(+13) -	-	-	
S + (CH ₃) ₂ C(CH ₃) ₂ → cy-(CH ₃) ₂ CC(CH ₃) ₂ S SULFUR ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KEE/PAR REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	8.5(+13) -	-	-	
S ₂ + O → S + SO SULFUR DIMER + OXYGEN ATOM 75 BEN/GEL REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	6.3(+11) -	0.5	0	
S ₂ + H → S + SH SULFUR DIMER + HYDROGEN ATOM 75 BEN/GEL REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	7.9(+12) -	0.5	8355	
S ₂ + S → S + S ₂ SULFUR DIMER + SULFUR ATOM 75 BEN/GEL REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	6.3(+11) -	0.5	0	
S ₂ + N → S + NS SULFUR DIMER + NITROGEN ATOM 75 BEN/GEL REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	6.3(+11) -	0.5	4000	
S ₂ + C → S + CS SULFUR DIMER + CARBON ATOM 75 BEN/GEL REACTION ORDER: 2. k/k _{ref} : 56.0 NOTE: k _{ref} : S + CH ₂ =CH ₂	298 298	6.3(+11) -	0.5	4000	

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
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 ₂ SULFUR MONOXIDE + OXYGEN ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		2.0(+11)	0.5	2770	
SO + O + N - SO ₂ + N SULFUR MONOXIDE + OXYGEN ATOM						
76 BAU/DRY	REACTION ORDER: 3. -----	298	6.7(+13)	-	-	0.7 1.3
SO + O ₂ - (SO ₂ + O) SULFUR MONOXIDE + OXYGEN MOLECULE						
76 BAU/DRY	REACTION ORDER: 2. -----	440-2100	4.5(+11)	0	3250±590	0.3 1.7
SO + H - O + SH SULFUR MONOXIDE + HYDROGEN ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	19930	
SO + H - S + OH SULFUR MONOXIDE + HYDROGEN ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		4.0(+12)	0.5	11200	
SO + S - O + S ₂ SULFUR MONOXIDE + SULFUR ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	11500	
SO + S - S + SO SULFUR MONOXIDE + SULFUR ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
SO + N - O + NS SULFUR MONOXIDE + NITROGEN ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		1.6(+12)	0.5	8254	
SO + N - S + NO SULFUR MONOXIDE + NITROGEN ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
SO + C - O + CS SULFUR MONOXIDE + CARBON ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
SO + C - S + CS SULFUR MONOXIDE + CARBON ATOM						
75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
SO ₂ + O - SO + O ₂ SULFUR DIOXIDE + OXYGEN ATOM						
76 BAU/DRY	REACTION ORDER: 2. -----	440-2100	1.3(+14)	-0.5	5980	0.3 1.7

CHEMICAL REACTIONS				T/K	A	B	E/R (in °K)	k factors f
NOTE: k ₁ = k _{k-1} ----- S ₂ + H + M → HS ₂ + M SULFUR DICHLORIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 3. -----				1660-2120	5.1(+15)	-	-	0.5 1.5
S ₂ + H ₂ → S ₂ + 2H SULFUR DICHLORIDE + HYDROPEROXYL FREE RADICAL 74 LLC REACTION ORDER: 2. NOTE: RATIO DATA VERSUS k _{ref} FOR REACTION H ₂ + H ₂ → H ₂ O ₂ + C ₂ -----				300	5.2(+8)	-	-	0.9 1.2
SH + O → S + OH MERCAPTO FREE RADICAL + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	4000	
SH + O → S + H MERCAPTO FREE RADICAL + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	0	
SH + H → S + H ₂ MERCAPTO FREE RADICAL + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----				298	1.5(+13)	-	-	0.5 1.5
SH + H → H + SH MERCAPTO FREE RADICAL + HYDROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	0	
SH + S → H + S ₂ MERCAPTO FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	0	
SH + S → S + SH MERCAPTO FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	4000	
SH + SH → H ₂ + S MERCAPTO FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. -----				295	7.8(+12)	-	-	0.5 1.5
SH + N → H + NS MERCAPTO FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	403	
SH + N → S + NH MERCAPTO FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	9060	
SH + C → H + CS MERCAPTO FREE RADICAL + CARBON ATOM 75 BEN/GGL REACTION ORDER: 2. -----					6.3(+11)	0.5	0	
SH + C → S + CH -----								

CHEMICAL REACTIONS

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
MERCAPTO FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $H_2S + O_3 \rightarrow H_2O + SO_2$ HYDROGEN SULFIDE + OZONE 76 BAU/DRY REACTION ORDER: 2. -----	298	4.0(+11)	0.5	6090	0.1 10.
$H_2S + H \rightarrow SH + H_2$ HYDROGEN SULFIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----	190-470	7.8(+12)	0	860±50	0.5 1.5
$H_2S + OH \rightarrow SH + H_2O$ 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
$H_2S + CH_3 \rightarrow SH + CH_4$ HYDROGEN SULFIDE + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----	300-600	2.00(+11)	0	2065±150	0.4 2.5
$N + O + M \rightarrow NO + M$ NITROGEN ATOM + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: N_2 -----	200-400	6.4(+16)	-0.5	0	0.5 1.5
$N + O_2 \rightarrow NO + O$ 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
$N + H + M \rightarrow NH + M$ NITROGEN ATOM + HYDROGEN ATOM 76 ENG REACTION ORDER: 3. -----	1500-2500	2.5(+17)	-0.5	0±1000	
$N + H_2 \rightarrow NH + H$ NITROGEN ATOM + HYDROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2. -----		2.5(+12)	0.5	18700	
$N + OH \rightarrow NO + H$ NITROGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$N + OH \rightarrow M \rightarrow HNO + M$ NITROGEN ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		1.3(+12)	0.5	17765	
$N + OH_2 \rightarrow NH + O_2$ NITROGEN ATOM + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 3. -----	1500-2500	1.00(+15)	-0.5	0	
$N + H_2O_2 \rightarrow NH + O_2$ NITROGEN ATOM + HYDROPEROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.00(+11)	0	0±2500	0.3 3.2

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f F
N + S₂ → NS + S NITROGEN ATOM + SULFUR DIMER 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
N + SO → NO + S NITROGEN ATOM + SULFUR MONOXIDE 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
N + SO → NS + O NITROGEN ATOM + SULFUR MONOXIDE 75 BEN/GGL REACTION ORDER: 2. -----		1.6(+12)	0.5	8254	
N + SH → NH + S NITROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	9060	
N + SH → NS + H NITROGEN ATOM + MERCAPTO FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	403	
N + N + M → N₂ + M NITROGEN ATOM 73 BAU/DRY 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 + N₂ → N₂ + N NITROGEN ATOM + NITROGEN MOLECULE 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
N + NO → N₂ + O NITROGEN ATOM + NITROGEN OXIDE(NO) 73 BAU/DRY 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/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
N + NO₂ → N₂ + O₂ NITROGEN ATOM + NITROGEN OXIDE(NO₂) 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	0±1500	
N + NO₂ → NO + NO NITROGEN ATOM + NITROGEN OXIDE(NO₂) 76 ENG REACTION ORDER: 2. -----	1500-2500	4.0(+12)	0	0±1500	0.2 5.0
N + NO₂ → N₂ + O NITROGEN ATOM + NITROGEN OXIDE(NO₂) 76 ENG REACTION ORDER: 2. -----	1500-2500	5.0(+12)	0	0±1500	0.5 2.0
N + N₂O → NO + N₂ -----					

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
1500-2500	5.0(+8)	0	5000+2500	0.3 3.2
	6.3(+11)	0.5	0	
	6.3(+11)	0.5	4000	
1500-2500	5.0(+10)	0.5	1500+2500	
1500-2500	1.0(+11)	0.5	1000+2500	
	6.3(+11)	0.5	0	
	6.3(+11)	0.5	4000	
	5.0(+12)	0.5	57300	
	3.2(+12)	0.5	38800	
1500-2500	2.00(+11)	0.5	1500+10000	0.1 10.
	1.0(+12)	0.5	6995	
	6.3(+11)	0.5	0	
1500-2500	6.3(+11)	0.7	20400+2500	0.3 3.2

NITROGEN ATOM + NITROGEN OXIDE(N₂O)
 76 ENG
 REACTION ORDER: 2.

 N + NH → N₂ + H
 NITROGEN ATOM + IMIDGEN FREE RADICAL
 75 BEN/GEL
 REACTION ORDER: 2.

 N + NH → NH + N
 NITROGEN ATOM + IMIDGEN FREE RADICAL
 75 BEN/GEL
 REACTION ORDER: 2.

 N + HNO → H + N₂O
 NITROGEN ATOM + NITROSYL HYDRIDE
 76 ENG
 REACTION ORDER: 2.

 N + HNO → NH + NO
 NITROGEN ATOM + NITROSYL HYDRIDE
 76 ENG
 REACTION ORDER: 2.

 N + NS → N₂ + S
 NITROGEN ATOM + NITROGEN SULFIDE(NS)
 75 BEN/GEL
 REACTION ORDER: 2.

 N + NS → NS + N
 NITROGEN ATOM + NITROGEN SULFIDE(NS)
 75 BEN/GEL
 REACTION ORDER: 2.

 N + CO → NC + C
 NITROGEN ATOM + CARBON MONOXIDE
 75 BEN/GEL
 REACTION ORDER: 2.

 N + CO → CN + C
 NITROGEN ATOM + CARBON MONOXIDE
 75 BEN/GEL
 REACTION ORDER: 2.

 N + CO₂ → NO + CO
 NITROGEN ATOM + CARBON DIOXIDE
 76 ENG
 REACTION ORDER: 2.

 N + CH → NH + C
 NITROGEN ATOM + METHYLIDENE FREE RADICAL
 75 BEN/GEL
 REACTION ORDER: 2.

 N + CH → CN + H
 NITROGEN ATOM + METHYLIDENE FREE RADICAL
 75 BEN/GEL
 REACTION ORDER: 2.

 N + CH₂ → NH + CH
 NITROGEN ATOM + METHYLIDENE FREE RADICAL
 76 ENG
 REACTION ORDER: 2.

 N + .CH₃ → C + HCN
 NITROGEN ATOM + FORMYL FREE RADICAL

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f
320-550 435	1.9(+11) -	0 -	926 -	
340	3.5(+10)	-	-	
320-550 435	1.6(+11) -	0 -	660 -	
320-550 435	2.3(+11) -	0 -	995 -	
320-550 435	3.4(+11) -	0 -	1055 -	
320-550 435	7.8(+10) -	0 -	277 -	
320-550 435	3.0(+11) -	0 -	1047 -	
320-550 435	5.3(+10) -	0 -	433 -	
320-55 435	4.6(+11) -	0 -	1233 -	

$N + CH_3C \equiv CCH_3 \rightarrow$ products
 NITROGEN ATOM + 2-BUTYNE
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH \equiv CH$.
 k/k_{ref} : 12.0

$N + CH_2-CHCH=CH_2 \rightarrow$ products
 NITROGEN ATOM + 1,3-BUTADIENE
 72 KER/PAR
 REACTION ORDER: 2.

$N + CH_3CH_2CH=CH_2 \rightarrow$ products
 NITROGEN ATOM + 1-BUTENE
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH_2=CH_2$.
 k/k_{ref} : 3.4

$N + cis-CH_3CH=CHCH_3 \rightarrow$ products
 NITROGEN ATOM + cis-2-BUTENE
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH_2=CH_2$.
 k/k_{ref} : 2.4

$N + trans-CH_3CH=CHCH_3 \rightarrow$ products
 NITROGEN ATOM + trans-2-BUTENE
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH_2=CH_2$.
 k/k_{ref} : 3.0

$N + (CH_3)_2C=CH_2 \rightarrow$ products
 NITROGEN ATOM + 1-PROPENE, 2-METHYL-
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH_2=CH_2$.
 k/k_{ref} : 4.1

$N + CH_3CH_2CH_2C \equiv CH \rightarrow$ products
 NITROGEN ATOM + 1-PENTINE
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH \equiv CH$.
 k/k_{ref} : 14.0

$N + (CH_3)_2C=CHCH_3 \rightarrow$ products
 NITROGEN ATOM + 2-BUTENE, 2-METHYL-
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH_2=CH_2$.
 k/k_{ref} : 3.5

$N + CH_3CH_2CH_2CH_2C \equiv CH \rightarrow$ products
 NITROGEN ATOM + 1-HEXYNE
 72 KER/PAR
 REACTION ORDER: 2.
 NOTE: k_{ref} : $N + CH \equiv CH$.
 k/k_{ref} : 14.0

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
$N + CH_3CH_2C \equiv CCH_2CH_3 \rightarrow$ products NITROGEN ATOM + 3-HEXYNE 72 KER/PAR REACTION ORDER: 2. k/k_{ref}: 14.0	320-550 435	3.4(+11) -	0 -	1102 -	
NOTE: k_{ref}: N + CH=CH $N + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products NITROGEN ATOM + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. k/k_{ref}: 3.5	320-550 435	1.7(+11) -	0 -	690 -	
NOTE: k_{ref}: N + CH₂=CH₂ $N_2 + O \rightarrow N + NO$ NITROGEN MOLECULE + OXYGEN ATOM 73 BAW/DRY REACTION ORDER: 2.	2000-5000	7.6(+13)	0	38000±150	0.5 2.0
NOTE: k₁ = k_{k-1} $N_2 + O + M \rightarrow N_2O + M$ NITROGEN MOLECULE + OXYGEN ATOM 73 BAW/DRY REACTION ORDER: 3. M: Ar	1300-2500	1.4(+13)	0	10400±1500	0.7 1.5
$N_2 + O_2 \rightarrow N_2O + O$ NITROGEN MOLECULE + OXYGEN MOLECULE 73 BAW/DRY REACTION ORDER: 2.	1200-2000	6.3(+13)	0	55200±2000	0.4 2.5
NOTE: k₁ = k_{k-1} $N_2 + H \rightarrow N + NH$ NITROGEN MOLECULE + HYDROGEN ATOM 75 BEN/GEL REACTION ORDER: 2.		2.0(+13)	0.5	75945	
$N_2 + S \rightarrow N + NS$ NITROGEN MOLECULE + SULFUR ATOM 75 BEN/GEL REACTION ORDER: 2.		4.0(+12)	0.5	55200	
$N_2 + N \rightarrow N + N_2$ NITROGEN MOLECULE + NITROGEN ATOM 75 BEN/GEL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
$N_2 + C \rightarrow N + CN$ NITROGEN MOLECULE + CARBON ATOM 75 BEN/GEL REACTION ORDER: 2.		1.3(+12)	0.5	22750	
$N_2 + CH \rightarrow N + HCN$ NITROGEN MOLECULE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	0	9560	
NOTE: REVISED ESTIMATE. $N_2 + CH \rightarrow NH + CN$ NITROGEN MOLECULE + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	3.2(+14)	0	46300±10000	
NOTE: k ESTIMATED. $N_2 + CH_2 \rightarrow NH + HCN$					

CHEMICAL REACTIONS			T/K	A	B	E/R (in °K)	k factors f F
NITROGEN MOLECULE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.			1500-2500	1.0(±14)	0	35230±10000	
N ₂ + M → N + N + M NITROGEN MOLECULE 76 ENG 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 → O + NO NITROGEN OXIDE(NO) + OXYGEN ATOM 75 BEN/GOL				6.3(±11)	0.5	0	
NO + O → N + O ₂ NITROGEN OXIDE(NO) + OXYGEN ATOM 73 BAU/DRY NOTE: k FACTORS INCREASING TO: f = 0.5; F = 2.0 AT 3000K. k ₁ = k ₁ -1			1000-3000	1.5(±9)	1.0	19500±150	0.7 1.3
NO + O + M → NO ₂ + M NITROGEN OXIDE(NO) + OXYGEN ATOM 73 BAU/DRY NOTE: M eff: O ₂ (1.0) AT 297K			200-500	1.1(±15)	0	-940±50	0.8 1.2
Ar(0.1) AT 297K			200-500	1.1(±14)	0	-940±50	0.8 1.2
H ₂ O(6.1) AT 297K			200-500	6.7(±15)	0	-940±50	0.8 1.2
D ₂ O(5.0) AT 297K			200-500	5.5(±15)	0	-940±50	0.8 1.2
SF ₆ (2.6) AT 297K			200-500	2.9(±15)	0	-940±50	0.8 1.2
N ₂ (1.4) AT 297K			200-500	1.5(±15)	0	-940±50	0.8 1.2
N ₂ O(2.1) AT 297K			200-500	2.3(±15)	0	-940±50	0.8 1.2
CO ₂ (2.1) AT 297K			200-500	2.3(±15)	0	-940±50	0.8 1.2
CH ₄ (2.2) AT 297K			200-500	2.4(±15)	0	-940±50	0.8 1.2
CF ₄ (2.2) AT 297K			200-500	2.4(±15)	0	-940±50	0.8 1.2
NO + O ₂ → NO ₂ + O NITROGEN OXIDE(NO) + OXYGEN MOLECULE 73 BAU/DRY NOTE: k ₁ = k ₁ -1			300-550	1.7(±12)	0	23400	0.8 1.3
NO + O ₃ → NO ₂ + O ₂ NITROGEN OXIDE(NO) + OZONE 73 BAU/DRY NOTE: k ₁ = k ₁ -1			200-350	8.9(±11)	0	1330±130	0.5 1.5
NO + H → O + NH NITROGEN OXIDE(NO) + HYDROGEN ATOM							

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
75 BEN/GOL $\text{N}_2 + \text{H} \rightarrow \text{N} + \text{GH}$ NITROGEN OXIDE(N ₂) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		5.0(+12)	0.5	38200	
$\text{N}_2 + \text{H} + \text{M} \rightarrow \text{HN}_2 + \text{M}$ NITROGEN OXIDE(N ₂) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		2.5(+12)	0.5	24460	
$\text{N}_2 + \text{H} + \text{M} \rightarrow \text{HN}_2 + \text{M}$ NITROGEN OXIDE(N ₂) + HYDROGEN ATOM 73 HAU/DRY REACTION ORDER: 3. 76 ENG -----	230-700 1500-2500	5.4(+15) 5.0(+15)	0 0	-300±100 -300±150	0.5 1.5 0.5 2.0
$\text{N}_2 + \text{S} \rightarrow \text{S} + \text{NS}$ NITROGEN OXIDE(N ₂) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. -----		1.0(+12)	0.5	17465	
$\text{N}_2 + \text{S} \rightarrow \text{N} + \text{S}_2$ NITROGEN OXIDE(N ₂) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. -----		4.0(+11)	0.5	17260	
$\text{N}_2 + \text{N} \rightarrow \text{e} + \text{N}_2$ NITROGEN OXIDE(N ₂) + NITROGEN ATOM 73 HAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 ABOVE 2000K -----	300-5000	1.6(+13)	-	-	0.8 1.2
$\text{N}_2 + \text{N} \rightarrow \text{N} + \text{N}_2$ NITROGEN OXIDE(N ₂) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_2 + \text{N}_2$ NITROGEN OXIDE(N ₂) + OXYGEN MOLECULE 72 KEN REACTION ORDER: 2. -----	1370-4300	1.3(+14)	0	38060±720	0.7 1.5
$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_2 + \text{N}_2$ NITROGEN OXIDE(N ₂) + OXYGEN MOLECULE 73 HAU/DRY REACTION ORDER: 2. -----	1200-2000	1.3(+12)	0	32100±1500	0.5 2.0
$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_2 + \text{N}_2$ NITROGEN OXIDE(N ₂) + OXYGEN MOLECULE 73 HAU/DRY REACTION ORDER: 3. -----	273-660	1.2(+9)	0	-530±100	0.5 1.5
$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_2 + \text{N}_2$ NITROGEN OXIDE(N ₂) + NITROGEN OXIDE(N ₂) 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	30200	0.01 100.
$\text{N}_2 + \text{N}_2 \rightarrow \text{N}_2 + \text{N}_2$ NITROGEN OXIDE(N ₂) + NITROGEN OXIDE(N ₂) 73 HAU/DRY REACTION ORDER: 3. -----	300-500	2.9(+7)	0	-400±500	0.4 2.5
$\text{N}_2 + \text{N}_3 \rightarrow \text{N}_2 + \text{N}_2$ NITROGEN OXIDE(N ₂) + NITROGEN OXIDE(N ₃) 72 KEN REACTION ORDER: 2. -----	298-547	1.5(+14)	0	1163±115	0.7 1.4

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f
----- NO + N₂O → NO₂ + N₂ NITROGEN OXIDE(N₂O) + NITROGEN OXIDE(N₂O) 76 ENG REACTION ORDER: 2. -----	1500-2500	2.0(±14)	0	25000	0.1 1.0
NO + HNO → N₂O + OH NITROGEN OXIDE(N₂O) + NITROGEN OXIDE(N₂O) 76 ENG REACTION ORDER: 2. -----	1500-2500	2.0(±12)	0	13000±2500	0.5 2.0
NO + C → CO + CN NITROGEN OXIDE(N₂O) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(±11)	0.5	0	
NO + C → N + CO NITROGEN OXIDE(N₂O) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(±11)	0.5	4000	
NO + CH → C + HCN NITROGEN OXIDE(N₂O) + METHYLIDINE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: K ESTIMATED.	1500-2500	2.0(±12)	0	0±1000	
NO + CH → N + CH₂ NITROGEN OXIDE(N₂O) + METHYLIDINE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: K ESTIMATED.	1500-2500	1.6(±13)	0	5000±3000	
NO + CH₂ → N + HCHO NITROGEN OXIDE(N₂O) + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: K ESTIMATED.	1500-2500	2.0(±12)	0	3500±2000	
NO + CH₃ → HNO + CH₃ NITROGEN OXIDE(N₂O) + FORMYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	2.0(±11)	0.5	1000±2500	0.3 3.2
NO + CN → N₂ + C₂ NITROGEN OXIDE(N₂O) + 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(N₂O) 76 ENG REACTION ORDER: 2. NOTE: M = Ar, CR N₂ OR O₂ GIVEN WITH CAUTION. 72 ION M: Ar	1500-2500	4.0(±20)	-1.5	75500±2500	0.3 3.2
NO₂ + O → NO + O₂ NITROGEN OXIDE(N₂O) + OXYGEN ATOM 73 BAU/DRY 76 ENG REACTION ORDER: 2. -----	3000-8000	8.00(±2)	-1.5	75500	
NO₂ + O → N + NO₃ + M NITROGEN OXIDE(N₂O) + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----	300-550 1500-2500	1.0(±13) 1.0(±13)	0 0	300±100 500±250	0.8 1.3 0.5 2.0

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f F
73 BAU/DRY NOTE: LIMITING HIGH PRESSURE K REACTION ORDER: 2. M: N ₂ K ₀ (LOW PRESSURE). -----	295	1.1(+13)	-	-	0.4 2.5
N ₂ + O ₃ → N ₂ O + O ₂ NITROGEN OXIDE(N ₂ O) + O ₂ 73 BAU/DRY REACTION ORDER: 2. -----	295	2.3(+16)	-	-	0.4 2.5
N ₂ + H → N ₂ O + OH NITROGEN OXIDE(N ₂ O) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. -----	286-302	5.9(+12)	0	3500	0.5 2.0
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + HYDROXYL FREE RADICAL 73 BAU/DRY REACTION ORDER: 3. M: H ₂ -----	298-630	3.5(+14)	0	740±500	0.5 1.5
N ₂ + O ₃ → N ₂ O + O ₂ NITROGEN OXIDE(N ₂ O) + O ₂ 76 ENG NOTE: K FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 633K. -----	1500-2500	3.2(+14)	0	750±500	0.5 2.0
N ₂ + O ₃ → N ₂ O + O ₂ NITROGEN OXIDE(N ₂ O) + O ₂ 76 ENG NOTE: K FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 633K. -----	300	5.0(+17)	-	-	0.4 1.6
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	5.0(+12)	0	0±1500	0.5 2.0
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	0±1500	0.5 2.0
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	4.0(+12)	0	0±1500	0.2 5.0
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	30200	0.01 100
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2. -----	300-500	2.9(+7)	0	-400±500	0.4 2.5
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2. -----	600-2000	2.0(+12)	0	13500±100	0.7 1.3
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(N ₂ O) 76 ENG NOTE: K FACTORS INCREASING SLIGHTLY ABOVE 1000K. -----	250-350	1.1(+13)	0	-1040	0.7 1.3
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(N ₂ O) 76 ENG NOTE: CORRECTED K VALUE (PERSONAL COMMUNICATION FROM DR. FAULCHER TO DR. BAMPSON). K ₁ = K ₂ -1 -----					
N ₂ + N → N ₂ + N ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(N ₂ O) 76 ENG NOTE: CORRECTED K VALUE (PERSONAL COMMUNICATION FROM DR. FAULCHER TO DR. BAMPSON). K ₁ = K ₂ -1 -----					

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
300-850	1.4(+11)	0	1610±500	0.4 2.5
300	2.3(+12)	-	-	0.4 2.5
300	1.0(+18)	-	-	0.5 2.0
1500-2500	2.0(+11)	0.5	2500±2500	0.3 3.2
500-800	1.9(+12)	0	14726±385	0.5 1.9
1500-2500	2.00(+12)	0	15000±1500	0.5 2.0
1400-2400	1.1(+16)	0	33000±750	0.8 1.3
299-547	1.5(+14)	0	1160±120	0.7 1.4
300-850	1.4(+11)	0	1600±500	0.4 2.5
300	2.3(+12)	-	-	0.4 2.5
300	1.0(+18)	-	-	0.5 2.0
500-1100	1.9(+11)	0	1990±110	0.8 1.3
1200-2000	1.0(+14)	0	14100±2000	0.4 2.5
1200-2000 900-2300	1.0(+14) 3.6(+13)	0 0	14000±1500 13700	0.5 2.0

73 BAU/DRY

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O₅) + NITROGEN OXIDE(N₂O₃)

73 BAU/DRY

REACTION ORDER: 2.

NOTE: LIMITING HIGH PRESSURE K

M IS A N₂O₅ + NO MIXTURE

REACTION ORDER: 3.

K₀(LOW PRESSURE). M IS A N₂O₅ + NO MIXTURE.

NITROGEN OXIDE(N₂O) + IMIDGEN FREE RADICAL

76 ENG

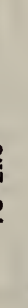
REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + CARBON MONOXIDE

72 ION

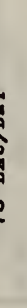
REACTION ORDER: 2.

76 ENG

NITROGEN OXIDE(N₂O)

73 BAU/DRY

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + NITROGEN OXIDE(N₂O)

72 ION

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + NITROGEN OXIDE(N₂O)

73 BAU/DRY

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + NITROGEN OXIDE(N₂O)

72 BAU/DRY

REACTION ORDER: 2.

NOTE: LIMITING HIGH-PRESSURE K. M IS A N₂O₅ + NO MIXTURE.K₁ = K₁₋₁

K₀(LOW PRESSURE). M IS A N₂O₅ + NO MIXTURE.

NITROGEN OXIDE(N₂O)

72 ION

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + OXYGEN ATOM

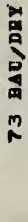
73 BAU/DRY

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + OXYGEN ATOM

73 BAU/DRY

REACTION ORDER: 2.

NITROGEN OXIDE(N₂O) + OXYGEN ATOM

72 ION

REACTION ORDER: 2.

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
NITROGEN OXIDE(N ₂ O) + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. -----		700-2500	7.6(+13)	0	7600±500	0.5 1.5
N ₂ O + H → N ₂ + NH NITROGEN OXIDE(N ₂ O) + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	1.0(+11)	0.5	15100±2500	0.3 3.2
N ₂ O + OH → N ₂ + H ₂ O NITROGEN OXIDE(N ₂ O) + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----		1500-2500	3.2(+13)	0	7550	
N ₂ O + N → N ₂ + NO NITROGEN OXIDE(N ₂ O) + NITROGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+8)	0	5000±2500	0.3 3.2
N ₂ O + NO → N ₂ + NO ₂ NITROGEN OXIDE(N ₂ O) + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. -----		1500-2500	2.0(+14)	0	25165	0.1 10.
N ₂ O + CO → N ₂ + CO ₂ NITROGEN OXIDE(N ₂ O) + CARBON MONOXIDE 76 ENG REACTION ORDER: 2. -----		1500-2500	1.0(+11)	0	10000±1500	0.5 2.0
N ₂ O + M → N ₂ + O + M NITROGEN OXIDE(N ₂ O) 73 BAU/DRY REACTION ORDER: 2. -----		1300-2500	5.0(+14)	0	29000±1500	0.7 1.5
N ₂ O ₄ → NO ₂ + NO ₂ NITROGEN OXIDE(N ₂ O ₄) 70 BEN/6°N REACTION ORDER: 1. -----		253-301	1.0(+16)	0	6600	
N ₂ O ₄ + M → NO ₂ + NO ₂ + M NITROGEN OXIDE(N ₂ O ₄) 73 BAU/DRY REACTION ORDER: 2. M: N ₂ -----		250-350	2.5(+17)	0	5550±500	0.7 1.3
N ₂ O ₅ + M → NO ₂ + NO ₃ + M NITROGEN OXIDE(N ₂ O ₅) 73 BAU/DRY REACTION ORDER: 1. NOTE: LIMITING HIGH-PRESSURE k. M IS A N ₂ O ₅ + NO MIXTURE. REACTION ORDER: 2. k ₀ (LOW PRESSURE). M IS A N ₂ O ₅ + NO MIXTURE. -----		300-340	5.7(+14)	0	10600	0.4 2.5
NB + O → H + NO IMIDGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----			1.3(+19)	0	9700	0.5 2.0
NH + O → N + OH IMIDGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----			6.3(+11)	0.5	0	
NH + O + M → HNO + M IMIDGEN FREE RADICAL + OXYGEN ATOM			6.3(+11)	0.5	4000	

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f	k factors F
76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+16)	-0.5	0+2500	0.3	3.2
NH + H → H + NH IMIDGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
NH + H → N + H ₂ IMIDGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000		
NH + OH → N + H ₂ O IMIDGEN FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	1000+2500	0.3	3.2
NH + H ₂ O → NH ₂ + H ₂ IMIDGEN FREE RADICAL + WATER 76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.5	1500+2500	0.3	3.2
NH + S → H + NS IMIDGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
NH + S → N + SH IMIDGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000		
NH + N → H + N ₂ IMIDGEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
NH + N → N + NH IMIDGEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000		
NH + NO ₂ → NH ₂ + NO IMIDGEN FREE RADICAL + NITROGEN OXIDE(NO ₂) 76 ENG	REACTION ORDER: 2. -----	1500-2500	2.0(+11)	0.5	2500+2500	0.3	3.2
NH + NH → H ₂ + N ₂ IMIDGEN FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+13)	0	0	0.1	10.
NH + C → H + CN IMIDGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
NH + C → N + CH IMIDGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000		
NH + CN → N + HCN IMIDGEN FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.5	1000+25000		

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	F
2000-3000	4.8(+14)	0	-8300±2500	0.5	2.0
----- $\text{NH}_2 \cdot + \text{M} \rightarrow \text{NH}_3 \cdot + \text{M}$ AMIDOGEN FREE RADICAL + HYDROGEN ATOM 73 BAU/DRY NOTE: $k_1 = 10^{-1}$ -----					
300-1000	1.5(+12)	0	3020±300	0.5	1.5
----- $\text{NH}_3 \cdot + \text{O} \rightarrow \text{NH}_2 \cdot + \text{OH}$ AMMONIA + OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 2. -----					
350-650	1.0(+11)	0	5100±500	0.3	1.3
----- $\text{NH}_3 \cdot + \text{CH}_3 \cdot \rightarrow \text{NH}_2 \cdot + \text{CH}_4$ AMMONIA + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----					
350-500	1.0(+11)	0	5535±500	0.3	1.3
----- $\text{ND}_3 \cdot + \text{CH}_3 \cdot \rightarrow \text{ND}_2 \cdot + \text{CH}_3\text{D}$ AMMONIA-D ₃ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----					
2000-3000	9.2(+15)	0	42400±2500	0.5	2.0
----- $\text{NH}_3 \cdot + \text{M} \rightarrow \text{H} \cdot + \text{NH}_2 \cdot + \text{M}$ AMMONIA 73 BAU/DRY REACTION ORDER: 2. -----					
250-500	1.3(+13)	0	1260±100	0.5	2.0
----- $\text{NH}_2\text{NH}_2 \cdot + \text{H} \rightarrow \text{NH}_2\text{NH} \cdot + \text{H}_2$ HYDRAZINE + HYDROGEN ATOM 73 BAU/DRY REACTION ORDER: 2. -----					
350-500	1.0(+11)	0	2515±500	0.5	2.0
----- $\text{NH}_2\text{NH}_2 \cdot + \text{CH}_3 \cdot \rightarrow \text{NH}_2\text{NH} \cdot + \text{CH}_4$ HYDRAZINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----					
350-500	7.2(+10)	0	3200±500	0.5	2.0
----- $\text{ND}_2\text{ND}_2 \cdot + \text{CH}_3 \cdot \rightarrow \text{ND}_2\text{ND} \cdot + \text{CH}_3\text{D}$ HYDRAZINE-D ₄ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----					
1250-1400	8.0(+13)	0	27700±1000	0.3	3.0
----- $\text{NH}_2\text{NH}_2 \cdot + \text{M} \rightarrow \text{NH}_2 \cdot + \text{NH}_2 \cdot + \text{M}$ HYDRAZINE 73 BAU/DRY REACTION ORDER: 2. -----					
1250-1400	4.0(+15)	0	20600±1000	0.3	3.0
----- $\text{HN}_3 \cdot + \text{CH}_3 \cdot \rightarrow \text{N}_3 \cdot + \text{CH}_4$ HYDRAZIC ACID + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----					
300-400	1.0(+11)	0	2100±500	0.5	2.0
----- $\text{HN}_3 \cdot + \text{O} \rightarrow \text{H} \cdot + \text{NO}_2$ NITROSYL HYDRIDE + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----					
1500-2500	5.0(+10)	0.5	0±2500	0.3	3.2

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
1500-2500	5.0(+11)	0.5	0+2500	0.3 3.2
1500-2500	1.0(+11)	0.5	3500+2500	0.3 3.2
2000	4.8(+12)	-	-	0.5 1.5
1500-2500	2.0(+11)	0.5	11600+2500	0.3 3.2
2000	3.6(+13)	-	-	0.5 1.5
1500-2500	1.0(+11)	0.5	1000+2500	0.3 3.2
1500-2500	5.0(+10)	0.5	1500+2500	0.3 3.2
1500-2500	2.0(+12)	0	13100+2500	0.5 2.0
1500-2500	1.0(+11)	0.5	3500+2500	0.3 3.2
1500-2500	6.3(+11)	0.5	0+2500	0.3 3.2
1500-2500	6.3(+11)	0.5	0+2500	0.3 3.2
1500-2500	5.0(+11)	0.5	0+2500	0.3 3.2
1500-2500	3.2(+11)	0.5	0+2500	0.3 3.2

$\text{HN} \cdot + \cdot \text{O} \rightarrow \text{NO} + \text{OH}$
 NITROSYL HYDRIIDE + OXYGEN ATOM
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \cdot \text{O} \rightarrow \text{NO} + \cdot \text{O}_2$
 NITROSYL HYDRIIDE + OXYGEN ATOM
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{H} \rightarrow \text{NH} + \text{H}_2$
 NITROSYL HYDRIIDE + HYDROGEN ATOM
 73 BAU/DRY
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{H} \rightarrow \text{NH} + \cdot \text{OH}$
 NITROSYL HYDRIIDE + HYDROGEN ATOM
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \cdot \text{OH} \rightarrow \text{NO} + \text{H}_2\text{O}$
 NITROSYL HYDRIIDE + HYDROXYL FREE RADICAL
 73 BAU/DRY
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{N} \rightarrow \text{N}_2 + \text{NH}$
 NITROSYL HYDRIIDE + NITROGEN ATOM
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{N} \rightarrow \text{N}_2 + \text{H}$
 NITROSYL HYDRIIDE + NITROGEN ATOM
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{NO} \rightarrow \cdot \text{OH} + \text{N}_2\text{O}$
 NITROSYL HYDRIIDE + NITROGEN OXIDE(N₂O)
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \cdot \text{CO} \rightarrow \text{NH} + \text{CO}_2$
 NITROSYL HYDRIIDE + CARBON MONOXIDE
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \cdot \text{CH} \rightarrow \text{NO} + \cdot \text{CH}_2$
 NITROSYL HYDRIIDE + METHYLIDINE FREE RADICAL
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{CH}_2 \rightarrow \text{NO} + \text{CH}_3\cdot$
 NITROSYL HYDRIIDE + METHYLENE FREE RADICAL
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{CH}_3\cdot \rightarrow \text{NO} + \text{CH}_4$
 NITROSYL HYDRIIDE + METHYL FREE RADICAL
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \cdot \text{CHO} \rightarrow \text{NO} + \text{HCHO}$
 NITROSYL HYDRIIDE + METHYL, OXO-, FREE RADICAL
 76 ENG
 REACTION ORDER: 2.

$\text{HN} \cdot + \text{CN} \rightarrow \text{NO} + \text{HCN}$

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
NITROXYL HYDRIDE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. ----- $\text{HNO}_3 + \text{OH} \rightarrow \text{NO}_3 + \text{H}_2\text{O}$ NITRIC ACID + HYDROXYL FREE RADICAL 73 HAU/DRY REACTION ORDER: 2. ----- $\text{HNO}_3 + \text{M} \rightarrow \text{NO}_2 + \text{OH} + \text{M}$ NITRIC ACID 73 HAU/DRY REACTION ORDER: 2. M: Ar ----- $\text{NS} + \text{O} \rightarrow \text{S} + \text{NO}$ NITROGEN SULFIDE(NS) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{O} \rightarrow \text{N} + \text{SO}$ NITROGEN SULFIDE(NS) + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{H} \rightarrow \text{S} + \text{NH}$ NITROGEN SULFIDE(NS) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{H} \rightarrow \text{N} + \text{SH}$ NITROGEN SULFIDE(NS) + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{S} \rightarrow \text{S} + \text{NS}$ NITROGEN SULFIDE(NS) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{S} \rightarrow \text{N} + \text{S}_2$ NITROGEN SULFIDE(NS) + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{N} \rightarrow \text{S} + \text{N}_2$ NITROGEN SULFIDE(NS) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{N} \rightarrow \text{N} + \text{NS}$ NITROGEN SULFIDE(NS) + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{C} \rightarrow \text{S} + \text{CN}$ NITROGEN SULFIDE(NS) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{NS} + \text{C} \rightarrow \text{N} + \text{CS}$ NITROGEN SULFIDE(NS) + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{C} + \text{O} + \text{M} \rightarrow \text{CO} + \text{M}$ CARBON ATOM + OXYGEN ATOM	1500-2500 300 800-1200	4.00(+11) 8.0(+10) 1.6(+15) 6.3(+11) 6.3(+11) 2.5(+12) 2.5(+12) 6.3(+11) 2.0(+11) 6.3(+11) 6.3(+11) 6.3(+11)	0.5 - 0 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	0±2500 - 15400±1500 0 4000 20735 15700 0 10870 0 4000 0 4000	0.3 3.2 0.5 2.0 0.4 2.5

CHEMICAL REACTIONS					T/K	A	B	E/R (in °K)	k factors f
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 500K. -----									
C6 + O → C + O ₂ CARBON MONOXIDE + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----						1.0(+12)	0.5	69300	
C6 + O ₂ → C6 ₂ + 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
C6 + H → O + CH CARBON MONOXIDE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----						2.5(+13)	0.5	88020	
C6 + H → C + OH CARBON MONOXIDE + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----						2.0(+13)	0.5	77755	
C6 + H + M → .CH6 + M CARBON MONOXIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: H ₂ NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 773K. -----					298-773	7.2(+14)	0	850±500	0.7 1.3
C6 + H + M → .CH6 + M CARBON MONOXIDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 3. -----					1500-2500	1.6(+20)	-1.5	0	0.3 3.2
C6 + OH → C6 ₂ + 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(cm ³ mole ⁻¹ s ⁻¹) = 10.83 + 3.94 x 10 ⁻⁴ T -----					250-2000	1.5(+ 7)	1.3	-385	0.8 1.2
C6 + H6 ₂ → C6 ₂ + OH CARBON MONOXIDE + HYDROPEROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. -----					700-1000	1.5(+14)	0	11900±1000	0.3 3.0
C6 + S → O + CS CARBON MONOXIDE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. -----						1.3(+12)	0.5	37600	
C6 + S → C + SO CARBON MONOXIDE + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. -----						4.0(+12)	0.5	66530	
C6 + N → O + CN CARBON MONOXIDE + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----						3.2(+12)	0.5	38800	
C6 + N → C + NO CARBON MONOXIDE + NITROGEN ATOM									

CHEMICAL REACTIONS

	T/K	A	B	E/R (in oK)	k factors f
75 BEN/GOL REACTION ORDER: 2. ----- $\text{C}\delta + \text{N}\delta_2 \rightarrow \text{C}\delta_2 + \text{N}\delta$ CARBON MONOXIDE + NITROGEN OXIDE($\text{N}\delta_2$) 72 KCN REACTION ORDER: 2. 76 ENG ----- $\text{C}\delta + \text{N}\delta_2 \rightarrow \text{C}\delta_2 + \text{N}_2$ CARBON MONOXIDE + NITROGEN OXIDE(N_2) 76 ENG REACTION ORDER: 2. ----- $\text{C}\delta + \text{H}\text{N}\delta \rightarrow \text{C}\delta_2 + \text{H}\delta$ CARBON MONOXIDE + NITROGEN HYDRIDE 76 ENG REACTION ORDER: 2. ----- $\text{C}\delta + \text{C} \rightarrow \text{C} + \text{C}_2$ CARBON MONOXIDE + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. ----- $\text{C}\delta + \text{CH}_3 \rightarrow \text{CH}_3\text{C}(\delta)$ CARBON MONOXIDE + METHYL FREE RADICAL 72 KCN REACTION ORDER: 2. ----- $\text{C}\delta + \text{M} \rightarrow \text{C} + \delta + \text{M}$ CARBON MONOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: K FACTORS CHANGING TO: f = 0.5; F = 1.5 OVER 10000K. M = Ar OR CO ----- $\text{C}\delta_2 + \delta \rightarrow \text{C}\delta + \delta_2$ CARBON DIOXIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: K FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K. $k_1 = k_{-1}$ ----- $\text{C}\delta_2 + \text{E} \rightarrow \text{C}\delta + \delta\text{H}$ CARBON DIOXIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2. ----- $\text{C}\delta_2 + \text{E}_2 \rightarrow \text{C}\delta + \text{H}_2\delta$ CARBON DIOXIDE + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2. ----- $\text{C}\delta_2 + \text{N} \rightarrow \text{C}\delta + \text{N}\delta$ CARBON DIOXIDE + NITROGEN ATOM 76 ENG REACTION ORDER: 2. ----- $\text{C}\delta_2 + \text{CH} \rightarrow \text{C}\delta + \cdot\text{CH}\delta$ CARBON DIOXIDE + METHYLDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. ----- $\text{C}\delta_2 + \text{M} \rightarrow \text{C}\delta + \delta + \text{M}$ CARBON DIOXIDE	57300 500-800 1500-2500 1500-2500 1500-2500 273-400 7000-15000 1500-3000 1000-3000 1500-2500 1500-2500 1500-2500 1500-2500	5.0(+12) 1.9(+12) 2.0(+12) 1.0(+11) 1.0(+11) 1.0(+12) 3.8(+8) 8.8(+29) 1.7(+13) 1.5(+14) 1.0(+9) 2.0(+11) 1.0(+10)	0.5 0 0 0 0.5 0 -3.5 0 0 0.5 0.5 0.5 0.5 0.5 0.5 0.5	14725+385 15000+1500 10000+1500 3500+2500 58025 128700+1800 26500+2500 13300+150 7550+2500 15000+10000 3000+2500	0.5 0.5 0.5 0.5 0.3 0.3 0.5 0.8 0.3 0.1 0.3 0.3

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+15)	0	5000+2500	0.5 2.0
CH + O → H + CO METHYLIDYNE FREE RADICAL + OXYGEN ATOM 75 BEN/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CH + O → C + OH METHYLIDYNE FREE RADICAL + OXYGEN ATOM 75 BEN/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
CH + O + M → CH ₂ + 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 ₂ → CH ₂ + 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/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CH + H → C + H ₂ METHYLIDYNE FREE RADICAL + HYDROGEN ATOM 75 BEN/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
CH + H + M → CH ₂ + 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 → CH ₂ + 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
CH + H ₂ → CH ₂ + H ₂ METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+10)	0.5	7550+2500	0.3 3.2
CH + H ₂ → CH ₂ + 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/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CH + S → C + SH METHYLIDYNE FREE RADICAL + SULFUR ATOM 75 BEN/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	4000	
CH + N → H + CN METHYLIDYNE FREE RADICAL + NITROGEN ATOM 75 BEN/GGL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	

CHEMICAL REACTIONS		T/K	A	B	E/R (in oK)	k factors f F
CH ₂ + O - CR + OH METHYLENE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	2.0(+11)	0.7	13000±2500	0.3 3.2
CH ₂ + O - CH ₂ + H METHYLENE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+11)	0.5	2000±2500	0.3 3.2
CH ₂ + O ₂ - HCHO + O METHYLENE FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+11)	0.5	3500±2500	0.3 3.2
CH ₂ + H - CH + H ₂ METHYLENE FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	3.2(+11)	0.7	2500±2500	0.3 3.2
CH ₂ + H ₂ - CH ₃ + H METHYLENE FREE RADICAL + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2. -----		1500-2500	3.2(+12)	0	3525±1500	
NOTE: k ESTIMATED.						
CH ₂ + OH - CH + H ₂ O METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+11)	0.5	3000±2500	0.3 3.2
CH ₂ + OH - CH ₃ + O METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----		1500-2500	5.0(+11)	0.5	3000±2500	0.3 3.2
CH ₂ + OH - HCHO + H METHYLENE FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----		1500-2500	1.0(+13)	0	2500	
NOTE: k ESTIMATED.						
CH ₂ + N - CH + NH METHYLENE FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2. -----		1500-2500	6.3(+11)	0.7	20400±2500	0.3 3.2
CH ₂ + N ₂ - HCN + NH METHYLENE FREE RADICAL + NITROGEN MOLECULE 76 ENG REACTION ORDER: 2. -----		1500-2500	1.0(+14)	0	35230±10000	
NOTE: k ESTIMATED.						
CH ₂ + NO - HCHO + N METHYLENE FREE RADICAL + NITROGEN OXIDE(NO) 76 ENG REACTION ORDER: 2. -----		1500-2500	2.0(+12)	0	3500±2000	
NOTE: k ESTIMATED.						
CH ₂ + HNO - CH ₃ + NO METHYLENE FREE RADICAL + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2. -----		1500-2500	6.3(+11)	0.5	0±2500	0.3 3.2
CH ₂ + CH ₂ - CH + CH ₃ ·						

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f
METHYLENE FREE RADICAL 76 ENG	REACTION ORDER: 2. -----			
$\text{CH}_2 + \text{CH}_4 \rightarrow \text{CH}_3 + \text{CH}_3$ METHYLENE FREE RADICAL + METHANE 76 ENG	REACTION ORDER: 2. -----	0.5	3000±2500	0.3 3.2
$\text{CH}_2 + \text{C}_2\text{H}_6 \rightarrow \text{CH}_3 + \text{C}_2\text{H}_5$ METHYLENE FREE RADICAL + METHYL, C ₂ H ₅ , FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	0.7	10000±2500	0.3 3.2
$\text{CH}_2 + \text{HCHO} \rightarrow \text{CH}_3 + \text{CHO}$ METHYLENE FREE RADICAL + FORMALDEHYDE 76 ENG	REACTION ORDER: 2. -----	0.7	500±2500	0.3 3.2
$\text{CH}_2 + \text{CN} \rightarrow \text{CH} + \text{HCN}$ METHYLENE FREE RADICAL + CYANOGEN FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	0	3270±1500	
NOTE: k ESTIMATED.				
$\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE 72 KEE/PAR	REACTION ORDER: 2. $k/k_{\text{ref}}: 1.27$ -----	-	-	
NOTE: $k_{\text{ref}}: {}^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$				
${}^3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE 72 KEE/PAR	REACTION ORDER: 2. $k/k_{\text{ref}}: 1.0$ -----	-	-	
NOTE: $k_{\text{ref}}: {}^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$				
${}^1\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-BUTENE 72 KEE/PAR	REACTION ORDER: 2. $k/k_{\text{ref}}: 1.63$ -----	-	-	
NOTE: $k_{\text{ref}}: {}^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$				
${}^3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-BUTENE 72 KEE/PAR	REACTION ORDER: 2. $k/k_{\text{ref}}: 1.6$ -----	-	-	
NOTE: $k_{\text{ref}}: {}^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$				
${}^1\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + cis-2-BUTENE 72 KEE/PAR	REACTION ORDER: 2. $k/k_{\text{ref}}: 1.37$ -----	-	-	
NOTE: $k_{\text{ref}}: {}^1\text{CH}_2 + \text{CH}_2=\text{CH}_2$				
${}^3\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + cis-2-BUTENE 72 KEE/PAR	REACTION ORDER: 2. $k/k_{\text{ref}}: 0.94$ -----	-	-	
NOTE: $k_{\text{ref}}: {}^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
297	-	-	-	
$^1\text{CH}_2 + \text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + trans-2-BUTENE 72 KEE/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	-	-	-	
$^3\text{CH}_2 + \text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + trans-2-BUTENE 72 KEE/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	-	-	-	
$^1\text{CH}_2 + (\text{CH}_3)_2\text{C=CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE, 2-METHYL- 72 KEE/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	-	-	-	
$^3\text{CH}_2 + (\text{CH}_3)_2\text{C=CH}_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 1-PROPENE, 2-METHYL- 72 KEE/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	-	-	-	
$^1\text{CH}_2 + (\text{CH}_3)_2\text{C=CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2-METHYL- 72 KEE/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	-	-	-	
$^3\text{CH}_2 + (\text{CH}_3)_2\text{C=CHCH}_3 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2-METHYL- 72 KEE/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	-	-	-	
$^1\text{CH}_2 + (\text{CH}_3)_2\text{C=C(CH}_3)_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 72 KEE/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	-	-	-	
$^3\text{CH}_2 + (\text{CH}_3)_2\text{C=C(CH}_3)_2 \rightarrow \text{products}$ METHYLENE FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 72 KEE/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 2.74$ NOTE: $k_{\text{ref}}: ^3\text{CH}_2 + \text{CH}_2=\text{CH}_2$ -----				
1500-2500	5.0(+13)	0	0	0.5 2.0
$\text{CH}_3 + \text{O} \rightarrow \text{HCHO} + \text{H}$ METHYL FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----				
1500-2500	3.2(+12)	0	34975+1500	
$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2 + \text{HO}_2$ METHYL FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----				

CHEMICAL REACTIONS

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

CHEMICAL REACTIONS					T/K	A	B	E/R (in °K)	k factors f	F
METHYL FREE RADICAL + AMMONIA 76 KER/PAR REACTION ORDER: 2. -----					350-650	1.0(+11)	0	5100±500	0.3	1.8
CH ₃ + ND ₃ → CH ₃ D + ND ₂ METHYL FREE RADICAL + AMMONIA-d ₃ 76 KER/PAR REACTION ORDER: 2. -----					350-500	1.0(+11)	0	5535±500	0.3	1.8
CH ₃ + NB ₂ NH ₂ → CH ₄ + NB ₂ NH. METHYL FREE RADICAL + HYDRAZINE 76 KER/PAR REACTION ORDER: 2. -----					350-500	1.0(+11)	0	2500±500	0.5	2.0
CH ₃ + ND ₂ ND ₂ → CH ₃ D + ND ₂ ND. METHYL FREE RADICAL + HYDRAZINE-d ₄ 76 KER/PAR REACTION ORDER: 2. -----					350-500	7.2(+10)	0	3200±500	0.5	2.0
CH ₃ + HN ₃ → CH ₄ + N ₃ METHYL FREE RADICAL + HYDRAZIC ACID 76 KER/PAR REACTION ORDER: 2. -----					300-400	1.0(+11)	0	2100±500	0.5	2.0
NOTE: TENTATIVE & VALUE.					1500-2500	5.0(+11)	0.5	0±2500	0.3	3.2
CH ₃ + HN ₂ → CH ₄ + N ₂ METHYL FREE RADICAL + NITROSYL HYDRIDE 76 KER/PAR REACTION ORDER: 2. -----					273-400	3.8(+8)	0	1968		
CH ₃ + C ₂ → CH ₃ C(2). METHYL FREE RADICAL + CARBON MONOXIDE 72 KGN REACTION ORDER: 2. -----					450-800	4.0(+11)	0	7045±250	0.7	1.3
CH ₃ + CH ₄ → CH ₄ + CH ₃ . METHYL FREE RADICAL + METHANE 76 KER/PAR REACTION ORDER: 2. -----					400-650	1.1(+11)	0	6995±250	0.7	1.3
CH ₃ + CHD ₃ → CH ₄ + CD ₃ . METHYL FREE RADICAL + METHANE-d ₃ 76 KER/PAR REACTION ORDER: 2. -----					400-650	2.5(+11)	0	7700±500	0.5	1.5
CH ₃ + CD ₄ → CH ₃ D + CD ₃ . METHYL FREE RADICAL + METHANE-d ₄ 76 KER/PAR REACTION ORDER: 2. -----					400-650	5.0(+10)	0	7200±500	0.5	1.5
CD ₃ + CH ₃ D → CD ₄ + CH ₃ . METHYL-d ₃ -FREE RADICAL + METHANE-d 76 KER/PAR REACTION ORDER: 2. -----					473-623	4.1(+12)	0	8960±250		
NOTE: TENTATIVE & VALUE.					1500-2500	3.2(+11)	0.5	0±2500	0.3	3.2
CD ₃ + CD ₄ → CD ₄ + CD ₃ . METHYL-d ₃ -FREE RADICAL + METHANE-d ₄ 72 KGN REACTION ORDER: 2. -----										
CH ₃ + .CH ₃ → CH ₄ + C ₂ METHYL FREE RADICAL + METHYL, CH ₃ ·, FREE RADICAL 76 ENG REACTION ORDER: 2.										

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
CH₃ • + HCHO → CH₄ + •CH₂O METHYL FREE RADICAL + FORMALDEHYDE 76 KEE/PAR CH₃ • + HCHO → CH₄ + •CH₂O METHYL FREE RADICAL + FORMALDEHYDE 76 ENG CH₃ • + DCD₂ → CH₃D + •CD₂ METHYL FREE RADICAL + FORMALDEHYDE-d₂ 76 KEE/PAR CH₃ • + CH₃OH → CH₄ + CH₃O• METHYL FREE RADICAL + METHANOL 76 KEE/PAR CH₃ • + CH₃OH → CH₄ + •CH₂OH METHYL FREE RADICAL + METHANOL 76 KEE/PAR CH₃ • + CH₃OH → CH₄ + CH₃O• + •CH₂OH METHYL FREE RADICAL + METHANOL 76 KEE/PAR CH₃ • + CD₃OH → CH₃D + •CD₂OH METHYL FREE RADICAL + METHAN-d₃-ol 76 KEE/PAR CH₃ • + CD₃OH → CH₄ + CD₃O• METHYL FREE RADICAL + METHAN-d₃-ol 76 KEE/PAR CD₃ • + CH₃OD → CD₃H + •CH₂OD METHYL-d₃ FREE RADICAL + METHANOL-d 76 KEE/PAR CD₃ • + CH₃OH → CD₄ + CH₃O• METHYL-d₃ FREE RADICAL + METHANOL 76 KEE/PAR NOTE: GIVEN WITH CAUTION CH₃ • + CH₃SH → CH₄ + CH₃S• + •CH₂SH METHYL FREE RADICAL + METHANETHIOL 76 KEE/PAR CH₃ • + CD₃SH → CH₄ + CD₃S• METHYL FREE RADICAL + METHANE-d₃-THIOL 76 KEE/PAR CH₃ • + CD₃SH → CH₃D + •CD₂SH METHYL FREE RADICAL + METHANE-d₃-THIOL 76 KEE/PAR	1.1(+11) 1.0(+10) 1.4(+11) 6.2(+10) 1.9(+11) 2.3(+11) 2.0(+11) 6.2(+10) 1.9(+11) 1.9(+11) 3.2(+10) 1.2(+8) 1.1(+11) 7.6(+10)	0 0.5 0 0 0 0 0 0 0 0 0 0 0 0	3070±500 3000±2500 3975±500 4900±500 5035±500 4900±500 5940±500 4900±500 5000±500 5700±1000 - 2050±500 4200±250	0.5 0.3 0.5 0.6 0.6 0.6 0.6 0.6 0.5 0.5 0.5 0.5 0.5 0.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f	F
CH ₃ ° + CN → CH ₂ ° + 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
CH ₃ ° + CH ₃ NH ₂ → CH ₄ ° + •CH ₂ NH ₂ METHYL FREE RADICAL + METHANAMINE 72 KON ----- REACTION ORDER: 2.	388-617	5.4(±11)	0	5020±500	0.3	3.0
CH ₃ ° + CH ₃ NH ₂ → CH ₄ ° + CH ₃ NH° + •CH ₂ NH ₂ METHYL FREE RADICAL + METHANAMINE 76 KEE/PAR ----- REACTION ORDER: 2.	350-650	2.1(±11)	0	4330±500	0.7	1.3
CH ₃ ° + CH ₃ ND ₂ → CH ₄ ° + •CH ₂ ND ₂ METHYL FREE RADICAL + METHANAMINE-d ₂ 76 KEE/PAR ----- REACTION ORDER: 2.	350-450	1.4(±11)	0	4530±500	0.7	1.3
CH ₃ ° + CH ₃ ND ₂ → CH ₃ D° + CH ₃ ND METHYL FREE RADICAL + METHANAMINE-d ₂ 76 KEE/PAR ----- REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-450	2.0(±11)	0	5135±1000	0.5	1.5
CH ₃ ° + CD ₃ NH ₂ → CH ₄ ° + CD ₃ NH° METHYL FREE RADICAL + METHAN-d ₃ -AMINE 76 KEE/PAR ----- REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	400-500	2.0(±11)	0	4530±750	0.5	2.0
CH ₃ ° + CD ₃ NH ₂ → CH ₃ T° + •CD ₂ NH ₂ METHYL FREE RADICAL + METHAN-d ₃ -AMINE 76 KEE/PAR ----- REACTION ORDER: 2.	400-500	7.2(±10)	0	5100±500	0.5	1.5
CH ₃ ° + CH ₃ NHNH ₂ → CH ₄ ° + CH ₃ N(•)NH ₂ + CH ₃ NHNH° + •CH ₂ NHNH ₂ METHYL FREE RADICAL + HYDRAZINE, METHYL- 76 KEE/PAR ----- REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	420	6.3(±8)	-	-	-	-
CH ₃ ° + HCONE ₂ → CH ₄ ° + ECONE° + •CONE ₂ METHYL FREE RADICAL + FORMANIDE 76 KEE/PAR ----- REACTION ORDER: 2.	350-500	3.6(±10)	0	3300±500	0.5	1.5
CH ₃ ° + HCOND ₂ → CH ₄ ° + •COND ₂ METHYL FREE RADICAL + FORMANIDE-N,N-d ₂ 76 KEE/PAR ----- REACTION ORDER: 2.	350-500	5.5(±10)	0	3575±500	0.5	2.0
CH ₃ ° + HCOND ₂ → CH ₃ D° + HCOND METHYL FREE RADICAL + FORMANIDE-N,N-d ₂ 76 KEE/PAR ----- REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-500	2.0(±11)	0	4900±500	0.5	2.0
CH ₃ ° + CH ₃ NO ₂ → CH ₄ ° + •CH ₂ NO ₂ METHYL FREE RADICAL + METHANE, NITRO- 76 KEE/PAR ----- REACTION ORDER: 2.	300-500	1.0(±11)	0	5100±750	0.5	2.5

CHEMICAL REACTIONS

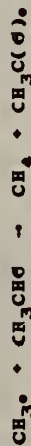
NOTE: TENTATIVE k VALUE.

CH₃ • + CH₃GNH₂ → CH₄ + CH₃GNH • METHYL FREE RADICAL + HYDROXYLAMINE, 6-METHYL- 76 KER/PAR REACTION ORDER: 2. ----- CH₃ • + CH₃CND₂ → CH₃D + CH₃CND • METHYL FREE RADICAL + HYDROXYLAMINE-N,N-d₂, 6-METHYL- 76 KER/PAR REACTION ORDER: 2. ----- CH₃ • + CH=CH → CH₄ + CH=C • METHYL FREE RADICAL + ETHYNE 76 KER/PAR REACTION ORDER: 2. ----- NOTE: GIVEN WITH CAUTION. ----- CH₃ • + CH=CH → CH₃CH=CH • METHYL FREE RADICAL + ETHYNE 72 KER/PAR REACTION ORDER: 2. ----- CH₃ • + CH₂=CH₂ → CH₄ + CH₂=CH • METHYL FREE RADICAL + ETHENE 76 KER/PAR REACTION ORDER: 2. ----- CH₃ • + CH₂=CH₂ → CH₃CH₂CH₂ • METHYL FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2. ----- CH₃ • + CH₂=CH₂ → CH₃CH₂CH₂ • + (CH₃)₂CH • METHYL FREE RADICAL + ETHENE 72 KCN REACTION ORDER: 2. ----- CH₃ • + CH₃-CH₃ → CH₄ + CH₃CH₂ • METHYL FREE RADICAL + ETHANE 76 KER/PAR REACTION ORDER: 2. ----- CH₃ • + CD₃CD₃ → CH₃D + CD₃CD₂ • METHYL FREE RADICAL + ETHANE-d₆ 76 KER/PAR REACTION ORDER: 2. ----- CD₃ • + CH₃CH₃ → CD₃H + CH₃CH₂ • METHYL-d₃ FREE RADICAL + ETHANE 72 KCN REACTION ORDER: 2. ----- CD₃ • + CH₃CD₃ → CD₃H + CD₃CH₂ • METHYL-d₃ FREE RADICAL + ETHANE-1,1,1-d₃ 76 KER/PAR REACTION ORDER: 2. ----- CD₃ • + CH₃CD₃ → CD₄ + CH₃CD₂ • METHYL-d₃ FREE RADICAL + ETHANE-1,1,1-d₃ 76 KER/PAR REACTION ORDER: 2. ----- CD₃ • + CD₃CD₃ → CD₄ + CD₃CD₂ • METHYL-d₃ FREE RADICAL + ETHANE-d₆ -----	T/K	A	B	E/R (in °K)	k factors f
300-500	5.0(+10)	0	2265±500	0.5	1.5
300-500	3.5(+10)	0	2970±500	0.5	1.5
473-773	-	-	7100		
371-479	2.5(+11)	0	3900		
350-650	4.2(+11)	0	5600±500	0.5	1.5
353-453	3.3(+11)	0	3900		
350-705	2.0(+11)	0	3575±105	0.8	1.3
400-800	5.6(+11)	0	5840±250	0.7	1.3
500-900	5.6(+11)	0	6600±250	0.7	1.3
350-800	1.0(+12)	0	6085±165	0.7	1.4
500-750	3.0(+11)	0	5900±250	0.7	1.3
500-750	4.3(+11)	0	6845±250	0.7	1.3

CHEMICAL REACTIONS

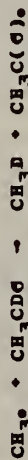
T/K	A	B	E/R (in °K)	k factors f
550-760	4.6(+11)	0	6405	
300-525	8.5(+10)	0	3000±250	0.4 1.6
300-500	1.0(+11)	0	3975±500	0.5 1.5
350-500	2.5(+11)	0	5435±750	0.5 2.0
350-550	2.0(+11)	0	4900±500	0.5 1.5
350-550	1.6(+11)	0	5635±500	0.5 1.5
350-550	3.0(+11)	0	4980±500	0.5 1.5
350-550	2.5(+11)	0	5900±500	0.5 1.5
350-550	1.6(+11)	0	5635±500	0.5 1.5
300-600	1.6(+11)	0	5135±500	0.6 1.4
400-625	7.9(+10)	0	4730±500	0.6 1.4
400-625	4.00(+11)	0	4900±500	0.6 1.4
400-625	5.1(+11)	0	4900±500	0.6 1.4

72 KGN REACTION ORDER: 2.



METHYL FREE RADICAL + ACETALDEHYDE

76 KHR/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + ACETALDEHYDE-1-d

76 KEE/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + CYRANE

76 KHR/PAR REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.



METHYL FREE RADICAL + FORMIC ACID METHYL ESTER

76 KHR/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + FORMIC ACID METHYL ESTER

76 KHR/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + FORMIC ACID METHYL ESTER

76 KHR/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER

76 KHR/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER

76 KHR/PAR REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.



METHYL FREE RADICAL + ACETIC ACID-d

76 KHR/PAR REACTION ORDER: 2.



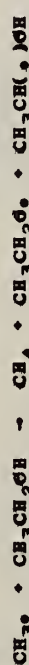
METHYL FREE RADICAL + ETHANOL

76 KEE/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + ETHANOL

76 KHR/PAR REACTION ORDER: 2.



METHYL FREE RADICAL + ETHANOL

76 KHR/PAR REACTION ORDER: 2.

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
400-550	7.1(+10)	0	4530±500	0.6 1.4
400-550	4.1(+11)	0	5735±500	0.6 1.4
400-525	4.4(+11)	0	4900±500	0.6 1.4
400-525	6.2(+10)	0	5135±500	0.5 2.0
300-550	4.2(+11)	0	5035±500	0.5 1.5
350-500	4.2(+11)	0	5000±1000	0.3 3.0
300-500	2.2(+11)	0	4800±500	0.5 2.0
303	3.5(+7)	-	-	0.5 2.0
350-600	5.4(+11)	0	5100±500	0.5 1.5
350-500	2.9(+11)	0	4200±500	0.5 2.0
350-500	2.0(+11)	0	4600±500	0.5 2.0
350-500	2.9(+11)	0	4200±500	0.5 2.0

CH₃ • CH₃CD₂OH → CH₄ + CH₃CD₂• • CH₂CD₂OH
METHYL FREE RADICAL + ETHAN-1,1-d₂-OL
76 KEE/PAR REACTION ORDER: 2.

CH₃ • CH₃CD₂OH → CH₃D + CH₃CD(•)OH
METHYL FREE RADICAL + ETHAN-1,1-d₂-OL
76 KEE/PAR REACTION ORDER: 2.

CD₃ • CH₃CH₂OD → CD₃H + CH₃CH(•)OD • CH₂CH₂OD
METHYL-d₃ FREE RADICAL + ETHANOL-d
76 KEE/PAR REACTION ORDER: 2.

CD₃ • CH₃CH₂OD → CD₄ + CH₃CH₂•
METHYL-d₃ FREE RADICAL + ETHANOL-d
76 KEE/PAR REACTION ORDER: 2.

CH₃ • CH₃•CH₃ → CH₄ + CH₃•CH₂•
METHYL FREE RADICAL + METHANE, GYXHS-
76 KEE/PAR REACTION ORDER: 2.

CH₃ • CH₃•CH₃ → CH₄ + CH₃•CH₂•
METHYL FREE RADICAL + PEROXIDE, DIMETHYL-
76 KEE/PAR REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE.

CD₃ • cy-CH₂CH₂S → CD₃H + cy-CH₂CH(•)S
METHYL-d₃ FREE RADICAL + THIIRANE
76 KEE/PAR REACTION ORDER: 2.

CH₃ • CH₃CH₂SH → CH₄ + CH₃CH₂S • CH₃CH(•)SH
• CH₂CH₂SH
METHYL FREE RADICAL + ETHANETHIOL
76 KEE/PAR REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE.

CH₃ • CH₃CN → CH₄ + •CH₂CN
METHYL FREE RADICAL + ACETONITRILE
76 KEE/PAR REACTION ORDER: 2.

CH₃ • CH₃CH₂NH₂ → CH₄ + CH₃CH₂NH • CH₃CH(•)NH₂
• CH₂CH₂NH₂
METHYL FREE RADICAL + ETHANAMINE
76 KEE/PAR REACTION ORDER: 2.

CH₃ • CH₃CH₂NH₂ → CH₄ + CH₃CH₂NH•
METHYL FREE RADICAL + ETHANAMINE
76 KEE/PAR REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE.

CH₃ • CD₃CH₂NH₂ → CH₄ + CH₃D + CD₃CH(•)NH₂ • CD₂CH₂NH₂
METHYL FREE RADICAL + ETHAN-2,2-d₃-AMINE
76 KEE/PAR REACTION ORDER: 2.

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
CH ₃ • CD ₃ CH ₂ NE ₂ → CH ₄ • CD ₃ CH ₂ NE. METHYL FREE RADICAL • ETHAN-2,2,2-d ₃ -AMINE 76 KHR/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.		423	4.0(±5)	-	-	
CH ₃ • (CH ₃) ₂ NH → CH ₄ • (CH ₃) ₂ N • • CH ₂ NHCH ₃ METHYL FREE RADICAL • METHANAMINE, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.		350-650	1.6(±11)	0	3500±500	0.5 2.0
CH ₃ • (CH ₃) ₂ NH → CH ₄ • (CH ₃) ₂ N • METHYL FREE RADICAL • METHANAMINE, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.		350-650	6.5(±10)	0	3200±500	0.5 2.0
CH ₃ • (CH ₃) ₂ ND → CH ₄ • • CH ₂ NDCH ₃ METHYL FREE RADICAL • METHANAMINE-D, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.		350-500	2.9(±11)	0	4400±500	0.5 1.5
CH ₃ • (CH ₃) ₂ ND → CH ₃ D • (CH ₃) ₂ N • METHYL FREE RADICAL • METHANAMINE-D, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.		350-500	1.0(±11)	0	4300±500	0.5 1.5
CH ₃ • CH ₃ N-NCH ₃ → CH ₄ • • CH ₂ N-NCH ₃ METHYL FREE RADICAL • DIAZENE, DIMETHYL- 76 KHR/PAR REACTION ORDER: 2.		300-500	1.1(±11)	0	3975±250	0.7 1.3
CH ₃ • CH ₃ N-NCH ₃ → (CH ₃) ₂ NN(•)CH ₃ METHYL FREE RADICAL • DIAZENE, DIMETHYL- 72 KON REACTION ORDER: 2.		300-450	5.0(±10)	0	3040±355	0.4 2.6
CD ₃ • CD ₃ N-NCD ₃ → CD ₄ • CD ₃ N-NCD ₃ METHYL-d ₃ FREE RADICAL • DIAZENE, DI(METHYL-d ₃)- 76 KHR/PAR REACTION ORDER: 2.		300-500	6.6(±10)	0	4125±500	0.5 1.5
CH ₃ • NE-CH ₂ CH ₂ NE ₂ → CH ₄ • • NHCH ₂ CH ₂ NE ₂ • NH ₂ CH(•)CH ₂ NE ₂ METHYL FREE RADICAL • 1,2-ETHANEDIAMINE 76 KHR/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.		350-500	3.8(±11)	0	4200±500	0.5 2.0
CH ₃ • NE-CH ₂ CH ₂ NE ₂ → CH ₄ • • NHCH ₂ CH ₂ NE ₂ METHYL FREE RADICAL • 1,2-ETHANEDIAMINE 76 KHR/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.		350-500	2.0(±11)	0	4430±500	0.5 2.0
CH ₃ • ND ₂ CH ₂ CH ₂ ND ₂ → CH ₄ • ND ₂ CH(•)CH ₂ ND ₂ METHYL FREE RADICAL • 1,2-ETHANEDIAMINE-d ₂ 76 KHR/PAR REACTION ORDER: 2.		350-500	2.0(±11)	0	4000±500	0.5 2.0
CH ₃ • ND ₂ CH ₂ CH ₂ ND ₂ → CH ₃ D • • NDCH ₂ CH ₂ ND ₂ METHYL FREE RADICAL • 1,2-ETHANEDIAMINE-d ₂ 76 KHR/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.		350-500	3.2(±11)	0	5100±500	0.5 2.0

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
350-500	1.7(+11)	0	2870±500	0.5 1.5
350-500	2.4(+11)	0	2970±500	0.5 1.5
350-500	3.2(+11)	0	4125±750	0.5 2.0
350-500	2.1(+11)	0	3400±500	0.5 1.5
350-500	2.5(+11)	0	2400±250	0.5 2.0
350-500	2.0(+11)	0	2700±500	0.5 2.0
400-600	7.9(+10)	0	3800±500	0.5 1.5
350-600	2.1(+11)	0	5235±500	0.5 1.5
350-600	1.0(+11)	0	5200±500	0.5 1.5
350-600	1.1(+11)	0	5235±500	0.5 1.5
350-600	1.4(+11)	0	5800±500	0.5 1.5
379-465	5.0(+11)	0	4400	

$\text{CH}_3^\bullet + (\text{CH}_3)_2\text{NNH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N}^\bullet\text{NH}_2$
METHYL FREE RADICAL + HYDRAZINE, 1,1-DIMETHYL-
76 KER/PAR REACTION ORDER: 2.

$\text{CH}_3^\bullet + (\text{CH}_3)_2\text{NNH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N}^\bullet\text{NH}_2 + \bullet\text{CH}_2\text{N}(\text{CH}_3)\text{NH}_2$
METHYL FREE RADICAL + HYDRAZINE, 1,1-DIMETHYL-
76 KER/PAR REACTION ORDER: 2.

$\text{CH}_3^\bullet + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_4 + \bullet\text{CH}_2\text{N}(\text{CH}_3)\text{ND}_2$
METHYL FREE RADICAL + HYDRAZINE- d_2 , 1,1-DIMETHYL-
76 KER/PAR REACTION ORDER: 2.
NOTE: TENTATIVE & VALUE.

$\text{CH}_3^\bullet + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{NND}^\bullet$
METHYL FREE RADICAL + HYDRAZINE- d_2 , 1,1-DIMETHYL-
76 KER/PAR REACTION ORDER: 2.

$\text{CH}_3^\bullet + \text{CH}_3\text{NNHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}(\bullet)\text{NHCH}_3 + \bullet\text{CH}_2\text{NNHCH}_3$
METHYL FREE RADICAL + HYDRAZINE, 1,2-DIMETHYL-
76 KER/PAR REACTION ORDER: 2.
NOTE: TENTATIVE & VALUE.

$\text{CH}_3^\bullet + \text{CH}_3\text{NDNDCH}_3 \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{N}(\bullet)\text{NDCH}_3$
METHYL FREE RADICAL + HYDRAZINE-1,2- d_2 , 1,2-DIMETHYL-
76 KER/PAR REACTION ORDER: 2.
NOTE: TENTATIVE & VALUE.

$\text{CH}_3^\bullet + \text{HCNCH}_3 \rightarrow \text{CH}_4 + \bullet\text{C}^\bullet\text{NCH}_3 + \text{HCN}(\bullet)\text{CH}_3$
METHYL FREE RADICAL + FORMAMIDE, N-METHYL-
76 KER/PAR REACTION ORDER: 2.

$\text{CH}_3^\bullet + \text{CH}_3\text{CONH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CONH}^\bullet + \bullet\text{CH}_2\text{CONH}_2$
METHYL FREE RADICAL + ACETAMIDE
76 KER/PAR REACTION ORDER: 2.

$\text{CH}_3^\bullet + \text{CH}_3\text{CONH}_2 \rightarrow \text{CH}_4 + \bullet\text{CH}_2\text{CONH}_2$
METHYL FREE RADICAL + ACETAMIDE
76 KER/PAR REACTION ORDER: 2.

$\text{CD}_3^\bullet + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_3\text{H} + \text{CD}_3\text{CONH}^\bullet$
METHYL FREE RADICAL + ACETAMIDE-2,2- d_3
76 KER/PAR REACTION ORDER: 2.

$\text{CD}_3^\bullet + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_4 + \bullet\text{CD}_2\text{CONH}_2$
METHYL FREE RADICAL + ACETAMIDE-2,2- d_3
76 KER/PAR REACTION ORDER: 2.

$\text{CH}_3^\bullet + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}^\bullet + \text{CH}_3\text{C}(\bullet)=\text{CHCH}_3$
METHYL FREE RADICAL + 1-PROPENE
72 KER/PAR REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE. CH_3 ADDITION OCCURS PREDOMINANTLY AT TERMINAL C ATOM.

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
373-483	2.0(±11)	0	4100	
350-600	1.4(±11)	0	4430±500	0.6 1.4
350-580	3.2(±10)	0	3775±300	0.5 2.0
353-453 453	1.7(±11)	0	3700	
550-750	2.0(±11)	0	4830±250	0.7 1.3
550-750	4.4(±11)	0	5735±250	0.7 1.3
550-750	2.5(±11)	0	5735±250	0.7 1.3
350-500	1.0(±11)	0	2970±500	0.4 1.6
350-700	3.5(±11)	0	4900±250	0.8 1.3
350-800	4.8(±11)	0	5735±250	0.8 1.3
350-500	2.5(±11)	0	5100±500	0.5 2.0
350-600	2.1(±11)	0	5035±500	0.5 1.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f F
$\text{CH}_3^\bullet + \text{CH}_3\text{COCDCD}_3 \rightarrow \text{CH}_4 + \bullet\text{CH}_2\text{COCDCD}_3$ METHYL FREE RADICAL + ACETIC ACID METHYL- d_3 ESTER 76 KER/PAR REACTION ORDER: 2.	350-650	1.9(+11)	0	5035*500	0.4 1.6
$\text{CH}_3^\bullet + \text{CD}_3\text{COCCH}_3 \rightarrow \text{CH}_4 + \text{CD}_3\text{COCCH}_2^\bullet$ METHYL FREE RADICAL + ACETIC- d_3 ACID METHYL ESTER 76 KER/PAR REACTION ORDER: 2.	400-600	1.7(+11)	0	5990*500	0.5 1.5
$\text{CH}_3^\bullet + \text{CH}_3\text{COCCH}_3 \rightarrow \text{CH}_4 + \bullet\text{CH}_2\text{COCCH}_3$ METHYL FREE RADICAL + CARBONIC ACID DIMETHYL ESTER 76 KER/PAR REACTION ORDER: 2.	350-500	3.2(+11)	0	5800*750	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3^\bullet + (\text{CH}_3)_2\text{CDCH} \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{C}(\bullet)\text{CH}$ METHYL FREE RADICAL + 2-PROPAN-2- d_1 -OL 76 KER/PAR REACTION ORDER: 2.	400-525	1.9(+11)	0	4900*500	0.6 1.4
$\text{CD}_3^\bullet + (\text{CH}_3)_2\text{CHOD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{C}(\bullet)\text{OD} + \bullet\text{CH}_2\text{CH}(\text{CH}_3)\text{OD}$ METHYL- d_3 FREE RADICAL + 2-PROPANOL- d 76 KER/PAR REACTION ORDER: 2.	400-525	1.5(+11)	0	3975*500	0.6 1.4
$\text{CH}_3^\bullet + \text{cy-CH}_2\text{CH}_2\text{CH}_2\text{S} \rightarrow \text{CH}_4 + \text{cy-CH}_2\text{CH}(\bullet)\text{CH}_2\text{S}$ METHYL FREE RADICAL + THIETANE 76 KER/PAR REACTION ORDER: 2.	300-450	3.2(+11)	0	4630*750	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3^\bullet + (\text{CH}_3)_2\text{CHSH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHS} + (\text{CH}_3)_2\text{C}(\bullet)\text{SH}$ $+ \bullet\text{CH}_2\text{CH}(\text{CH}_3)\text{SH}$ METHYL FREE RADICAL + 2-PROPANETHIOL 76 KER/PAR REACTION ORDER: 2.	303	4.1(+7)	-	-	0.5 2.0
NOTE: TENTATIVE k VALUE.					
$\text{CD}_3^\bullet + \text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}(\bullet)\text{CN} + \bullet\text{CH}_2\text{CH}_2\text{CN}$ METHYL- d_3 FREE RADICAL + PROPANENITRILE 76 KER/PAR REACTION ORDER: 2.	400-600	3.6(+11)	0	4330*500	0.5 1.5
$\text{CH}_3^\bullet + (\text{CH}_3)_3\text{N} \rightarrow \text{CH}_4 + \bullet\text{CH}_2\text{N}(\text{CH}_3)_2$ 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
$\text{CH}_3^\bullet + \text{HCN}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \bullet\text{CN}(\text{CH}_3)_2 + \text{HC}(\bullet)(\text{CH}_3)\text{NCH}_2^\bullet$ METHYL FREE RADICAL + FORMAMIDE, N,N-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.	400-600	6.3(+10)	0	3600*500	0.5 1.5
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3^\bullet + \text{CH}_3\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\bullet)\text{C}\equiv\text{CH}$ $+ \bullet\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} + \text{CH}_3\text{CH}_2\text{C}\equiv\text{C}\bullet$ METHYL FREE RADICAL + 1-BUTYNE 76 KER/PAR REACTION ORDER: 2.	456-620	1.9(+12)	0	5135*500	0.6 1.4
NOTE: TENTATIVE k VALUE.					
$\text{CH}_3^\bullet + \text{CH}_3\text{C}\equiv\text{CCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}\equiv\text{CCH}_2^\bullet$ METHYL FREE RADICAL + 2-BUTYNE 76 KER/PAR REACTION ORDER: 2.					

CHEMICAL REACTIONS

CHEMICAL REACTIONS		T/K	A	B	E/R (in OK)	k factors f
76 KER/PAR	REACTION ORDER: 2.	486-619	1.1(+12)	0	4900*500	0.6 1.4
NOTE: INITIATIVE k VALUE.						
CH ₃ • CH ₃ -CHCH-CH ₂ → CH ₃ CH ₂ CH(•)CH-CH ₂	-----					
METHYL FREE RADICAL • 1,3-BUTADIENE						
72 KER/PAR	REACTION ORDER: 2.	353-453	8.1(+10)	0	2065	
CH ₃ • CH ₂ -CHCH-CH ₂ → CH ₃ CH ₂ CH(•)CH-CH ₂	-----					
•CH ₂ CH(CH ₃)CH-CH ₂						
METHYL FREE RADICAL • 1,3-BUTADIENE						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 12.0	453	-	-	-	
NOTE: k _{ref} : CH ₃ • CH ₂ -CH ₂						
CH ₃ • CH ₃ CH ₂ CH-CH ₂ → CH ₄ • CH ₃ CH(•)CH-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
CH ₃ • CH ₃ CH ₂ CH-CH ₂ → CH ₃ CH ₂ CH(•)CHCH ₃	-----					
•CH ₃ CH ₂ CH(CH ₃)CH ₂ •						
METHYL FREE RADICAL • 1-BUTENE						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 0.7	353-453 453	1.0(+11)	0	3600	
NOTE: k _{ref} : CH ₃ • CH ₂ -CH ₂						
CH ₃ • cis-CH ₃ CH-CHCH ₃ → CH ₄ • CH ₃ CH-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
CH ₃ • cis-CH ₃ CH-CHCH ₃ → (CH ₃) ₂ CHCH(•)CH ₃	-----					
METHYL FREE RADICAL • cis-2-BUTENE						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 0.2	353-453 453	4.5(+10)	0	3675	
NOTE: k _{ref} : CH ₃ • CH ₂ -CH ₂						
CH ₃ • trans-CH ₃ CH-CHCH ₃ → CH ₄ • CH ₃ CH-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
CH ₃ • trans-CH ₃ CH-CHCH ₃ → (CH ₃) ₂ CHCH(•)CH ₃	-----					
METHYL FREE RADICAL • trans-2-BUTENE						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 0.4	353-453 453	1.4(+11)	0	4075	
NOTE: k _{ref} : CH ₃ • CH ₂ -CH ₂						
CH ₃ • (CH ₃) ₂ C-CH ₂ → CH ₄ • CH ₂ C(CH ₃)-CH ₂	-----					
METHYL FREE RADICAL • 1-PHOPENE, 2-METHYL-						
76 KER/PAR	REACTION ORDER: 2.	350-600	3.0(+11)	0	4500*500	0.6 1.4
CH ₃ • (CH ₃) ₂ C-CH ₂ → (CH ₃) ₃ CCH ₂ • • (CH ₃) ₂ C(•)CH ₂ CH ₃	-----					
METHYL FREE RADICAL • 1-PROPENE, 2-METHYL-						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 1.1	353-453 453	1.4(+11)	0	3475	
NOTE: k _{ref} : CH ₃ • CH ₂ -CH ₂						

CHEMICAL REACTIONS

T/K	A	B	E/R (ln OK)	k factors f F
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + BUTANE 76 KBR/PAR REACTION ORDER: 2.	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 KBN REACTION ORDER: 2.	1.6(+11)	0	4540±150	0.7 1.4
$\text{CD}_3 \cdot + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_2\cdot$ METHYL-d ₃ FREE RADICAL + BUTANE-2,2,3,3-d ₄ 76 KBR/PAR REACTION ORDER: 2.	4.8(+11)	0	5735±250	0.7 1.3
$\text{CD}_3 \cdot + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_4 + \text{CH}_3\text{CD}_2\text{CD}(\cdot)\text{CH}_3$ METHYL-d ₃ FREE RADICAL + BUTANE-2,2,3,3-d ₄ 76 KBR/PAR REACTION ORDER: 2.	4.5(+11)	0	5735±250	0.7 1.3
$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C} \cdot + (\text{CH}_3)_2\text{CHCH}_2\cdot$ METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2.	8.3(+10)	0	4000±500	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C} \cdot$ METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2.	9.6(+10)	0	3975±250	0.7 1.3
$\text{CD}_3 \cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{CDCH}_2\cdot$ METHYL-d ₃ FREE RADICAL + PROPANE-2-d, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2.	6.0(+11)	0	5735±250	0.7 1.3
$\text{CD}_3 \cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_4 + (\text{CH}_3)_3\text{C} \cdot$ METHYL-d ₃ FREE RADICAL + PROPANE-2-d, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2.	1.2(+11)	0	4800±250	0.7 1.3
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{CHC}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + 2-BUTENAL 76 KBR/PAR NOTE: TENTATIVE & VALUE.	1.0(+11)	0	3400±500	0.4 2.5
$\text{CH}_3 \cdot + \text{CH}_3\text{COCCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{COCCH}_2\cdot$ METHYL FREE RADICAL + 2,3-BUTANEDIONE 76 KBR/PAR REACTION ORDER: 2.	2.2(+11)	0	4300±500	0.5 1.5
$\text{CH}_3 \cdot + (\text{CH}_3\text{C}_6\text{H}_5) \rightarrow \text{CH}_4 + \text{CH}_3\text{C}_6\text{H}_5\text{CCH}_2\cdot$ METHYL FREE RADICAL + ACETIC ACID ANHYDRIDE 76 KBR/PAR REACTION ORDER: 2.	1.8(+11)	0	4830±500	0.6 1.4
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + BUTANAL 76 KBR/PAR NOTE: TENTATIVE & VALUE.	1.0(+11)	0	2970±500	0.4 1.6
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHC}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + ISOBUTANAL 76 KBR/PAR NOTE: TENTATIVE & VALUE.				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	k factors F
350-500	1.0(±11)	0	2970±500	0.4	1.6
METHYL FREE RADICAL + PROPANAL, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.					
350-500	1.0(±11)	0	2970±500	0.4	1.6
300-500	8.2(±10)	0	3700±500	0.5	1.5
347-455	1.3(±10)	0	3675		
350-500	2.5(±11)	0	5000±500	0.5	2.0
350-500	2.5(±11)	0	4980±500	0.5	2.0
400-500	2.5(±11)	0	4200±750	0.5	2.0
303	5.9(±7)	-	-	0.5	2.0
350-600	2.5(±11)	0	3975±500	0.5	2.0
426	3.2(±7)	-	-	0.5	2.0
350-500	2.2(±11)	0	3550±500	0.5	2.0

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
420	2.6(+7)	-	-	0.5 2.0
350-600	2.0(+11)	0	4200±500	0.5 1.5
350-600	1.6(+11)	0	4125±500	0.5 1.5
450-650	4.5(+11)	0	4500±500	0.6 1.4
258	-	-	4060	
298	-	-	4125	
298	-	-	3500	
450-600	4.4(+11)	0	4225±7500	0.5 1.5
400-500	4.9(+11)	0	4300±500	0.5 1.5
453	-	-	-	
403-455	1.4(+10)	0	3070	

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f	
76 KER/PAR	REACTION ORDER: 2.	350-800	4.8(+11)	0	5800±250	0.7	1.3
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$							
$\cdot\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$							
METHYL FREE RADICAL + PENTANE							
76 KER/PAR	REACTION ORDER: 2.	350-800	6.0(+11)	0	4830±250	0.7	1.3
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$							
METHYL FREE RADICAL + BUTANE, 2-METHYL-							
76 KER/PAR	REACTION ORDER: 2.	350-750	9.6(+10)	0	3975±250	0.7	1.3
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$							
METHYL FREE RADICAL + BUTANE, 2-METHYL-							
76 KER/PAR	REACTION ORDER: 2.	350-750	2.0(+11)	0	4830±250	0.7	1.3
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$							
$\cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$							
METHYL FREE RADICAL + BUTANE, 2-METHYL-							
76 KER/PAR	REACTION ORDER: 2.	350-750	7.1(+11)	0	5800±250	0.7	1.3
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3)_4\text{C} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\cdot$							
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
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\cdot)\text{CH}_3$							
METHYL FREE RADICAL + PENTANAL							
76 KER/PAR	REACTION ORDER: 2.	350-500	1.0(+11)	0	3000±500	0.4	1.6
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\cdot)\text{CH}_3$							
METHYL FREE RADICAL + BUTANAL, 2-METHYL-							
76 KER/PAR	REACTION ORDER: 2.	350-500	1.0(+11)	0	3200±500	0.5	2.0
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)\text{CH}_3$							
METHYL FREE RADICAL + BUTANAL, 3-METHYL-							
76 KER/PAR	REACTION ORDER: 2.	350-500	1.0(+11)	0	3070±500	0.4	1.6
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CCCHO} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CC}(\cdot)\text{CH}_3$							
METHYL FREE RADICAL + PROPANAL, 2,2-DIMETHYL-							
76 KER/PAR	REACTION ORDER: 2.	350-500	1.0(+11)	0	3170±500	0.5	2.0
NOTE: TENTATIVE & VALUE.							

$\text{CH}_3 \cdot + (\text{CH}_3\text{CH}_2)_2\text{CCO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{C}(\text{CH}_3)_2\text{CH}_3$							
$\cdot\text{CH}_2\text{CH}_2\text{CCCH}_2\text{CH}_3$							
METHYL FREE RADICAL + 3-PENTANONE							
76 KER/PAR	REACTION ORDER: 2.	300-450	1.9(+11)	0	3675±500	0.5	1.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$\text{CH}_3 \cdot + (\text{CH}_3\text{CD}_2)_2\text{C}\dot{\text{C}}\text{H} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{C}\dot{\text{C}}\text{H}_2\text{CH}_2 \cdot$ METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d ₄ 76 IER/PAR REACTION ORDER: 2.	500-600	2.0(+11)	0	5535±500	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3\text{CD}_2)_2\text{C}\dot{\text{C}}\text{H} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CD}_2\text{C}\dot{\text{C}}\text{H}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d ₄ 76 IER/PAR REACTION ORDER: 2.	500-600	1.3(+11)	0	4200±500	0.5 2.0
$\text{CH}_3 \cdot + \text{HC}\dot{\text{C}}\text{H}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_4 + \cdot\text{C}\dot{\text{C}}\text{H}(\text{CH}_2)_3\text{CH}_3$ $+ \text{HC}\dot{\text{C}}\text{H}(\cdot)(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{HC}\dot{\text{C}}\text{H}_2\text{CH}(\cdot)(\text{CH}_2)\text{CH}_3$ $+ \text{HC}\dot{\text{C}}\text{H}_2\text{CH}_2\text{CH}(\cdot)(\text{CH}_3) \rightarrow \text{HC}\dot{\text{C}}\text{H}(\text{CH}_2)_3\text{CH}_2$ METHYL FREE RADICAL + FORMIC ACID BUTYL ESTER 76 IER/PAR REACTION ORDER: 2.	350-500	2.5(+11)	0	4980±500	0.5 2.0
NOTE: TENTATIVE & VALUE.					
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{C}\dot{\text{C}}\text{HCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{C}\dot{\text{C}}\text{HCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{C}\dot{\text{C}}\text{H}(\cdot)\text{CH}_3 \rightarrow \cdot\text{CH}_2\text{CH}_2\text{C}\dot{\text{C}}\text{HCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{C}\dot{\text{C}}\text{HCH}_2\text{CH}_2 \cdot$ METHYL FREE RADICAL + PROPANOIC ACID ETHYL ESTER 76 IER/PAR REACTION ORDER: 2.	300-650	2.5(+11)	0	4125±500	0.5 1.5
$\text{CH}_3 \cdot + (\text{CH}_3\text{CH}_2)_2\text{NCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)\text{CH}_3$ $+ \cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)\text{CH}_3 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{NCH}_2 \cdot$ METHYL FREE RADICAL + ETHANAMINE, N-ETHYL-N-METHYL- 76 IER/PAR REACTION ORDER: 2.	420	3.0(+7)	-	-	0.5 2.0
NOTE: TENTATIVE & VALUE.					
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NCON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{CON}(\text{CH}_3)_2$ METHYL FREE RADICAL + UREA TETRAMETHYL- 76 IER/PAR REACTION ORDER: 2.	350-550	2.0(+11)	0	3975±500	0.5 1.5
$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH-CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)(\text{CH}(\text{CH}_3)_2)$ METHYL FREE RADICAL + cis-2-HEXENE 72 IER/PAR REACTION ORDER: 2.	298	-	-	4060	
$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH-CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)(\text{CH}_3)$ METHYL FREE RADICAL + cis-2-HEXENE 72 IER/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 IER/PAR REACTION ORDER: 2.	298	-	-	3450	
$\text{CH}_3 \cdot + \text{cis-}(\text{CH}_3)_2\text{CHCH-CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)(\text{CH}(\text{CH}_3)_2)$ METHYL FREE RADICAL + cis-2-PENTENE, 4-METHYL- 72 IER/PAR REACTION ORDER: 2.	298	-	-	4390	
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}-(\text{CH}_3)\text{C}\dot{\text{C}}\text{H}_2 \cdot$ METHYL FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 76 IER/PAR REACTION ORDER: 2.	403-614	7.8(+11)	0	4400±500	0.6 1.4
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{C}\dot{\text{C}}(\cdot)(\text{CH}_3)_2$					

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f
403-453 453	1.0(+10) -	0 -	3400 -	
METHYL FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. NOTE: $k_{ref} = CH_3 \cdot + CH_2=CH_2$ $k/k_{ref} = 0.2$ ----- $CH_3 \cdot + CH_3(CH_2)_4CH_3 \rightarrow CH_4 + CH_3(CH_2)_4CH_2 \cdot$ METHYL FREE RADICAL + HEXANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- $CH_3 \cdot + CH_3(CH_2)_4CH_3 \rightarrow CH_4 + CH_3CH_2CH_2CH_2CH_2CH_3$ $+ CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ METHYL FREE RADICAL + HEXANE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- $CH_3 \cdot + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + \cdot CH_3CH_2CH(CH_3)CH(CH_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- $CH_3 \cdot + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2C(\cdot)CH(CH_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- $CH_3 \cdot + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2CHC(\cdot)(CH_3)_2$ $+ \cdot CH_3CH(CH_3)CH(CH_3)_2$ METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KER REACTION ORDER: 2. ----- $CD_3 \cdot + (CH_3)_2CHCH(CH_3)_2 \rightarrow CD_3H + (CH_3)_2C(\cdot)CH(CH_3)_2$ $+ \cdot CH_2CH(CH_3)CH(CH_3)_2$ METHYL-d3 FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KER REACTION ORDER: 2. ----- $CH_3 \cdot + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2C(\cdot)CH(CH_3)_2$ $+ \cdot CH_2CH(CH_3)CH(CH_3)_2$ METHYL FREE RADICAL + PROPANE, 2,2'-DIBIS- 76 KER/PAR REACTION ORDER: 2. ----- $CH_3 \cdot + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2C(\cdot)CH(CH_3)_2$ $+ \cdot CH_2CH(CH_3)CH(CH_3)_2$ METHYL FREE RADICAL + PEROXIDE, BIS(1-METHYLETHYL)- 76 KER/PAR REACTION ORDER: 2. ----- $CH_3 \cdot + CH_3CH=NC(CH_3)_3 \rightarrow CH_4 + CH_3C(\cdot)=NC(CH_3)_3$ $+ \cdot CH_2CH=NC(CH_3)_3 + CH_3CH=NC(CH_3)_2CH_2 \cdot$ METHYL FREE RADICAL + PROPANIMINE, N-ETHYLIDENE-2-METHYL- 76 KER/PAR REACTION ORDER: 2. -----				
350-800	4.8(+11)	0	5800±250	0.7 1.3
350-800	7.9(+11)	0	4830±250	0.7 1.3
350-750	9.5(+11)	0	5800±250	0.7 1.3
350-750	1.9(+11)	0	3975±250	0.7 1.3
300-500	5.0(+10)	0	3445	
439-566	4.7(+11)	0	4525	
400-600	2.1(+11)	0	4100±500	0.5 2.0
300-450	2.3(+11)	0	4100±500	0.5 1.5
350-500	8.9(+10)	0	3925±500	0.5 1.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CNECH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{N}(\text{CH}_3)_2$ $(\text{CH}_3)_2\text{C}(\cdot)\text{N}(\text{CH}_3)_2$ METHYL FREE RADICAL + 2-PROPANAMINE, N-(1-METHYLETHYL)- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-500	2.0(+11)	0	3370±750	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3\text{CH}_2)_3\text{N} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$ $\cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2$ METHYL FREE RADICAL + ETHANAMINE, N,N-DIETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-600	5.0(+11)	0	4000±500	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_3\text{C}\cdot$ METHYL FREE RADICAL + PENTANE, 3-ETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$\text{CH}_3 \cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{CHCH}(\cdot)(\text{CH}_3)$ METHYL FREE RADICAL + PENTANE, 3-ETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	6.0(+11)	0	4830±250	0.7 1.3
$\text{CH}_3 \cdot + (\text{CH}_3\text{CH}_2)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3\text{CH}_2)_2\text{CHCH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + PENTANE, 3-ETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
$\text{CH}_3 \cdot + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot$ METHYL FREE RADICAL + OCTANE 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-800	4.8(+11)	0	5800±250	0.7 1.3
$\text{CH}_3 \cdot + \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $\text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)(\text{CH}_3)$ METHYL FREE RADICAL + OCTANE 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-800	1.2(+12)	0	4830±250	0.7 1.3
$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCCH}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	2.0(+11)	0	4830±250	0.7 1.3
$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCCH}_2\text{C}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ $\cdot\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ METHYL FREE RADICAL + PENTANE, 2,2,4-TRIMETHYL- 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
----- CH₄ + CH₂ → CH₃ + CH₃ METHANE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.3(±12)	0.7	10000±2500	0.3 3.2
CH₄ + CH₃ → CH₃ + CH₄ METHANE + METHYL FREE RADICAL 76 KBr/PAr REACTION ORDER: 2. -----	450-800	4.0(±11)	0	7045±250	0.7 1.3
CH₃D + CD₃ → CH₃ + CD₄ METHANE-d + METHYL-d₃ FREE RADICAL 76 KBr/PAr REACTION ORDER: 2. NOTE: TENTATIVE & VALUE. -----	400-650	5.0(±10)	0	7200±500	0.5 1.5
CHD₃ + CH₃ → CD₃ + CH₄ METHANE-d₃ + METHYL FREE RADICAL 76 KBr/PAr REACTION ORDER: 2. NOTE: TENTATIVE & VALUE. -----	400-650	1.1(±11)	0	6995±250	0.7 1.3
CD₄ + CH₃ → CD₃ + CDH₃ METHANE-d₄ + METHYL FREE RADICAL 76 KBr/PAr REACTION ORDER: 2. -----	370-550	2.5(±11)	0	7700±500	0.5 1.5
CD₄ + CD₃ → CD₃ + CD₄ METHANE-d₄ + METHYL-d₃ FREE RADICAL 72 ION REACTION ORDER: 2. -----	473-623	4.1(±12)	0	8960±250	
CH₄ + CN → HCN + CH₃ METHANE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(±11)	0.7	2500±2500	0.3 3.2
CH₄ + M → CH₃ + H + M METHANE 76 ENG REACTION ORDER: 2. -----	1500-2500	2.0(±17)	0	44035±1000	0.5 2.0
CH₃D → CD + H METHYL, CH₃-d, FREE RADICAL 70 BEN/G'N REACTION ORDER: 1. -----	298	5.0(±13)	0	9560	
CH₃D + D → CD₂ + H METHYL, CH₃-d, FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: & ESTIMATED. -----	1500-2500	3.2(±11)	0	0±1500	
CH₃D + D → CD + CH₃ METHYL, CH₃-d, FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: & ESTIMATED. -----	1500-2500	3.2(±11)	1.0	250±1500	
CH₃D + D₂ → CD + HD₂ METHYL, CH₃-d, FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: & ESTIMATED. -----	1500-2500	1.6(±12)	0	1500±2500	

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
1500-2500	1.6(+12)	0.5	0.2500	0.3 3.2
1500-2500	3.2(+10)	1.0	0.1500	
1500-2500	1.0(+14)	0	1500.1500	
1500-2500	1.0(+14)	0	0.1000	
1500-2500	2.0(+11)	0.5	1000.2500	0.3 3.2
1500-2500	2.0(+11)	0.5	1000.2500	0.3 3.2
1500-2500	3.2(+11)	0.5	0.2500	0.3 3.2
1500-2500	3.2(+10)	0.7	500.2500	0.3 3.2
1500-2500	3.2(+10)	0.7	500.2500	0.3 3.2
1500-2500	3.2(+11)	0.5	0.2500	0.3 3.2
1500-2500	1.6(+11)	0.5	0.2500	0.3 3.2
1500-2500	2.0(+11)	0.5	0.2500	0.3 3.2

CHEMICAL REACTIONS					T/K	A	B	E/R (in °K)	k factors f	k factors F
FORMALDEHYDE + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----					1500-2500	1.0(+11)	1.0	1750±1000	0.5	2.0
HCHO + O → products FORMALDEHYDE + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2. -----					300	9.0(+10)	-	-	0.7	1.3
HCHO + O → products FORMALDEHYDE-d + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2. -----					300	4.9(+10)	-	-	0.7	1.3
HCHO + H → .CHO + H ₂ FORMALDEHYDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. -----					1500-2500	1.3(+10)	1.0	1600	0.3	3.2
HCHO + OH → .CHO + H ₂ O FORMALDEHYDE + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----					1500-2500	3.2(+10)	1.0	0±1500	0.5	2.0
HCHO + H ₂ → .CHO + H ₂ O ₂ FORMALDEHYDE + HYDROPEROXYL FREE RADICAL 74 ILC REACTION ORDER: 2. NOTE: k FACTORS ARE: f = 0.1; F = 10. AT 300K. -----					300-800	1.0(+12)	0	4000	0.7	1.5
HCHO + CH → .CHO + CH ₂ FORMALDEHYDE + METHYLIDINE FREE RADICAL 76 ENG REACTION ORDER: 2. -----					1500-2500	1.0(+11)	0.7	2000±2500	0.3	3.2
HCHO + CH ₂ → .CHO + CH ₃ FORMALDEHYDE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----					1500-2500	2.0(+11)	0	3270±1500	-	-
HCHO + CH ₃ → .CHO + CH ₄ FORMALDEHYDE + METHYL FREE RADICAL 76 BEN/FAR REACTION ORDER: 2. -----					300-500 1500-2500	1.1(+11) 1.0(+10)	0 0.5	3070±500 3000±2500	0.5 0.3	1.5 3.2
DCDO + CH ₃ → .CDO + CH ₃ D FORMALDEHYDE-d + METHYL FREE RADICAL 76 BEN/FAR REACTION ORDER: 2. -----					300-500	1.4(+11)	0	3975±500	0.5	1.5
HCHO + CN → .CHO + HCN FORMALDEHYDE + CYANOGEN FREE RADICAL 76 ENG REACTION ORDER: 2. -----					1500-2500	1.3(+11)	0.7	1500±2500	0.3	3.2
HCHO + M → .CHO + H + M FORMALDEHYDE 76 ENG REACTION ORDER: 2. -----					1500-2500	3.2(+17)	0	43800±2500	0.3	3.2
.CH ₂ OH → HCHO + H METHYL, HYDROXY-, FREE RADICAL 70 BEN/G'N REACTION ORDER: 2. -----					673-773	1.1(+13)	0	14600		

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
CH₃O. + O → HCHO + OH METHOXY FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(±14)	0	0±1500	
CH₃O. + O₂ → HCOO + HO₂ METHOXY FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(±12)	0	3000±1500	
CH₃O. + H → HCHO + H₂ METHOXY FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(±14)	0	0±1500	
CH₃O. + OH → HCHO + H₂O METHOXY FREE RADICAL + HYDROXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(±13)	0	0±1500	
CH₃O. + N → HCHO + NH METHOXY FREE RADICAL + NITROGEN ATOM 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	1.0(±14)	0	0±1500	
CH₃O. + M → HCHO + H + M METHOXY FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	4.0(±40)	-1.5	11375±1500	
CH₃OH + CH₃ → CH₂OH + CH₄ METHANOL + METHYL FREE RADICAL 76 IHR/PAR REACTION ORDER: 2.	350-500	1.9(±11)	0	5035±500	0.6 1.4
CH₃OH + CH₃ → CH₃O. + CH₄ METHANOL + METHYL FREE RADICAL 76 IHR/PAR REACTION ORDER: 2.	350-550	6.2(±10)	0	4900±500	0.6 1.4
CH₃OD + CD₃ → CH₂OD + CD₃H METHANOL-d + METHYL-d₃ FREE RADICAL 76 IHR/PAR REACTION ORDER: 2.	400-500	2.3(±11)	0	4930±500	0.6 1.4
CH₃OD + CD₃ → CH₃O. + CD₄ METHANOL-d + METHYL-d₃ FREE RADICAL 76 IHR/PAR REACTION ORDER: 2. NOTE: GIVEN WITH CAUTION.	400-500	1.9(±11)	0	5000±500	0.5 2.0
CD₃OH + CH₃ → CD₂OH + CH₃D. METHANOL-d₃ + METHYL FREE RADICAL	400-500	3.2(±10)	0	5700±1000	0.5 2.0

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
76 KEE/PAR $\text{CD}_3\text{OH} + \text{CH}_3^{\bullet} \rightarrow \text{CD}_3\text{O}^{\bullet} + \text{CH}_4$ METHAN- d_3 -OL + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. ----- $\text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}^{\bullet} + \text{OH}^{\bullet}$ HYDROPEROXIDE, METHYL 70 BEN/G'N REACTION ORDER: 1. 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. ----- $\text{CS} + \text{O} \rightarrow \text{S} + \text{CO}$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{O} \rightarrow \text{SC} + \text{C}$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN 75 HEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{H} \rightarrow \text{S} + \text{CH}$ CARBON MONOSULFIDE FREE RADICAL + HYDROGEN ATOM 75 HEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{H} \rightarrow \text{SH} + \text{C}$ CARBON MONOSULFIDE FREE RADICAL + HYDROGEN ATOM 75 HEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{S} \rightarrow \text{S} + \text{CS}$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{S} \rightarrow \text{C} + \text{S}_2$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{S} + \text{M} \rightarrow \text{CS}_2 + \text{M}$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 3. NOTE: $k_1 = 10^{-1}$ ----- $\text{CS} + \text{N} \rightarrow \text{S} + \text{CN}$ CARBON MONOSULFIDE FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{N} \rightarrow \text{C} + \text{NS}$ CARBON MONOSULFIDE FREE RADICAL + NITROGEN ATOM 75 HEN/GGL REACTION ORDER: 2. ----- $\text{CS} + \text{C} \rightarrow \text{S} + \text{C}_2$	370-550 370-550 565-651 300	2.0(+11) 6.2(+10) 7.9(+14) 1.3(+13) 6.3(+11) 1.6(+12) 1.3(+13) 2.0(+13) 6.3(+11) 1.6(+12) 8.7(+13) 1.3(+12) 4.0(+12)	0 0 0 - 0.5 0.5 0.5 0.5 0.5 0 0.5 0.5	5940+500 4900+500 21640 - 0 28940 50930 48870 0 40463 4370 1160 37200	0.6 1.4 0.5 1.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
CARBON MONOSULFIDE FREE RADICAL + CARBON ATOM 75 BEN/GGL REACTION ORDER: 2. -----		5.0(+11)	0.5	20435	
CS + C → C + CS					
CARBON MONOSULFIDE FREE RADICAL + CARBON ATOM 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CS ₂ + O → CS + SO					
CARBON DISULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----	200-1000	2.2(+13)	0	700	0.7 1.3
CS ₂ + O → COS + S					
CARBON DISULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----	302	2.2(+11)	-	-	0.5 1.5
CS ₂ + S → CS + S ₂					
CARBON DISULFIDE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2. -----	298	3.9(+11)	-	-	0.5 1.5
CS ₂ + M → CS + S + M					
CARBON DISULFIDE 76 BAU/DRY REACTION ORDER: 2. M: AR -----	1800-3700	2.6(+15)	0	38950±9000	0.5 1.5
COS + O → CO + SO					
CARBON OXIDE SULFIDE + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 ABOVE 300K. -----	190-1200	1.6(+13)	0	2250±250	0.5 1.5
COS + H → CO + HS					
CARBON OXIDE SULFIDE 76 BAU/DRY REACTION ORDER: 2. -----	298	1.3(+10)	-	-	0.8 1.3
COS + S → CO + S ₂					
CARBON OXIDE SULFIDE + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 2. -----	230-2600	1.7(+12)	0	2050±230	0.3 3.0
CH ₃ S. + CH=CH → CH ₃ SCH=CH. METHYLTHIO FREE RADICAL + ETHYLENE 72 KER/PAR REACTION ORDER: 2. -----	298-333	7.9(+ 7)	-	-	
CH ₃ S. + CH ₂ =CH ₂ → CH ₃ SCH ₂ CH ₂ . METHYLTHIO FREE RADICAL + ETHYLENE 72 KER/PAR REACTION ORDER: 2. -----	298	4.8(+ 8)	-	-	
CH ₃ S. + CH ₃ CH=CHCH ₃ → CH ₃ CH(SCH ₃)CH ₂ CH ₃ METHYLTHIO FREE RADICAL + 2-BUTENE 72 KER/PAR REACTION ORDER: 2. NOTE: cis-trans EQUILIBRIUM - WEIGHTED K. -----	298-333	1.6(+ 9)	-	-	
CH ₃ SH → CH ₃ + SH METHANETHIOL 70 BEN/O'N REACTION ORDER: 1. -----	1005-1102	3.2(+15)	0	38550	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$\text{CH}_3\text{SH} + \text{CH}_3 \rightarrow \text{CH}_3\text{S} \cdot + \cdot\text{CH}_2\text{SH} + \text{CH}_4$ METHANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	303	1.2(+8)	-	-	0.5 2.0
$\text{CD}_3\text{SH} + \text{CH}_3 \rightarrow \text{CD}_3\text{S} \cdot + \cdot\text{CH}_2\text{SH} + \text{CH}_4$ METHANE- d_3 -THIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	400-500	1.1(+11)	0	2065*500	0.5 2.0
$\text{CD}_3\text{SH} + \text{CH}_3 \rightarrow \cdot\text{CD}_2\text{SH} + \text{CH}_3\text{D}$ METHANE- d_3 -THIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	400-500	7.6(+10)	0	4200*250	0.5 2.0
$\text{CN} + \text{O} \rightarrow \text{N} + \text{CO}$ CYANOGEN FREE RADICAL + OXYGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	0*2500	0.3 3.2
$\text{CN} + \text{O} \rightarrow \text{N} + \text{C}$ CYANOGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		1.3(+12)	0.5	14545	
$\text{CN} + \text{O}_2 \rightarrow \text{N} + \text{CO}$ CYANOGEN FREE RADICAL + OXYGEN MOLECULE 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+11)	0	0*5000	0.3 3.2
$\text{CN} + \text{H} \rightarrow \text{N} + \text{CH}$ CYANOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+12)	0.5	49775	
$\text{CN} + \text{H} \rightarrow \text{NH} + \text{C}$ CYANOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		1.0(+13)	0.5	52745	
$\text{CN} + \text{H} + \text{M} \rightarrow \text{HCN} + \text{M}$ CYANOGEN FREE RADICAL + HYDROGEN ATOM 76 ENG REACTION ORDER: 3. -----	1500-2500	3.2(+16)	-0.5	0*2500	0.3 3.2
$\text{CN} + \text{H}_2 \rightarrow \text{HCN} + \text{H}$ CYANOGEN FREE RADICAL + HYDROGEN MOLECULE 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	2500*1500	
$\text{CN} + \text{OH} \rightarrow \text{HCN} + \text{O}$ CYANOGEN FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	1500*1500	
$\text{CN} + \text{S} \rightarrow \text{N} + \text{CS}$ CYANOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$\text{CN} + \text{S} \rightarrow \text{C} + \text{NS}$ CYANOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL REACTION ORDER: 2. -----		2.0(+12)	0.5	32010	

NOTE: k ESTIMATED.

NOTE: k ESTIMATED.

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f F
CN + N → C + N ₂ CYANOGEN FREE RADICAL + NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CN + N ₂ → C ₂ + N ₂ CYANOGEN FREE RADICAL + NITROGEN OXIDE(N ₂ O) 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+11)	0	0+2500	0.3 3.2
CN + NB → HCN + N CYANOGEN FREE RADICAL + IMIDGEN FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.5	1000+2500	0.3 3.2
CN + HN ₂ → HCN + N ₂ CYANOGEN FREE RADICAL + NITROGEN HYDRIDE 76 ENG REACTION ORDER: 2. -----	1500-2500	4.0(+11)	0.5	0+2500	0.3 3.2
CN + C → N + C ₂ CYANOGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. -----		2.5(+11)	0.5	19300	
CN + C → C + CN CYANOGEN FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CN + CH ₂ → HCN + CH CYANOGEN FREE RADICAL + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	2500+1500	
NOTE: K ESTIMATED.					
CN + CH ₃ → HCN + CH ₂ CYANOGEN FREE RADICAL + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.7	1500+2500	
CN + CH ₄ → HCN + CH ₃ CYANOGEN FREE RADICAL + METHANE 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+11)	0.7	2500+2500	0.3 3.2
CN + C ₂ H ₂ → C ₂ + HCN CYANOGEN FREE RADICAL + ETHYLENE 76 ENG REACTION ORDER: 2. -----	1500-2500	2.0(+11)	0.5	0+2500	0.3 3.2
CN + HCHO → HCN + CH ₂ CYANOGEN FREE RADICAL + FORMALDEHYDE 76 ENG REACTION ORDER: 2. -----	1500-2500	1.3(+11)	0.7	1500+2500	0.3 3.2
C(N ₂) ₄ → C(N ₂) ₃ + N ₂ METHANE, TETRANITRO- 70 BEN/GOL REACTION ORDER: 1. -----	443-506	3.4(+17)	0	20575	
HCN + OH → CN + H ₂ O HYDROCYANIC ACID + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	2.0(+11)	0.6	2500+2500	0.3 3.2

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
350-650 REACTION ORDER: 2. -----	2.1(+11)	0	4330±500	0.7 1.3
388-617 REACTION ORDER: 2. -----	5.4(+11)	0	5020±500	0.3 3.0
350-450 REACTION ORDER: 2. -----	2.0(+11)	0	5135±1000	0.5 1.5
350-450 REACTION ORDER: 2. -----	1.4(+11)	0	4530±500	0.7 1.3
400-500 REACTION ORDER: 2. -----	7.2(+10)	0	5100±500	0.5 1.5
400-500 REACTION ORDER: 2. -----	2.0(+11)	0	4530±750	0.5 2.0
498-723 REACTION ORDER: 1. -----	1.0(+13)	0	17600	
746-862 REACTION ORDER: 1. -----	5.0(+16)	-	32600	
420 REACTION ORDER: 2. -----	6.3(+8)	-	-	
633-698 REACTION ORDER: 1. -----	7.9(+12)	0	19800	
350-500 REACTION ORDER: 2. -----	3.6(+10)	0	3300±5000	0.5 1.5
350-500 REACTION ORDER: 2. -----	2.0(+11)	0	4900±500	0.5 2.0

CHEMICAL REACTIONS					T/K	A	B	E/R (in °K)	k factors f	F
NOTE: TENTATIVE k VALUE.										
HCND ₂ + CH ₃ → •CND ₂ + CH ₄ FORMAMIDE-N,N-d ₂ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.					350-500	5.5(+10)	0	3575±500	0.5	2.0
CH ₃ CN ₂ → CH ₃ • + N ₂ NITROUS ACID METHYL ESTER 70 BEN/GdN REACTION ORDER: 1.					453-513	4.0(+15)	0	20700		
CH ₃ CN ₂ → CH ₃ • + N ₂ METHANE, NITRO- 70 BEN/GdN REACTION ORDER: 1.					660	4.0(+15)	0	29700		
CH ₃ CN ₂ + CH ₃ • → •CH ₂ CN ₂ + CH ₄ METHANE, NITRO- 76 KER/PAR REACTION ORDER: 2.					300-500	1.0(+11)	0	5100±750	0.4	2.5
NOTE: TENTATIVE k VALUE.										
CH ₃ CN ₂ → CH ₃ • + N ₂ NITRIC ACID METHYL ESTER 70 BEN/GdN REACTION ORDER: 1.					483-513	3.2(+15)	0	20030		
CH ₃ CNH ₂ + CH ₃ • → CH ₃ CNH• + CH ₄ HYDROXYLAMINE, O-METHYL-, 76 KER/PAR REACTION ORDER: 2.					300-500	5.0(+10)	0	2265±500	0.5	1.5
CH ₃ CND ₂ + CH ₃ • → CH ₃ CND• + CH ₃ D HYDROXYLAMINE-N,N-d ₂ , O-METHYL-, 76 KER/PAR REACTION ORDER: 2.					300-500	3.5(+10)	0	2970±500	0.5	1.5
C ₂ + O → C + CO CARBON DIMER + OXYGEN ATOM 75 BEN/GdL REACTION ORDER: 2.						6.3(+11)	0.5	0		
C ₂ + H → C + CH CARBON DIMER + HYDROGEN ATOM 75 BEN/GdL REACTION ORDER: 2.						1.6(+13)	0.5	30450		
C ₂ + S → C + CS CARBON DIMER + SULFUR ATOM 75 BEN/GdL REACTION ORDER: 2.						6.3(+11)	0.5	0		
C ₂ + N → C + CN CARBON DIMER + NITROGEN ATOM 75 BEN/GdL REACTION ORDER: 2.						6.3(+11)	0.5	0		
C ₂ + C → C + C ₂ CARBON DIMER + CARBON ATOM 75 BEN/GdL REACTION ORDER: 2.						6.3(+11)	0.5	0		
CO ₂ + CH=CH → products CARBON OXIDE(C ₂ O) + ETHYNE										

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 0.3$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + CH_3CH=CH_2 \rightarrow CCl + CH_3CH=C-CH_2$ CARBON OXIDE(C2O) + 1-FROPENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 5.7$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + CH_3C=CH_3 \rightarrow$ Products CARBON OXIDE(C2O) + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 8.5$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + CH_2=CHCH=CH_2 \rightarrow CCl + CH_2=C-CHCH=CH_2$ CARBON OXIDE(C2O) + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 210.$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CH=C-CH_2 + CCl$ CARBON OXIDE(C2O) + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 7.0$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + cis-CH_3CH=CHCH_3 \rightarrow CCl + cis-CH_3CH=C-CHCH_3$ CARBON OXIDE(C2O) + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 9.1$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + trans-CH_3CH=CHCH_3 \rightarrow CCl + trans-CH_3CH=C-CHCH_3$ CARBON OXIDE(C2O) + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 10.6$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + (CH_3)_2C=CH_2 \rightarrow CCl + (CH_3)_2C=C-CH_2$ CARBON OXIDE(C2O) + 1-FROPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 50.0$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + (CH_3)_2C=CHCH_3 \rightarrow CCl + (CH_3)_2C=C-CHCH_3$ CARBON OXIDE(C2O) + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 100.$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + (CH_3)_2C=C(CH_3)_2 \rightarrow CCl + (CH_3)_2C=C-C(CH_3)_2$ CARBON OXIDE(C2O) + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 250.$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ ----- $CCl + (CH_3)_2C=C-C(CH_3)_2 \rightarrow CCl + (CH_3)_2C=C-C(CH_3)_2$ CARBON OXIDE(C2O) + 2,3-PENTADIENE, 2,4-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 113.$ NOTE: $k_{ref}: CCl + CH_2=CH_2$ -----	304	-	-	-	
	297	-	-	-	
	304	-	-	-	
	298	-	-	-	
	298	-	-	-	
	297	-	-	-	
	297	-	-	-	
	298	-	-	-	
	298	-	-	-	
	304	-	-	-	

CHEMICAL REACTIONS

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
$\text{CH}_3\text{CH} + \text{d} \rightarrow \text{products}$ ETHYNE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----	200-700	1.4(+13)	0	1500	0.8 1.2
$\text{CH}_3\text{CH} + \text{OB} \rightarrow \text{CH}_3\text{C} + \text{H}_2\text{d}$ ETHYNE + HYDROXYL FREE RADICAL 72 KER REACTION ORDER: 2. -----	300-2000	7.6(+12)	0	2335+400	0.5 2.1
$\text{CH}_3\text{CH} + \text{S} \rightarrow \text{cy-CH-CHS}$ ETHYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. -----	298	1.7(+11)	-	-	
$\text{CH}_3\text{CH} + \text{N} \rightarrow \text{C}_2\text{H}_2\text{N}$ ETHYNE + NITROGEN ATOM 72 KER/PAR NOTE: UPPER LIMIT. -----	440	2.0(+9)	-	-	
$\text{CH}_3\text{CH} + \text{CH}_3 \rightarrow \text{CH}_3\text{C} + \text{CH}_4$ ETHYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	473-773	-	-	7100	
$\text{CH}_3\text{CH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH-CH}_3$ ETHYNE + METHYL FREE RADICAL 72 KER/PAR NOTE: GIVEN WITH CAUTION. -----	371-479	2.5(+11)	0	3900	
$\text{CH}_3\text{CH} + \text{CH}_3\text{S} \rightarrow \text{CH}_3\text{SCH-CH}_3$ ETHYNE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	298-333	7.9(+7)	-	-	
$\text{CH}_3\text{CH} + \text{CCO} \rightarrow \text{products}$ ETHYNE + CARBON OXIDE(C_2d) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}} = 0.3$ -----	304	-	-	-	
$\text{CH}_3\text{CH} + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH-CH}_3$ ETHYNE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	373-473	5.0(+10)	0	3500	
$\text{CH}_3\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH-CH}_3$ ETHYNE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	3475	5.0(+10)	0		
$\text{CH}_3\text{CH} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{CCH-CH}_3$ ETHYNE + ETHYL, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	363-577	1.0(+11)	0	3875	
$\text{cis-CDH-CDH} \rightarrow \text{trans-CDH-CHD}$ $\text{cis-ETHENE-1,2-d}_2$ 70 KER/6'N REACTION ORDER: 1. -----	723-823	1.0(+13)	0	32700	

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
$\text{CH}_2=\text{CH}_2 + \theta \rightarrow \text{cy-CH}_2\text{CH}_2\theta$ ETHENE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----	200-500	3.3(+12)	0	565	0.8 1.2
$\text{CH}_2=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\cdot$ ETHENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. -----	298	9.3(+13)	0	1410	
$\text{CH}_2=\text{CH}_2 + \text{H} + \text{M} \rightarrow \text{CH}_3\text{CH}_2\cdot + \text{M}$ ETHENE + HYDROGEN ATOM 72 ION REACTION ORDER: 3. M: H_2 -----	298-813	5.6(+17)	0.5	495	
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_2=\text{CH}\cdot + \text{H}_2\text{O}$ ETHENE + HYDROXYL FREE RADICAL 72 ION REACTION ORDER: 2. -----	3500-1400	1.6(+14)	0	2831+445	0.4 2.4
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \cdot\text{CH}_2\text{CH}_2\text{OH}$ ETHENE + HYDROXYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----		1.1(+12)	-	-	0.8 1.3
$\text{CH}_2=\text{CH}_2 + \text{H}_2 \rightarrow \text{products}$ ETHENE + HYDROPEROXYL FREE RADICAL 74 LI6 REACTION ORDER: 2. NOTE: RATIO DATA VERSUS kref. FOR $\text{H}_2 + \text{C}_6 \rightarrow \text{C}_6\text{H}_2 + \text{OH}$ K FACTORS MIGHT BE HIGH. -----	300	1.0(+7)	-	-	0.1 10.
$\text{CH}_2=\text{CH}_2 + \text{S} \rightarrow \text{cy-CH}_2\text{CH}_2\text{S}$ ETHENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. -----	298	8.1(+11)	-	-	
$\text{CH}_2=\text{CH}_2 + \text{N} \rightarrow \text{products}$ ETHENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. -----	320-550	2.0(+10)	0	353	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_2=\text{CH}\cdot + \text{CH}_4$ ETHENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-650	4.2(+11)	0	5600+500	0.5 1.5
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ ETHENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	353-453	3.3(+11)	0	3900	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot + (\text{CH}_3)_2\text{CH}\cdot$ ETHENE + METHYL FREE RADICAL 72 ION REACTION ORDER: 2. -----	350-705	2.0(+11)	0	3575+105	0.8 1.3
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{S}\cdot \rightarrow \text{CH}_3\text{SCH}_2\text{CH}_2\cdot$ ETHENE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	298	4.8(+8)	-	-	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ ETHENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	348-482	1.6(+11)	0	3675	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ ETHENE + PROPYL FREE RADICAL 72 KER/PAR NOTE: TENTATIVE k VALUE.	375-503	1.9(+10)	0	3070	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{CH}\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ ETHENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR NOTE: TENTATIVE k VALUE.	340-457	6.9(+10)	0	3475	
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot$ ETHENE + BUTYL FREE RADICAL 72 KER/PAR NOTE: TENTATIVE k VALUE.	352-405	2.3(+10)	0	3370	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_3\text{C}\cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2\cdot$ ETHENE + ETHYL, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR NOTE: TENTATIVE k VALUE.	300-650	2.8(+10)	0	3575	
$\text{CH}_2=\text{CH}_2 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot \rightarrow (\text{CH}_3)_2\text{CH}(\text{CH}_2)_3\text{CH}_2\cdot$ ETHENE + BUTYL, 3-METHYL-, FREE RADICAL 72 KER/PAR 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 KEN 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 KEN REACTION ORDER: 2.	473-823	3.0(+11)	0	5435	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}=\text{CH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}\cdot$ ETHYL FREE RADICAL + ETHYLENE 72 KER/PAR REACTION ORDER: 2.	373-473	5.0(+10)	0	3500	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}\cdot$ ETHYL FREE RADICAL + ETHYLENE 72 KER/PAR REACTION ORDER: 2.	348-482	1.6(+11)	0	3675	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{C}(\text{CH}_3)-\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ ETHYL FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2.	375-465	3.2(+11)	0	4630	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHCH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ ETHYL FREE RADICAL + 2-PENTENE-1-OL 72 KER/PAR REACTION ORDER: 2.	323-415	1.9(+11)	0	3901	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHCN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + 2-PHENYLETHYLENE 72 KER/PAR REACTION ORDER: 2.	323-454	6.2(+10)	0	1700	

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
298	-	-	3675	
298	-	-	4265	
298	-	-	4350	
303-417	7.8(+10)	0	3475	
323-454	1.5(+10)	0	2500	
323-754	3.1(+10)	0	2600	
312-400	2.5(+11)	0	2300	
298	-	-	4300	
298	-	-	3620	
308-448	2.5(+11)	0	3900	
300-520	2.8(+11)	0	3986+100	0.4 2.2

$\text{CH}_3\text{CH}_2^\bullet + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\bullet)\text{CH}_2\text{CH}_3$
 ETHYL FREE RADICAL + 1-BUTENE
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{cis-CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\bullet)\text{CH}_3$
 ETHYL FREE RADICAL + cis-2-BUTENE
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{trans-CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\bullet)\text{CH}_3$
 ETHYL FREE RADICAL + trans-2-BUTENE
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{CH}_3\text{COCCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COCCH}(\bullet)\text{CH}_2\text{CH}_3$
 $+ \text{CH}_3\text{COCCH}(\text{CH}_2\text{CH}_3)\text{CH}_2^\bullet$
 ETHYL FREE RADICAL + ACETIC ACID ETHENYL ESTER
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{cis-CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\bullet)\text{CN}$
 $+ \text{CH}_3\text{CH}(\bullet)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$
 ETHYL FREE RADICAL + cis-2-BUTENENITRILE
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{trans-CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\bullet)\text{CN}$
 $+ \text{CH}_3\text{CH}(\bullet)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$
 ETHYL FREE RADICAL + trans-2-BUTENENITRILE
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{CH}_2=\text{C}(\text{CH}_3)\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\bullet)(\text{CH}_3)\text{CN}$
 $+ \text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CN}$
 ETHYL FREE RADICAL + 2-PHENYLENITRILE, 2-METHYL-
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\bullet)\text{CH}_3$
 ETHYL FREE RADICAL + cis-2-PENTENE
 72 KER/PAR REACTION ORDER: 2.

NOTE: CRITICAL ENERGY OF REACTION.

$\text{CH}_3\text{CH}_2^\bullet + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\bullet)\text{CH}_2\text{CH}_3$
 ETHYL FREE RADICAL + 1-BUTENE, 3-METHYL-
 72 KER/PAR REACTION ORDER: 2.

NOTE: CRITICAL ENERGY OF REACTION.

$\text{CH}_3\text{CH}_2^\bullet + \text{CH}_3\text{COCCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COCCH}_2\text{CH}(\bullet)\text{CH}_2\text{CH}_3$
 $+ \text{CH}_3\text{COCCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2^\bullet$
 ETHYL FREE RADICAL + ACETIC ACID 2-PHENYENYL ESTER
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{CH}_3\text{CH}_2\text{COCCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \bullet\text{CH}_2\text{CH}_2\text{COCCH}_2\text{CH}_3$
 ETHYL FREE RADICAL + 3-PENTANONE
 72 KER/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2^\bullet + \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow$
 $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\bullet)(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$\cdot \text{CH}_2\text{C}(\text{CH}_2)(\text{CH}_2\text{CH}_2)_2\text{C}(\text{CH}_3)_2\text{CH}_2$ ETHYL FREE RADICAL + 1,3-BUTADIENE, 2,3-DIMETHYL- 72 KBR/PAR REACTION ORDER: 2. -----	318-414	1.6(+11)	0	2265	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-HEXENE 72 KBR/PAR REACTION ORDER: 2. -----	338-435	3.9(+10)	0	3400	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + PROPANOIC ACID 2-PROPENYL ESTER 72 KBR/PAR REACTION ORDER: 2. -----	352-435	2.5(+11)	0	3875	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_3$ ETHYL FREE RADICAL + BUTANE, 1-ETHENYLOXY- 72 KBR/PAR REACTION ORDER: 2. -----	303-435	2.5(+10)	0	3070	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_4\text{C}=\text{CH} \rightarrow \text{CH}_3((\text{CH}_2)_4\text{C}(\cdot)-\text{CHCH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH}\cdot$ ETHYL FREE RADICAL + 1-HEPTYNE 72 KBR/PAR REACTION ORDER: 2. -----	300-455	3.9(+11)	0	4430	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-HEPTENE 72 KBR/PAR REACTION ORDER: 2. -----	359-439	6.2(+10)	0	3500	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 \rightarrow$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-HUTENE, 2,3,3-TRIMETHYL- 72 KBR/PAR REACTION ORDER: 2. -----	322-364	7.8(+9)	0	2800	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}=\text{C}(\text{CH}_3)_2 \rightarrow$ $(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)(\text{CH}_3)\text{CH}=\text{C}(\text{CH}_3)_2$ $\cdot (\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_2\text{CH}_3)\text{CH}=\text{C}(\text{CH}_3)_2$ ETHYL FREE RADICAL + 2,4-HEXADIENE, 2,5-DIMETHYL- 72 KBR/PAR REACTION ORDER: 2. -----	328-420	6.2(+10)	0	3300	
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-OCTENE 72 KBR/PAR REACTION ORDER: 2. -----	339-425	1.2(+11)	0	3825	
$\text{CH}_3\text{CH}_2\cdot + (\text{CH}_3)_3\text{CCCH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow$ $(\text{CH}_3)_3\text{CCCH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot (\text{CH}_3)_3\text{CCCH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + 1-PENTENE, 2,4,4-TRIMETHYL- 72 KBR/PAR REACTION ORDER: 2. -----	309-364	1.9(+10)	0	2870	
$\text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\cdot + \text{CH}_3\cdot$					

CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f F
ETHANE 70 BEN/C'N REACTION ORDER: 1. ----- CH ₃ CH ₃ + O → CH ₃ CH ₂ • + OH ETHANE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2. ----- CH ₃ CH ₃ + H → CH ₃ CH ₂ • + H ₂ ETHANE + HYDROGEN ATOM 72 ION REACTION ORDER: 2. ----- CH ₃ CH ₃ + OH → CH ₃ CH ₂ • + H ₂ O ETHANE + HYDROXYL FREE RADICAL 72 ION REACTION ORDER: 2. ----- CH ₃ CH ₃ + H ₂ O → CH ₃ CH ₂ • + H ₂ O ₂ ETHANE + HYDROPEROXYL FREE RADICAL 74 IIC REACTION ORDER: 2. ----- NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k _{ref} FOR H ₂ O + CO → HC + CO ₂ ----- CH ₃ CH ₃ + CH ₃ • → CH ₃ CH ₂ • + CH ₄ ETHANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CH ₃ CH ₃ + CD ₃ • → CH ₃ CH ₂ • + CD ₃ H ETHANE + METHYL-d ₃ FREE RADICAL 72 ION REACTION ORDER: 2. ----- CH ₃ CD ₃ + CD ₃ • → CH ₃ CD ₂ • + CD ₄ ETHANE-1,1,1-d ₃ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CD ₃ CH ₃ + CD ₃ • → CD ₃ CH ₂ • + CD ₃ H ETHANE-1,1,1-d ₃ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CD ₃ CD ₃ + CH ₃ • → CD ₃ CD ₂ • + CH ₃ D ETHANE-d ₆ + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CD ₃ CD ₃ + CD ₃ • → CD ₃ CD ₂ • + CD ₄ ETHANE-d ₆ + METHYL-d ₃ FREE RADICAL 72 ION REACTION ORDER: 2. ----- CH ₂ =C=O + O → products ETHENONE + OXYGEN ATOM 73 HER/HUI REACTION ORDER: 2. ----- H ₂ CC-COOH → HCCOH + CO ₂ ETHANEDIC ACID 70 BEN/C'N REACTION ORDER: 1. -----	298-858	5.6(+16)	0	45045	
		2.5(+13)	0	3200	0.7 1.3
	285-1440	1.0(+14)	0	4815470	0.8 1.2
		1.3(+14)	0	1998	
	300-1000	1.0(+12)	0	7000	0.1 10.
		5.6(+11)	0	58404250	0.7 1.3
	390-800	1.0(+12)	0	60854165	0.7 1.4
	500-750	4.3(+11)	0	68454250	0.7 1.3
		3.0(+11)	0	59004250	0.7 1.3
	500-900	5.6(+11)	0	66004250	0.7 1.3
		4.6(+11)	0	6405	
	298	5.3(+11)	-	-	0.7 1.3
	390-420	7.9(+11)	0	15100	

CHEMICAL REACTIONS

Chemical Reaction	T/K	A	B	E/R (in °K)	k factors f
$\text{CH}_3\text{C}(\text{O})\cdot \rightarrow \text{CH}_3\cdot + \text{CO}$ ETHYL, 1-CXG-, FREE RADICAL 72 KGN REACTION ORDER: 1.0 -----	273-413	1.5(+10)	0	6790±115	0.7 1.4
$\text{CH}_3\text{C}(\text{O})\cdot \rightarrow \text{CH}_3\cdot + \text{CO}$ ETHYL, 1-CXG-, FREE RADICAL 70 EHN/6'N REACTION ORDER: 1.0 -----		2.0(+10)	0	7550	
$\text{CH}_3\text{CHO} + \text{O} \rightarrow \text{products}$ ACETALDEHYDE + OXYGEN ATOM 73 HHE/HUI REACTION ORDER: 2.0 -----	298-500	1.4(+13)	0	1140	0.5 2.0
$\text{CH}_3\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\text{O})\cdot + \text{CH}_4$ ACETALDEHYDE + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	300-525	8.5(+10)	0	3000±250	0.4 1.6
$\text{CH}_3\text{CHO} + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}(\text{O})\cdot + \text{CH}_3\text{D}$ ACETALDEHYDE-1-d + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	300-500	1.0(+11)	0	3975±500	0.5 1.5
$\text{cy-CH}_2\text{CH}_2\text{O} + \text{O} \rightarrow \text{products}$ OXIRANE + OXYGEN ATOM 73 HHR/HUI REACTION ORDER: 2.0 -----	298	7.0(+8)	-	-	0.6 1.5
$\text{cy-CH}_2\text{CH}_2\text{O} + \text{CH}_3\cdot \rightarrow \text{cy-CH}_2\text{CH}(\text{O})\text{O} + \text{CH}_4$ OXIRANE + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	350-500	2.5(+11)	0	5435±750	0.5 2.0
$\text{HCOOCH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{COOCH}_3 + \text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	350-550	2.0(+11)	0	4900±500	0.5 1.5
$\text{HCOOCH}_3 + \text{CH}_3\cdot \rightarrow \text{HCOOCH}_2\cdot + \text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	350-550	1.6(+11)	0	5635±500	0.5 1.5
$\text{HCOOCH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{COOCH}_3 + \text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	350-550	3.0(+11)	0	4980±500	0.5 1.5
$\text{DCOOCH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{COOCH}_3 + \text{CH}_3\text{D}$ FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----	350-550	2.5(+11)	0	5900±500	0.5 1.5
$\text{DCOOCH}_3 + \text{CH}_3\cdot \rightarrow \text{DCOOCH}_2\cdot + \text{CH}_4$ FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.0 -----		1.6(+11)	0	5635±500	0.5 1.5
NOTE: TENTATIVE K VALUE. $\text{CH}_3\text{COOH} \rightarrow \text{CH}_3\text{-C}(\text{O})\cdot + \text{H}_2\text{O}$ ACETIC ACID 70 BEN/6'N NOTE: SUSPECT VALUE.	773-973	8.9(+12)	0	33970	

CHEMICAL REACTIONS

Chemical Reactions	T/K	A	B	E/R (in OK)	k factors f
$\text{CH}_3\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_4$ ACETIC ACID-d + METHYL FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\cdot + \text{C}_6\text{H}_5$ ETHOXY FREE RADICAL 70 BEN/d'N ----- $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{products}$ ETHANGL + OXYGEN ATOM 73 KER/HUI ----- $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_4$ ETHANGL + METHYL FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{C}_6\text{H}_5 + \text{CH}_4$ ETHANGL + METHYL FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}_6\text{H}_5 + \cdot\text{CH}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_4$ ETHANGL + METHYL FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CD}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CD}(\cdot)\text{C}_6\text{H}_5 + \text{CH}_3\text{D}$ ETHAN-1,1-d ₂ -GL + METHYL FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CD}_2\text{CH}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CD}_2\text{C}_6\text{H}_5 + \text{CH}_4$ ETHAN-1,1-d ₂ -GL + METHYL FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CH}_2\text{CD}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}_6\text{H}_5 + \text{CD}_4$ ETHANGL-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{CH}_2\text{CD}_2\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{C}_6\text{H}_5 + \text{CD}_3\text{H}$ ETHANGL-d + METHYL-d ₃ FREE RADICAL 76 KER/PAR ----- $\text{CH}_3\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\cdot + \text{C}_6\text{H}_5$ METHANE, OXYBIS- 70 BEN/d'N ----- $\text{CH}_3\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{products}$ METHANE, OXYBIS- + OXYGEN ATOM 73 KER/HUI ----- $\text{CH}_3\text{C}_6\text{H}_5 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{C}_6\text{H}_4\cdot + \text{CH}_4$ METHANE, OXYBIS- + METHYL FREE RADICAL 76 KER/PAR -----	300-600 488-468 298 400-625 400-625 400-625 400-550 400-550 400-525 400-525 750-820 200-500 300-550	1.6(+11) 2.5(+13) 8.7(+10) 7.9(+10) 4.0(+11) 5.1(+11) 4.1(+11) 7.1(+10) 6.2(+10) 4.4(+11) 1.0(+16) 5.9(+12) 4.2(+11)	0 0 - 0 0 0 0 0 0 0 0 0 0	5135*500 8805 - 4730*500 4900*500 4900*500 5735*500 4530*500 5135*500 4900*500 40765 1520 5035*500	0.6 1.4 0.6 1.5 0.6 1.4 0.6 1.4 0.6 1.4 0.6 1.4 0.6 1.4 0.5 2.0 0.6 1.4 0.5 2.0 0.7 1.3 0.5 1.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$\text{CH}_3\text{SOCH}_3 \rightarrow \text{CH}_3\text{O} \cdot + \text{CH}_3\text{O} \cdot$ PEROXIDE, DIMETHYL- 70 BEN/6'N REACTION ORDER: 1. -----	393-452	4.0(+15)	0	18570	
$\text{CH}_3\text{SOCH}_3 + \text{CH}_3\text{O} \cdot \rightarrow \text{CH}_3\text{SOCH}_2\text{O} \cdot + \text{CH}_4$ PEROXIDE, DIMETHYL- + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE. -----	350-500	4.2(+11)	0	5000±1000	0.3 3.0
$\text{CH}_3\text{CH}_2\text{SOCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{O} \cdot + \text{CH}_3$ HYDROPEROXIDE, ETHYL- 70 BEN/6'N REACTION ORDER: 1. -----	553-653	2.2(+15)	0	21640	
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CD}_3\text{O} \cdot \rightarrow \text{cy-CH}_2\text{CH}_2\text{O} \cdot + \text{CD}_3\text{H}$ THYRANE + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	300-500	2.2(+11)	0	4800±500	0.5 2.0
$\text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_3\text{CH}_2\text{S} \cdot + \text{H}_2\text{S}$ ETHANETHIOL 70 BEN/6'N REACTION ORDER: 1. -----	785-938	1.0(+13)	0	25900	
$\text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_3\text{CH}_2\text{S} \cdot + \text{SH}$ ETHANETHIOL 70 BEN/6'N REACTION ORDER: 1. -----	785-938	6.3(+15)	0	36336	
$\text{CH}_3\text{CH}_2\text{SH} + \text{CH}_3\text{O} \cdot \rightarrow \text{CH}_3\text{CH}_2\text{SO} \cdot + \text{CH}_3\text{CH}(\text{O})\text{SH}$ $+ \text{CH}_2\text{CH}_2\text{SO} \cdot + \text{CH}_4$ ETHANETHIOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE. -----	303	3.5(+7)	-	-	0.5 2.0
$\text{CH}_3\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SO}_2\text{O} \cdot + \text{CH}_3$ METHANE, SULFONYLHIS- 70 BEN/6'N REACTION ORDER: 1. -----	783-913	2.0(+14)	0	30500	
$\text{CH}_3\text{NC} \rightarrow \text{CH}_3\text{CN}$ METHANE, ISOCYAN- 70 BEN/6'N REACTION ORDER: 1. -----	472-533	4.0(+13)	0	19325	
$\text{CH}_3\text{CN} + \text{CH}_3\text{O} \cdot \rightarrow \text{CH}_2\text{CH} \cdot + \text{CH}_4$ ACETONITRILE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-600	5.4(+11)	0	5100±500	0.7 1.5
$\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\text{O} \cdot \rightarrow \text{CH}_3\text{CH}_2\text{NH} \cdot + \text{CH}_3\text{CH}(\text{O})\text{NH}_2$ $+ \text{CH}_2\text{CH}_2\text{NH}_2 \cdot + \text{CH}_4$ ETHANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CH}_3\text{CH}_2\text{NH}_2 + \text{CH}_3\text{O} \cdot \rightarrow \text{CH}_3\text{CH}_2\text{NH} \cdot + \text{CH}_4$ ETHANAMINE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE. -----	350-500	2.0(+11)	0	4600±500	0.5 2.0

CHEMICAL REACTIONS

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f F
$\text{CD}_3\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{D} + \text{CD}_3\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CD}_2\text{CH}_2\text{NH}_2$ ETHAN-2,2-d ₃ -AMINE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4200±500	0.5 2.0
$\text{CD}_3\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \text{CD}_3\text{CH}_2\text{NH} + \text{CH}_4$ ETHAN-2,2-d ₃ -AMINE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	423	4.0(+5)	-	-	-
NOTE: TENTATIVE k VALUE.					
$(\text{CH}_3)_2\text{NH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} + \cdot\text{CH}_2\text{NH}(\text{CH}_3) + \text{CH}_4$ METHANAMINE, N-METHYL- + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	350-650	1.6(+11)	0	3500±500	0.5 2.0
$(\text{CH}_3)_2\text{NH} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} + \text{CH}_4$ METHANAMINE, N-METHYL- + METHYL FREE RADICAL 76 KHR/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 KHR/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4400±500	0.5 1.5
$(\text{CH}_3)_2\text{ND} + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{N} + \text{CH}_3\text{D}$ METHANAMINE-d, N-METHYL- + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	4300±500	0.5 1.5
$\text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{N}=\text{N} \cdot$ DIAZENE, DIMETHYL- 70 BEN/6'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 KHR/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 KCN REACTION ORDER: 2.	300-450	5.0(+10)	0	3040±355	-
$\text{CD}_3\text{N}=\text{NCD}_3 + \text{CD}_3 \rightarrow \cdot\text{CD}_2\text{N}=\text{NCD}_3 + \text{CD}_4$ DIAZENE, DI(METHYL-d ₃)- + METHYL-d ₃ FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	300-500	6.6(+10)	0	4125±500	-
$\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \cdot\text{NHCH}_2\text{CH}_2\text{NH}_2$ $+ \text{NH}_2\text{CH}(\cdot)\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANEDIAMINE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	350-500	3.8(+11)	0	4200±500	-
$\text{NH}_2\text{CH}_2\text{CH}_2\text{NH}_2 + \text{CH}_3 \rightarrow \cdot\text{NHCH}_2\text{CH}_2\text{NH}_2 + \text{CH}_4$ ETHANEDIAMINE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	4430±500	-
NOTE: TENTATIVE k VALUE.					
$\text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3 \rightarrow \cdot\text{NDCH}_2\text{CH}_2\text{ND}_2 + \text{CH}_3\text{D}$					

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
ETHANEDI(AMINE-d ₂) + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-500	3.2(±11)	0	5100±500	
ND ₂ CH ₂ CH ₂ ND ₂ + CH ₃ • → ND ₂ CH(•)CH ₂ ND ₂ + CH ₄ ETHANEDI(AMINE-d ₂) + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.0(±11)	0	4025±500	
(CH ₃) ₂ NNH ₂ + CH ₃ • → (CH ₃) ₂ NNH• + CH ₄ HYDRAZINE, 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	1.7(±11)	0	2870±500	
(CH ₃) ₂ NNH ₂ + CH ₃ • → (CH ₃) ₂ NNH• + •CH ₂ N(CH ₃)NH ₂ + CH ₄ HYDRAZINE, 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.4(±11)	0	2970±500	
(CH ₃) ₂ NNND ₂ + CH ₃ • → (CH ₃) ₂ NNND• + CH ₄ HYDRAZINE-d ₂ , 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.1(±11)	0	3400±500	
(CH ₃) ₂ NNND ₂ + CH ₃ • → CH ₂ N(CH ₃)ND ₂ + CH ₄ HYDRAZINE-d ₂ , 1,1-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	3.2(±11)	0	4125±750	
NOTE: TENTATIVE & VALUE.					
CH ₃ NHCH ₃ + CH ₃ • → CH ₃ N(•)NHCH ₃ + •CH ₂ NHCH ₃ + 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 & VALUE.					
CH ₃ NDNDCH ₃ + CH ₃ • → CH ₃ N(•)NDCH ₃ + CH ₄ HYDRAZINE-d ₂ , 1,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-500	2.0(±11)	0	2700±500	
NOTE: TENTATIVE & VALUE.					
CH ₃ CH=NCH → CH ₃ CH=N• + CH ACETALDEHYDE, EXIME 70 BEN/6°N REACTION ORDER: 1.	603-713	6.8(±12)	0	23655	
HCNCH ₃ + CH ₃ • → •CNHCH ₃ + HCN(•)CH ₃ • HCNCH ₃ + CH ₄ FORMAMIDE, N-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	400-600	7.9(±10)	0	3800±500	
CH ₃ CNH ₂ + CH ₃ • → CH ₃ CNH• + •CH ₂ CNH ₂ + CH ₄ ACETAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	2.1(±11)	0	5235±500	
CH ₃ CNH ₂ + CH ₃ • → •CH ₂ CNH ₂ + CH ₄ ACETAMIDE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.	350-600	1.0(±11)	0	5200±500	
CD ₃ CNH ₂ + CD ₃ • → •CD ₂ CNH ₂ + CD ₄					

CHEMICAL REACTIONS

T/K	A	B	E/R (ln OK)	k factors f
PREDOMINANTLY AT TERMINAL C ATOM. ----- $\text{CH}_3\text{C}=\text{CH} + (\text{CH}_3)_2\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\cdot)\text{CH}_3$ 1-PROPENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR NOTE: SUSPECT K VALUE.				
360-439	1.9(+9)	0	2870	
----- $\text{CH}_3\text{C}=\text{CH} + (\text{CH}_3)_3\text{C}\cdot \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}\cdot$ $(\text{CH}_3)_3\text{CC}=\text{C}(\cdot)\text{CH}_3$ 1-PROPENE + ETHYL-, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR NOTE: SUSPECT K VALUE.				
360-439	5.0(+8)	0	2770	
----- $\text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
373-483	2.0(+11)	0	4100	
----- $\text{CH}_3-\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)$ 1,2-PROPADIENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
379-465	3.2(+11)	0	4630	
----- $\text{CH}_2=\text{C}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}\cdot \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
366-473	3.6(+10)	0	3660	
NOTE: TENTATIVE K VALUE.				
----- $\text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\cdot + \text{H}$ 1-PROPENE 70 BEN/σ'N REACTION ORDER: 1.				
953-1143	2.0(+15)	0	44900	
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{C} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\cdot$ 1-PROPENE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2.				
200-500	2.5(+12)	0	38	0.8 1.2
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\cdot$ 1-PROPENE + HYDROGEN ATOM 72 KER/PAR 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.				
298	7.2(+12)	0	600	
NOTE: ARRHENIUS PARAMETERS ARE MINIMUM VALUES OF THEIR HIGH PRESSURE LIMITS.				
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2 + \text{CH}_3\text{CH}(\text{CH})\text{CH}_2\cdot$ 1-PROPENE + HYDROXYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
300	6.6(+12)	-	-	
NOTE: ADDITION TO TERMINAL CARBON OF DOUBLE BOND IS PREDOMINANTLY 95%.				
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM				

CHEMICAL REACTIONS

T/K	A	B	E/R (in OK)	k factors f
363-577	5.0(+10)	0	3475	
72 KER/PAR NOTE: TENTATIVE & VALUE. REACTION ORDER: 2. ----- $(CH_3)_2CH \cdot + CH_2=CH_2 \rightarrow (CH_3)_2CHCH_2CH_2 \cdot$ ETHYL, 1-METHYL-, FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2. -----				
340-457	6.9(+10)	0	3475	
72 KER/PAR NOTE: SUSPECT & VALUE. REACTION ORDER: 2. ----- $(CH_3)_2CH \cdot + CH_3C \equiv CH \rightarrow (CH_3)_2CHCH \cdot C \cdot (CH_3)$ ETHYL, 1-METHYL-, FREE RADICAL + 1-BUTYNE 72 KER/PAR REACTION ORDER: 2. -----				
360-439	1.90(+9)	0	2870	
72 KER/PAR NOTE: TENTATIVE & VALUE. REACTION ORDER: 2. ----- $(CH_3)_2CH \cdot + CH_2=C=CH_2 \rightarrow (CH_3)_2CHCH_2C \cdot (CH_3)$ ETHYL, 1-METHYL-, FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2. -----				
366-473	3.6(+10)	0	3600	
72 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $(CH_3)_2CH \cdot + CH_3CH_2CH=CH_2 \rightarrow (CH_3)_2CHCH_2CH \cdot (CH_3)$ ETHYL, 1-METHYL-, FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. -----				
298	-	-	3480	
72 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $(CH_3)_2CH \cdot + cis-CH_3CH=CHCH_3 \rightarrow CH_3CH[CH(CH_3)_2]CH \cdot (CH_3)$ ETHYL, 1-METHYL-, FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. -----				
298	-	-	3950	
72 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $(CH_3)_2CH \cdot + trans-CH_3CH=CHCH_3 \rightarrow CH_3CH[CH(CH_3)_2]CH \cdot (CH_3)$ ETHYL, 1-METHYL-, FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. -----				
298	-	-	4065	
72 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $CH_3CH_2CH_3 + e \rightarrow \text{products}$ PROPANE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----				
298	5.0(+9)	-	-	0.7 2.0
72 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $CH_3CH_2CH_3 + H \rightarrow (CH_3)_2CH \cdot + CH_3CH_2CH_2 \cdot + H_2$ PROPANE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. -----				
332-933	1.0(+13)	0	3130±180	
74 IIG NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} FOR $H_2 + H_2 \rightarrow H_2^+ + H_2^-$ ----- $CH_3CH_2CH_3 + H_2 \rightarrow (CH_3)_2CH \cdot + H_2^+$ PROPANE + HYDROGEN ATOM 74 IIG REACTION ORDER: 2. -----				
300-1000	2.0(+11)	0	5300	
76 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $CH_3CH_2CH_3 + CH_3 \cdot \rightarrow (CH_3)_2CH \cdot + CH_4$ PROPANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----				
550-750	2.0(+11)	0	4820±250	
76 KER/PAR NOTE: CRITICAL ENERGY OF REACTION. ----- $CH_3CH_2CH_3 + CD_3 \cdot \rightarrow (CH_3)_2CH \cdot + CD_4$ PROPANE-2,2-d ₂ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----				
550-750	2.5(+11)	0	5735±250	

CHEMICAL REACTIONS

T/K	A	B	E/R (ln OK)	k factors f F
550-750	4.4(+11)	0	5735±250	
$\text{CH}_3\text{CD}_2\text{CH}_3 + \text{CD}_3 \rightarrow \text{CH}_3\text{CD}_2\text{CH}_2 + \text{CD}_3\text{H}$ PROPANE-2,2-d ₂ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
365-435	3.2(+12)	0	20130	
$\text{CH}_3\text{CCH}_2 + \text{CH}_3 \rightarrow \text{CH}_3 + \text{CH}_2\text{-C}^{\bullet}\text{-d}$ PROPYL, 2-oxo-, FREE RADICAL 70 BEN/G'N REACTION ORDER: 1.				
350-500	1.0(+11)	0	2970±500	
$\text{CH}_3\text{CH}_2\text{CCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3) + \text{CH}_4$ PROPANOL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
NOTE: TENTATIVE k VALUE.				
990-1101	1.8(+16)	0	40765	
$(\text{CH}_3)_2\text{CCH}_3 + \text{CH}_3\text{C}(\text{CH}_3) + \text{CH}_3$ I-PROPANONE 70 BEN/G'N REACTION ORDER: 1.				
298-873	4.6(+13)	0	4220±20	
$(\text{CH}_3)_2\text{CCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CCH}_2 + \text{H}_2$ 2-PROPANONE + HYDROGEN ATOM 72 KGN REACTION ORDER: 2.				
350-700	3.5(+11)	0	4900±250	
$(\text{CH}_3)_2\text{CCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CCH}_2 + \text{CH}_4$ 2-PROPANONE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
350-800	4.8(+11)	0	5735±250	
$(\text{CD}_3)_2\text{CCH}_3 + \text{CD}_3 \rightarrow \text{CD}_3\text{CCH}_2 + \text{CD}_4$ 2-PROPANE-1,1,1,2,2,3,3-d ₆ + METHYL-d ₃ FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
323-415	1.9(+11)	0	3901	
$\text{CH}_2=\text{CHCH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ $+ \text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{CH}_2$ 2-PROPEN-1-ol + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
648-920	2.5(+12)	0	24300	
$\text{HCCHCH}_2\text{CH}_3 \rightarrow \text{HCCH} + \text{CH}_2\text{-CH}_2$ FORMIC ACID ETHYL ESTER 70 BEN/G'N REACTION ORDER: 1.				
350-500	2.5(+11)	0	5100±500	
$\text{HCCHCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{HCCHCH}_2\text{CH}_2 + \text{HCCHCH}(\text{CH}_3)\text{CH}_3 + \text{CH}_4$ FORMIC ACID ETHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
NOTE: TENTATIVE k VALUE.				
350-600	2.1(+11)	0	5035±500	
$\text{CH}_3\text{CCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_2\text{CCH}_2\text{CH}_3 + \text{CH}_4$ ACETIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
350-650	1.9(+11)	0	5035±500	
$\text{CH}_3\text{CCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_2\text{CCH}_2\text{CH}_3 + \text{CH}_4$ ACETIC ACID METHYL-d ₃ ESTER + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.				
$\text{CD}_3\text{CCH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CD}_3\text{CCH}_2\text{CH}_2 + \text{CH}_4$ ACETIC-d ₃ ACID METHYL ESTER + METHYL FREE RADICAL				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
400-600	1.7(+11)	0	5990±500	
350-500	3.2(+11)	0	5800±750	
298	1.3(+11)	-	-	0.6 1.5
400-525	1.9(+11)	0	4590±500	
400-525	1.5(+11)	0	3975±500	
553-653	3.2(+15)	0	21640	
300-450	3.2(+11)	0	4630±750	
303	4.1(+7)	-	-	
323-454	6.2(+10)	0	1700	
958-1038	1.3(+14)	0	36600	
400-600	3.6(+11)	0	4330±500	
350-600	4.7(+11)	0	4600±500	
348-378	1.3(+17)	0	20300	

76 KER/PAR REACTION ORDER: 2.

 $\text{CH}_3\text{OCOCCH}_3 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{OCOCCH}_3 + \text{CH}_4$
 CARBONIC ACID DIMETHYL ESTER + METHYL FREE RADICAL
 REACTION ORDER: 2.
 76 KER/PAR

 $(\text{CH}_3)_2\text{CHOH} + \text{O} \rightarrow \text{products}$
 2-PROPANOL + OXYGEN ATOM
 73 KER/HUI
 REACTION ORDER: 2.

 $(\text{CH}_3)_2\text{CDOH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OH} + \text{CH}_3\text{D}$
 2-PROPAN-2-d-OL + METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

 $(\text{CH}_3)_2\text{CHOH} + \text{CD}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{OH} + \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{OD} + \text{CD}_3\text{H}$
 2-PROPANOL-d + METHYL-d₃ FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

 $(\text{CH}_3)_2\text{CHOH} \rightarrow (\text{CH}_3)_2\text{CHO}\cdot + \text{OH}$
 HYDROPEROXIDE, 1-METHYLETHYL
 70 BEN/G'N
 REACTION ORDER: 1.

 $\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{CH}_3\cdot \rightarrow \text{cy-CH}_2\text{CH}_2\text{CH}_2\text{SCH}_3 + \text{CH}_4$
 THETANE + METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.
 NOTE: TENTATIVE k VALUE.

 $(\text{CH}_3)_2\text{CHSH} + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{CHS}\cdot + (\text{CH}_3)_2\text{C}(\cdot)\text{SH}$
 $+ \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{SH} + \text{CH}_4$
 2-PROPANETHIOL + METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.
 NOTE: TENTATIVE k VALUE.

 $\text{CH}_2=\text{CHCN} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$
 2-PROPENITRILE + ETHYL FREE RADICAL
 72 KER/PAR
 REACTION ORDER: 2.

 $\text{CH}_3\text{CH}_2\text{CN} \rightarrow \text{CH}_3\cdot + \cdot\text{CH}_2\text{CN}$
 PROPANENITRILE
 70 BEN/G'N
 REACTION ORDER: 1.

 $\text{CH}_3\text{CH}_2\text{CN} + \text{CD}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}_2\text{CN} + \text{CD}_3\text{H}$
 PROPANENITRILE + METHYL-d₃ FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

 $(\text{CH}_3)_3\text{N} + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_4$
 METHANINE, N,N-DIMETHYL-, + METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

 $\text{O}_2\text{NOCCH}_2\text{CH}(\text{ONOC}_2\text{H}_5)_2 \rightarrow \text{products}$
 1,2,3-TRIFLUOROTRINITRILE
 70 BEN/G'N
 REACTION ORDER: 1.

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f
353-373	1.6(+15)	0	18800	
$\text{C}_2\text{N}_6\text{CH}_2\text{CH}(\text{ONO}_2)\text{CH}_3 \rightarrow \text{products}$ 1,2-PROPANEDICL, DINITRATE 70 BEN/G'N REACTION ORDER: 1. -----				
358-383	1.6(+15)	0	19175	
400-600	6.3(+10)	0	3600*500	
$\text{C}_2\text{N}_6\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO}_2 \rightarrow \text{products}$ 1,3-PROPANEDICL, DINITRATE 70 BEN/G'N REACTION ORDER: 1. -----				
687-733	2.50(+13)	0	24005	
800-1000	2.0(+11)	0	20130	
443-483	1.6(+16)	0	20230	
443-483	3.2(+16)	0	18600	
300	9.0(+11)	-	-	0.7 1.4
320-550 435	3.5(+11)	0	1125	
456-620	1.9(+12)	0	5135*500	
298	1.9(+13)	-	-	
320-550 435	1.9(+11)	0	526	
$\text{HCN}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \text{CN}(\text{CH}_3)_2 + \text{HC}-(\text{CH}_3)\text{NCH}_2 + \text{CH}_4$ FORMAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
$\text{CH}_3\text{CH}_2\text{CH}_2\text{NO}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HONO}$ PROPANE, 1-NITRO- 70 BEN/G'N REACTION ORDER: 1. -----				
$\text{CH}_3\text{CH}(\text{NO}_2)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HONO}$ PROPANE, 2-NITRO- 70 BEN/G'N REACTION ORDER: 1. -----				
$\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}$ NITROUS ACID PEROXY ESTER 70 BEN/G'N REACTION ORDER: 1. -----				
$(\text{CH}_3)_2\text{CHONO}_2 \rightarrow (\text{CH}_3)_2\text{CHO} + \text{NO}$ NITROUS ACID, 1-METHYL ETHYL ESTER 70 BEN/G'N REACTION ORDER: 1. -----				
$\text{CH}=\text{CC}=\text{CH} + \text{O} \rightarrow \text{products}$ 1,3-BUTADIENE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----				
$\text{CH}_3\text{CH}_2\text{C}=\text{CH} + \text{N} \rightarrow \text{products}$ 1-BUTYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 13.0				
NOTE: k _{ref} : CH ₃ CH + N -----				
$\text{CH}_3\text{CH}_2\text{C}=\text{CH} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}(\text{O})\text{C}=\text{CH} + \text{CH}_2\text{CH}_2\text{C}=\text{CH}$ + $\text{CH}_3\text{CH}_2\text{C}=\text{C} + \text{CH}_4$ 1-BUTYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
$\text{CH}_3\text{C}=\text{CCH}_3 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{C}=\text{C}(\text{CH}_3)\text{S}$ 2-BUTYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. -----				
$\text{CH}_3\text{C}=\text{CCH}_3 + \text{N} \rightarrow \text{products}$ 2-BUTYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. k/k _{ref} : 12.0				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f F
NOTE: k_{ref} : $CH_3CH \cdot N$ ----- $CH_3COCH_3 + CH_3 \rightarrow CH_3C=CH_2 + CH_4$ 2-BUTYNE + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----				
486-619	1.1(+12)	0	4900±500	
----- $CH_3COCH_3 + CCl_4 \rightarrow$ products 2-BUTYNE + CARBON OXIDE(C_2O) 72 KHE/PAR REACTION ORDER: 2. k/k_{ref} : 8.5 NOTE: k_{ref} : $CH_2=CH_2 + CCl_4$ ----- -----				
304	-	-	-	
----- $CH_2=CHCH=CH_2 + C \rightarrow$ products 1,3-BUTADIENE + OXYGEN ATOM 73 KHE/EUI REACTION ORDER: 2. -----				
298-400	3.4(+12)	0	- 380	0.7 1.3
----- $CH_2=CHCH=CH_2 + H \rightarrow CH_2=CHCH(\cdot)CH_3 + CH_2=CHCH_2CH_2 \cdot$ 1,3-BUTADIENE + HYDROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. NOTE: AVERAGED k . -----				
298	4.10(+13)	0	655	
300	-	-	-	
NOTE: k_{ref} : $CH_3CH=CH_2 + H$ ----- ----- $CH_2=CHCH=CH_2 + S \rightarrow cy-(CH_2=CH)CHCH_2S$ 1,3-BUTADIENE + SULFUR ATOM 72 KHE/PAR REACTION ORDER: 2. -----				
298	6.0(+13)	-	-	
----- $CH_2=CHCH=CH_2 + N \rightarrow$ products 1,3-BUTADIENE + NITROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. -----				
340	3.5(+10)	-	-	
----- $CH_2=CHCH=CH_2 + ^1CH_2 \rightarrow$ products 1,3-BUTADIENE + METHYLENE FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. k/k_{ref} : 3.2 NOTE: k_{ref} : $CH_2=CH_2 + ^1CH_2$ ASSUMING 10% 3CH_2 ----- -----				
297	-	-	-	
----- $CH_2=CHCH=CH_2 + CH_3 \rightarrow CH_3CH_2CH(\cdot)CH=CH_2$ 1,3-BUTADIENE + METHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. -----				
353-453	8.1(+10)	0	2065	
----- $CH_2=CHCH=CH_2 + CH_3 \rightarrow CH_3CH_2CH(\cdot)CH=CH_2$ 1,3-BUTADIENE + METHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. k/k_{ref} : 12.0 NOTE: k_{ref} : $CH_2=CH_2 + CH_3$ ----- -----				
435	-	-	-	
----- $CH_2=CHCH=CH_2 + CCl_4 \rightarrow CH_2=C=CHCH=CH_2 + CCl_4$ 1,3-BUTADIENE + CARBON TETRACHLORIDE 72 KHE/PAR REACTION ORDER: 2. k/k_{ref} : 210. NOTE: k_{ref} : $CH_2=CH_2 + CCl_4$ ----- -----				
298	-	-	-	
----- $CH_3CH_2CH=CH_2 + O \rightarrow cy-(CH_3CH_2)CHCH_2O$ 1-BUTENE + OXYGEN ATOM -----				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
NOTE: k_{ref} : $CH_2=CH_2 + N$ ----- $cis-CH_3CH=CHCH_3 + ^1CH_2 \rightarrow$ products $cis-2-BUTENE + METHYLENE FREE RADICAL$ 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 1.37				
297	-	-	-	
NOTE: k_{ref} : $CH_2=CH_2 + ^1CH_2$ ----- $cis-CH_3CH=CHCH_3 + ^3CH_2 \rightarrow$ products $cis-2-BUTENE + METHYLENE FREE RADICAL$ 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 0.94				
297	-	-	-	
NOTE: k_{ref} : $CH_2=CH_2 + ^3CH_2$ ----- $cis-CH_3CH=CHCH_3 + CH_3 \rightarrow CH_3CH=CHCH_2 + CH_4$ $cis-2-BUTENE + METHYL FREE RADICAL$ 76 KER/PAR REACTION ORDER: 2.				
350-650	1.8(+11)	0	4100±500	
$cis-CH_3CH=CHCH_3 + CH_3 \rightarrow (CH_3)_2CHCH(•)CH_3$ $cis-2-BUTENE + METHYL FREE RADICAL$ 72 KER/PAR REACTION ORDER: 2.				
353-453	4.5(+10)	0	3675	
NOTE: k_{ref} : $CH_2=CH_2 + CH_3$ ----- $cis-CH_3CH=CHCH_3 + CCl \rightarrow cis-CH_3CH=C=CHCH_3 + CCl$ $cis-2-BUTENE + CARBON OXIDE(C_2O)$ 72 KER/PAR REACTION ORDER: 2. k/k_{ref} : 9.1				
297	-	-	-	
NOTE: k_{ref} : $CH_2=CH_2 + CCl$ ----- $cis-CH_3CH=CHCH_3 + CH_3CH_2 \rightarrow CH_3CH(CH_2CH_3)CH(•)CH_3$ $cis-2-BUTENE + ETHYL FREE RADICAL$ 72 KER/PAR REACTION ORDER: 2.				
298	-	-	4265	
NOTE: CRITICAL ENERGY OF REACTION. ----- $cis-CH_3CH=CHCH_3 + CH_3CH_2CH_2 \rightarrow CH_3CH(CH_2CH_2CH_3)CH(•)CH_3$ $cis-2-BUTENE + PROPYL FREE RADICAL$ 72 KER/PAR REACTION ORDER: 2.				
298	-	-	4370	
$cis-CH_3CH=CHCH_3 + (CH_3)_2CH \rightarrow CH_3CH(CH_3)_2CH(•)CH_3$ $cis-2-BUTENE + ETHYL, 1-METHYL-, FREE RADICAL$ 72 KER/PAR REACTION ORDER: 2.				
298	-	-	3950	
$trans-CH_3CH=CHCH_3 + O \rightarrow$ products $trans-2-BUTENE + OXYGEN ATOM$ 73 KER/HUI REACTION ORDER: 2.				
298	1.4(+13)	-	-	0.7 1.3
$trans-CH_3CH=CHCH_3 + H \rightarrow CH_3CH_2CH(•)CH_3$ $trans-2-BUTENE + HYDROGEN ATOM$ 72 KER/PAR REACTION ORDER: 2.				
298	5.6(+11)	-	-	
NOTE: AVERAGE k . ----- $trans-CH_3CH=CHCH_3 + S \rightarrow cy-(CH_3CH)CH(CH_3)S$				
300	-	-	-	
NOTE: k_{ref} : $CH_3CH=CH_2 + H$ -----				

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
trans-2-BUTENE + SULFUR ATOM 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + S$ $k/k_{ref}: 20.0$	298 298	1.4(+13) -	- -	- -	
trans-CH ₃ CH=CHCH ₃ + N → products trans-2-BUTENE + NITROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + N$ $k/k_{ref}: 3.0$	320-550 435	3.4(+11) -	0 -	1055 -	
trans-CH ₃ CH=CHCH ₃ + ¹ CH ₂ → products trans-2-BUTENE + METHYLENE FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + ^1CH_2$ $k/k_{ref}: 1.39$	297	-	-	-	
trans-CH ₃ CH=CHCH ₃ + ³ CH ₂ → products trans-2-BUTENE + METHYLENE FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + ^3CH_2$ $k/k_{ref}: 0.89$	297	-	-	-	
trans-CH ₃ CH=CHCH ₃ + CH ₃ → CH ₃ CH=CHCH ₂ + CH ₄ trans-2-BUTENE + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + ^3CH_2$ $k/k_{ref}: 0.89$	350-500 353-453	1.0(+12) 1.4(+11)	0 0	4830±500 4075	
trans-CH ₃ CH=CHCH ₃ + CH ₃ → (CH ₃) ₂ CHCH(•)CH ₃ trans-2-BUTENE + METHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + CH_3$ $k/k_{ref}: 0.4$	453	-	-	-	
trans-CH ₃ CH=CHCH ₃ + CCl ₄ → CH ₃ CH=C-CHCH ₃ + CCl ₃ trans-2-BUTENE + CARBON TETRACHLORIDE 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + CCl_4$ $k/k_{ref}: 10.6$	297	-	-	-	
trans-CH ₃ CH=CHCH ₃ + CH ₃ CH ₂ • → CH ₃ CH(CH ₃)CH ₂ CH ₃ trans-2-BUTENE + ETHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + CCl_4$ $k/k_{ref}: 10.6$	298	-	-	4350	
trans-CH ₃ CH=CHCH ₃ + CH ₃ CH ₂ CH ₂ • → CH ₃ CH(CH ₃)CH ₂ CH ₂ CH ₃ trans-2-BUTENE + PROPYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + CCl_4$ $k/k_{ref}: 10.6$	298	-	-	4515	
trans-CH ₃ CH=CHCH ₃ + (CH ₃) ₂ CH• → CH ₃ CH(CH ₃) ₂ CH ₃ trans-2-BUTENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. NOTE: $k_{ref}: CH_2=CH_2 + CCl_4$ $k/k_{ref}: 10.6$	298	-	-	4065	

CHEMICAL REACTIONS

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f F
$(CH_3)_2C=CH_2 \rightarrow \cdot CH_2C(CH_3)=CH_2 + H$ 1-PROPENE, 2-METHYL- 70 BEN/6'N REACTION ORDER: 1. -----	930-1082	1.0(+17)	0	44400	
$(CH_3)_2C=CH_2 + \delta \rightarrow cy-[(CH_3)_2]CCH_2^\delta$ 1-PROPENE, 2-METHYL-, + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2. -----	298	1.2(+13)	-	-	0.7 1.3
$(CH_3)_2C=CH_2 + H \rightarrow (CH_3)_3C\cdot$ 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. -----	298	3.1(+13)	0	755	
$(CH_3)_2C=CH_2 + H \rightarrow (CH_3)_2CHCH_2\cdot$ 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. -----	298	1.3(+11)	-	-	
NOTE: CALCULATED ON THE BASIS OF 0.5% NON-TERMINAL ADDITION OF H TO $(CH_3)_2C=CH_2$. -----					
$(CH_3)_2C=CH_2 + H \rightarrow (CH_3)_3C\cdot + (CH_3)_2CHCH_2\cdot$ 1-PROPENE, 2-METHYL-, + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 2.52$ NOTE: $k_{ref}: CH_3CH=CH_2 + H$ -----	300	-	-	-	
$(CH_3)_2C=CH_2 + H_2 \rightarrow$ products 1-PROPENE, 2-METHYL-, + HYDROPEROXYL FREE RADICAL 74 ILG REACTION ORDER: 2. -----	300	1.0(+ 8)	-	-	0.1 10.
NOTE: SUGGESTED k VALUE.					
$(CH_3)_2C=CH_2 + S \rightarrow cy-[(CH_3)_2]CCH_2S$ 1-PROPENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. -----	298 298	4.0(+13)	- -	- -	
NOTE: $k_{ref}: CH_2=CH_2 + S^*(^1D)$ $k/k_{ref}: 50.0$					
$(CH_3)_2C=CH_2 + S^*(^1D) \rightarrow cy-[(CH_3)_2]CCH_2S$ 1-PROPENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 3.5$ -----	300	-	-	-	
NOTE: $k_{ref}: CH_2=CH_2 + S^*(^1D)$					
$(CH_3)_2C=CH_2 + N \rightarrow$ products 1-PROPENE, 2-METHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. -----	320-550	7.8(+10)	0	277	
$(CH_3)_2C=CH_2 + N \rightarrow$ products 1-PROPENE, 2-METHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 4.1$ -----	435	-	-	-	
NOTE: $k_{ref}: CH_2=CH_2 + N$					
$(CH_3)_2C=CH_2 + ^1CH_2 \rightarrow$ products 1-PROPENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 1.96$ -----	297	-	-	-	
NOTE: $k_{ref}: CH_2=CH_2 + ^1CH_2$					

CHEMICAL REACTIONS	T/K	A	B	E/R. (in °K)	k factors f F
----- $(CH_3)_2C=CH_2 + {}^3CH_2 \rightarrow$ products 1-PROPENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KHE/FAR REACTION ORDER: 2. k/k_{ref}: 2.86 NOTE: k_{ref}: $CH_2=CH_2 + {}^3CH_2$	297	-	-		
----- $(CH_3)_2C=CH_2 + CH_3 \rightarrow$ $CH_2C(CH_3)=CH_2 + CH_4$ 1-PROPENE, 2-METHYL-, + METHYL FREE RADICAL 76 KHE/FAR REACTION ORDER: 2.	350-600	3.0(+11)	0	4500±500	0.6 1.4
----- $(CH_3)_2C=CH_2 + CH_3 \rightarrow$ $(CH_3)_3CCH_2 + (CH_3)_2C(•)CH_2CH_3$ 1-PROPENE, 2-METHYL-, + METHYL FREE RADICAL 72 KHE/FAR REACTION ORDER: 2. k/k_{ref}: 1.1	353-453	1.4(+11)	0	3475	
----- NOTE: k_{ref}: $CH_2=CH_2 + CH_3$ $(CH_3)_2C=CH_2 + CCl_4 \rightarrow$ $(CH_3)_2C=CH_2 + CCl_4$ 1-PROPENE, 2-METHYL-, + CARBON TETRACHLORIDE 72 KHE/FAR REACTION ORDER: 2. k/k_{ref}: 50.0	297	-	-		
----- NOTE: k_{ref}: $CH_2=CH_2 + CCl_4$ $CH_3CH_2CH_2CH_2 + CH_3CH_2 + CH_2=CH_2$ BUTYL FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.	334-689	4.0(+13)	0	14600	
----- $CH_3CH_2CH_2CH_2 + CH_2=CH_2 \rightarrow$ $CH_3(CH_2)_4CH_2$ BUTYL FREE RADICAL + ETHYLENE 72 KHE/FAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	352-405	2.3(+10)	0	3370	
----- $CH_3CH_2CH(•)CH_3 \rightarrow$ $CH_3CH=CH_2 + CH_3$ PROPYL, 1-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.	523-622	1.4(+14)	0	17060	
----- $CH_3CH_2CH(•)CH_3 + CH_3CH=CH_2 \rightarrow$ $CH_3CH_2CH(CH_3)CH(CH_3)CH_2$ + $CH_3CH_2CH(CH_3)CH_2CH(•)CH_3$ PROPYL, 1-METHYL-, FREE RADICAL + 1-PROPENE 72 KHE/FAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	381-412	6.3(+10)	0	3725	
----- $(CH_3)_2CHCH_2 + CH_3 + CH_3CH=CH_2$ PROPYL, 2-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.	299-691	1.6(+14)	0	16455	
----- $(CH_3)_2CHCH_2 + (CH_3)_3CCH_2 + H$ PROPYL, 2-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.	299-691	5.0(+13)	0	18420	
----- $(CH_3)_3C + (CH_3)_2C=CH_2 + H$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.	300-897	4.0(+14)	0	21700	0.2 5.0

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
363-577	1.0(+11)	0	3875	
$(CH_3)_3C \cdot + CH=CH \rightarrow (CH_3)_3CCH=CH \cdot$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHYNE 72 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
300-650	2.8(+10)	0	3575	
360-439	5.0(+8)	0	2770	
653-803	4.0(+17)	0	43230	
653-803	1.9(+17)	0	41170	
298-650	3.0(+13)	0	2920	0.7 1.3
298-650	4.6(+13)	0	2410	0.7 1.3
320-930	4.1(+12)	0	2637±320	0.5 2.0
300-1000	5.0(+11)	0	5285	0.1 10.
350-500	1.6(+11)	0	4540±150	0.7 1.4
350-750	4.0(+11)	0	4830±250	0.7 1.3
600-750	4.5(+11)	0	5735±250	0.7 1.3
$(CH_3)_3C \cdot + CH_3C=CH \rightarrow (CH_3)_3CC(CH_3)=CH \cdot + (CH_3)_3CCH=C(\cdot)OH_3$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHYNE 72 KEE/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.				
$(CH_3)_3C \cdot + CH_2=CH_2 \rightarrow (CH_3)_3CCH_2CH_2 \cdot$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + ETHENE 72 KEE/PAR REACTION ORDER: 2.				
$(CH_3)_3C \cdot + CH_3C=CH \rightarrow (CH_3)_3CC(CH_3)=CH \cdot + (CH_3)_3CCH=C(\cdot)OH_3$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL + 1-PROPENE 72 KEE/PAR REACTION ORDER: 2. NOTE: SUSPECT k VALUE.				
$CH_3CH_2CH_2CH_3 \rightarrow CH_3 \cdot + CH_3CH_2CH_2 \cdot$ BUTANE 70 BEN/6'N REACTION ORDER: 1. NOTE: k ESTIMATED.				
$CH_3CH_2CH_2CH_3 \rightarrow CH_3CH_2 \cdot + CH_3CH_2 \cdot$ BUTANE 70 BEN/6'N REACTION ORDER: 1. NOTE: k ESTIMATED.				
$CH_3CH_2CH_2CH_3 + 6 \rightarrow CH_3CH_2CH_2CH_2 \cdot + 6H$ BUTANE + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2.				
$CH_3CH_2CH_2CH_3 + 6 \rightarrow CH_3CH_2CH_2CH(\cdot)CH_3 + 6H$ BUTANE + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2.				
$CH_3CH_2CH_2CH_3 + H \rightarrow CH_3CH_2CH(\cdot)CH_3 + H_2$ BUTANE + HYDROGEN ATOM 72 K6N REACTION ORDER: 2.				
$CH_3CH_2CH_2CH_3 + H_2 \rightarrow CH_3CH_2CH(\cdot)CH_3 + H_2$ BUTANE + HYDROPEROXYL FREE RADICAL 74 IIG REACTION ORDER: 2.				
NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} for $H_2 + H_2 \rightarrow H_2 + 2H$				
$CH_3CH_2CH_2CH_3 + CH_3 \cdot \rightarrow CH_3CH_2CH(\cdot)CH_3$ $+ CH_3CH_2CH_2CH_2 \cdot + CH_4$ BUTANE + METHYL FREE RADICAL 72 K6N REACTION ORDER: 2.				
$CH_3CH_2CH_2CH_3 + CH_3 \cdot \rightarrow CH_3CH_2CH(\cdot)CH_3 + CH_4$ BUTANE + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2.				
$CH_3CD_2CH_2CH_3 + CD_3 \cdot \rightarrow CH_3CD_2CD(\cdot)CH_3 + CD_4$ BUTANE-2,2,3,3-d ₄ + METHYL-d ₃ FREE RADICAL 76 KEE/PAR REACTION ORDER: 2.				

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors 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 ₄ + METHYL-d ₃ FREE RADICAL 76 KHR/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
$(\text{CH}_3)_3\text{CH} + \text{H}_2 \rightarrow (\text{CH}_3)_3\text{C} \cdot + \text{H}_2^{\delta 2}$ PROPANE, 2-METHYL-, + HYDROPEROXYL FREE RADICAL 74 IIC REACTION ORDER: 2.	300-1000	1.0(±11)	0	3500	0.1 10.
NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k_{ref} for $\text{H}_2 + \text{H}_2 \rightarrow \text{H}_2^{\delta 2} + \text{H}_2$					
$(\text{CH}_3)_3\text{CH} + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{C} \cdot + \text{CH}_4$ PROPANE, 2-METHYL-, + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	550-750	9.6(±10)	0	3975±250	0.7 1.3
$(\text{CH}_3)_3\text{CH} + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{C} \cdot + (\text{CH}_3)_2\text{CHCH}_2 \cdot + \text{CH}_4$ PROPANE, 2-METHYL-, + METHYL FREE RADICAL 76 KHR/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 ₃ FREE RADICAL 76 KHR/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 ₃ FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	550-750	6.0(±11)	0	5735±250	0.7 1.3
$\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}(\cdot) + \text{CH}_4$ 2-BUTENAL + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	350-500	1.0(±11)	0	3400±500	0.4 2.5
NOTE: TENTATIVE k VALUE.					
$\text{CH}_2=\text{CHCH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2$ 3-BUTENOIC ACID 70 HHR/G'N REACTION ORDER: 1.	587-651	2.2(±11)	0	20435	
$\text{CH}_3\text{COCH}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{COCH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COCH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ACETIC ACID ETHENYL ESTER + ETHYL FREE RADICAL 72 KHR/PAR REACTION ORDER: 2.	303-417	7.8(±10)	0	3475	
$\text{CH}_3\text{COCHCH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{COCHCH}_2 \cdot + \text{CH}_4$ 2,3-BUTANEDIONE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.	300-800	2.2(±11)	0	4300±500	0.5 1.5
$\text{CH}_3\text{COCHCH}_3 \rightarrow \text{CH}_3\text{C}(\cdot) + \text{CH}_3\text{C}(\cdot)$ 2,3-BUTANEDIONE 70 HHR/G'N REACTION ORDER: 1.	626-698	1.6(±16)	0	33970	

CHEMICAL REACTIONS

T/K	A	B	E/R. (in °K)	k factors f F
553-646	1.0(+12)	0	17365	
300-500	1.8(+11)	0	4830±500	0.6 1.4
363-463	1.8(+14)	0	14845	
300-500	8.2(+10)	0	3700±500	0.5 1.5
613-673	1.3(+12)	0	24006	
347-455	1.3(+10)	0	3675	
350-500	2.5(+11)	0	5000±500	0.5 2.0
721-811	4.0(+12)	0	22145	
350-500	2.5(+11)	0	4980±500	0.5 2.0
725-883	3.9(+12)	0	24155	
573-648	4.0(+12)	0	21640	
418-453	8.1(+10)	0	11825	

$(CH_3CO)_2O \rightarrow CH_3COOH + CH_2=C=O$
 ACETIC ACID ANHYDRIDE
 70 BEN/G'N REACTION ORDER: 1.

 $(CH_3CO)_2O + CH_3O \rightarrow CH_3COOCH_2O + CH_4$
 ACETIC ACID ANHYDRIDE + METHYL FREE RADICAL
 76 KER/PAR REACTION ORDER: 2.

 $CH_3C(=O)OCC(=O)CH_3 \rightarrow CH_3C(=O)O + CH_3C(=O)O$
 PEROXIDE, DIACETYL
 70 BEN/G'N REACTION ORDER: 1.

 $CH_3CH_2COCH_3 + CH_3O \rightarrow CH_3CH(=O)COCH_3 + CH_2CH_2COCH_3$
 $+ CH_3CH_2COCH_2O + CH_4$
 2-BUTANONE + METHYL FREE RADICAL
 76 KER/PAR REACTION ORDER: 2.

 $HCOCCH_2CH_2CH_3 \rightarrow HCOCCH_3 + CH_3CH=CH_2$
 FORMIC ACID PROPYL ESTER
 70 BEN/G'N REACTION ORDER: 1.

 $HCOCCH_2CH_2CH_3 + CH_3O \rightarrow HCOCCH_2CH_2CH_3 + CH_4$
 FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL
 72 KGN REACTION ORDER: 2.

 $HCOCCH_2CH_2CH_3 + CH_3O \rightarrow HCOCCH_2CH_2CH_3 + HCOCCH(=O)CH_2CH_3$
 $+ HCOCCH_2CH(=O)CH_3 + HCOCCH_2CH_2CH_2O + CH_4$
 FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL
 76 KER/PAR REACTION ORDER: 2.
 NOTE: TENTATIVE k VALUE.

 $HCOCCH(CH_3)_2 \rightarrow HCOCCH_3 + CH_3CH=CH_2$
 FORMIC ACID 1-METHYLETHYL ESTER
 70 BEN/G'N REACTION ORDER: 1.

 $HCOCCH(CH_3)_2 + CH_3O \rightarrow HCOCCH(CH_3)_2 + HCOCCH(=O)(CH_3)_2$
 $+ HCOCCH(CH_3)CH_2O + CH_4$
 FORMIC ACID 1-METHYLETHYL ESTER + METHYL FREE RADICAL
 76 KER/PAR REACTION ORDER: 2.
 NOTE: TENTATIVE k VALUE.

 $CH_3COOCH_2CH_3 \rightarrow CH_3COOH + CH_2=CH_2$
 ACETIC ACID ETHYL ESTER
 70 BEN/G'N REACTION ORDER: 1.

 $CH_3COOCH_2CH_3 \rightarrow CH_3OH + CO_2 + CH_2=CH_2$
 CARBONIC ACID ETHYL METHYL ESTER
 70 HEN/G'N REACTION ORDER: 1.

 $CH_3CH(=O)OCH_2CH_3 \rightarrow CH_3CHO + CH_3CH_2O$
 ETHYL, 1-ETHOXY-, FREE RADICAL
 70 HEN/G'N REACTION ORDER: 1.
 NOTE: logA PROBABLY LOW.

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
----- $\text{CH}_3\text{CH}(\text{C}_6\text{H}_5)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}^\bullet + \text{CH}_3\text{CH}_2\text{C}^\bullet$ ETHOXY, 1-ETHYL-, FREE RADICAL 70 BEN/6'N REACTION ORDER: 1. NOTE: ESTIMATED ARRHENIUS PARAMETERS (VERY LIKELY LOWER LIMITS). -----	423-463	1.0(+14)	0	8800	
----- $(\text{CH}_3)_3\text{CO}^\bullet \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3^\bullet$ ETHOXY, 1,1-DIMETHYL-, FREE RADICAL 70 BEN/6'N REACTION ORDER: 1. NOTE: TENTATIVE k. -----	393-453	3.2(+13)	0	8300	
----- $(\text{CH}_3)_3\text{COH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{O}$ 2-PROPANOL, 2-METHYL- 70 BEN/6'N REACTION ORDER: 1. -----	1050-1300	2.5(+13)	0	31001	
----- $\text{CH}_3\text{CH}_2\text{C}^\bullet\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2^\bullet + \text{CH}_3\text{CH}_2\text{C}^\bullet$ ETHANE, 1,1'-OXYBIS- 70 BEN/6'N REACTION ORDER: 1. NOTE: k PRECEABLY RELIABLE. -----	833-913	1.0(+18)	0	42275	
----- $\text{CH}_3\text{CH}_2\text{C}^\bullet\text{CH}_2\text{CH}_3 + \text{CH}_3^\bullet \rightarrow \text{CH}_3\text{CH}_2\text{C}^\bullet\text{CH}(\text{C}_6\text{H}_5)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{C}^\bullet\text{CH}_2\text{CH}_3 + \text{CH}_4$ ETHANE, 1,1'-OXYBIS-, METHYL FREE RADICAL 76 KEE/PAP REACTION ORDER: 2. -----	400-500	2.5(+11)	0	4200±750	0.5 2.0
----- $\text{CH}_3\text{CH}_2\text{C}^\bullet\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2^\bullet + \text{CH}_3\text{CH}_2\text{C}^\bullet$ PEROXIDE, DIETHYL 70 BEN/6'N REACTION ORDER: 1. -----	413-518	4.0(+15)	0	18770	
----- $(\text{CH}_3)_3\text{COH} \rightarrow (\text{CH}_3)_3\text{CO}^\bullet + \text{H}^\bullet$ HYDROPEROXIDE, 1,1-DIMETHYLETHYL 70 BEN/6'N REACTION ORDER: 1. -----	553-653	4.0(+15)	0	21640	
----- $(\text{CH}_3)_3\text{CSH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{S}$ 2-PROPANETHIOL, 2-METHYL- 70 BEN/6'N REACTION ORDER: 1. -----	950-1230	2.5(+13)	0	27830	
----- $(\text{CH}_3)_3\text{CSH} + \text{CH}_3^\bullet \rightarrow (\text{CH}_3)_3\text{CS}^\bullet + \text{CH}_2\text{C}(\text{CH}_3)_2\text{SE} + \text{CH}_4$ 2-PROPANETHIOL, 2-METHYL-, METHYL FREE RADICAL 76 KEE/PAP REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----	303	5.9(+7)	-	-	
----- $\text{CH}_2=\text{CHCH}_2\text{SC}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2^\bullet + \text{CH}_3\text{SC}_2^\bullet$ 1-PROPENE, 3-METHYLSULFONYL- 70 BEN/6'N REACTION ORDER: 1. -----	633-733	1.3(+14)	0	24006	
----- $\text{cis-CH}_3\text{CH=CHCN} \rightarrow \text{trans-CH}_3\text{CH=CHCN}$ cis-2-BUTENENITRILE 70 BEN/6'N REACTION ORDER: 1. -----	573-633	5.0(+12)	0	28030	
----- $\text{cis-CH}_3\text{CH=CHCN} + \text{CH}_3\text{CH}_2^\bullet \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\text{C}_6\text{H}_5)\text{CN}$ $+ \text{CH}_3\text{CH}(\text{C}_6\text{H}_5)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ -----					

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
323-454	1.5(+10)	0	2500	
323-754	3.1(+10)	0	2600	
312-400	2.5(+11)	0	2300	
350-600	2.5(+11)	0	3975±500	0.5 2.0
543-605	2.0(+16)	0	25165	
426	3.2(+7)	-	-	0.5 2.0
350-500	2.2(+11)	0	3550±500	0.5 2.0
420	2.6(+7)	-	-	0.5 2.0
466-539	2.5(+14)	0	18170	
640-859	4.0(+11)	0	22345	

cis-2-BUTENENITRILE + ETHYL FREE RADICAL
72 KEE/PAR
REACTION ORDER: 2.

trans-CH₃CH=CHCN + CH₃CH₂• → CH₃CH(CF₂CH₃)CH(•)CN
+ CH₃CH(•)CH(CH₂CH₃)CN
trans-2-BUTENENITRILE + ETHYL FREE RADICAL
72 KEE/PAR
REACTION ORDER: 2.

CH₂=C(CH₃)CN + CH₃CH₂• → CH₃CH₂CH₂C(•)(CH₃)CN
+ •CH₂C(CH₃)(CH₂CH₃)CN
2-PROPENENITRILE, 2-METHYL-, + ETHYL FREE RADICAL
72 KEE/PAR
REACTION ORDER: 2.

CH₃CH=NN-CHCH₃ + CH₃• → CH₃C(•)-NN-CHCH₃
+ •CH₂CH=NN-CHCH₃ + CH₄
ACETALDEHYDE ETHYLIDENEHYDRAZONE + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

CH₃CH₂N=NCH₂CH₃ → CH₃CH₂N=N• + CH₃CH₂•
DIAZENE, DIETHYL-
70 BEN/6°N
REACTION ORDER 1.

CH₃N=NCH(CH₃)₂ → CH₃N=N• + (CH₃)₂CH•
DIAZENE, METHYL(1-METHYLETHYL)-
70 BEN/6°N
REACTION ORDER 1.

CH₃CH₂CH₂CH₂NH₂ + CH₃• → CH₃CH₂CH₂CH₂NH•
+ CH₃CH₂CH₂CH(•)NH₂ + •CH₂CH₂CH₂CH₂NH₂
1-BUTANAMINE + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE.

(CH₃CH₂)₂NH + CH₃• → (CH₃CH₂)₂N• + CH₃CH(•)NHCH₂CH₃
+ •CH₂CH₂NECH₂CH₃ + CH₄
ETHANAMINE, N-ETHYL-, + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE.

CH₃CH₂N(CH₃)₂ + CH₃• → CH₃CH(•)N(CH₃)₂ + •CH₂CH₂N(CH₃)₂
+ CH₃CH₂N(CH₃)CH₂• + CH₄
ETHANAMINE, N,N-DIMETHYL-, + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

NOTE: TENTATIVE & VALUE.

(CH₃)₂NN-NN(CH₃)₂ → (CH₃)₂NN=N• + (CH₃)₂N•
2-TETRAZENE, 1,1,4,4-TETRAMETHYL-
70 BEN/6°N
REACTION ORDER: 1.

CH₃CH₂CH=CH₂ → CH₃CH• + CH₂=CH₂
ETHENE, ETHENYL-
70 BEN/6°N
REACTION ORDER: 1.

CH₂=CHCH₂CH₂CH₂ → CH₃CH=CH₂ + HCH•

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f F
643-685	4.5(+11)	0	20635	
350-500	1.0(+11)	0	2970±500	0.4 1.6
350-500	1.0(+11)	0	2970±500	0.4 1.6
350-600	1.6(+11)	0	4125±500	0.5 1.5
350-600	2.0(+11)	0	4200±500	0.5 1.5
443-485	2.0(+16)	0	20400	
320-550 435	3.0(+11) -	0	1047 -	
298	2.8(+12)	-	-	0.7 1.3
298 300	8.3(+11) -	- -	- -	
298	8.1(+12)	-	-	
450-650	4.5(+11)	0	4500±500	0.6 1.4

3-BUTEN-1-OL

70 BEN/6'N

REACTION ORDER: 1.

 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)\text{CH}_3 + \text{CH}_4$

BUTANAL + METHYL FREE RADICAL

REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

 $(\text{CH}_3)_2\text{CHCH}_2 + \text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHC}(\cdot)\text{CH}_3 + \text{CH}_4$

PROPANAL, 2-METHYL-, + METHYL FREE RADICAL

REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

 $\text{CH}_3\text{CON}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2\cdot + \text{CH}_4$

ACETAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL

REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

 $\text{CH}_3\text{CON}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \cdot\text{CH}_2\text{CON}(\text{CH}_3)_2$
+ $\text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2\cdot + \text{CH}_4$

ACETAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL

REACTION ORDER: 2.

76 KER/PAR

 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CONH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot + \text{NH}_2$

NITROUS ACID BUTYL ESTER

REACTION ORDER: 1.

70 BEN/6'N

 $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{N} \rightarrow \text{products}$

1-PENTYNE + NITROGEN ATOM

REACTION ORDER: 2.

72 KER/PAR

NOTE: k_{ref} : $\text{CHCH} + \text{N}$ k/k_{ref} : 14.0

 $\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \cdot\text{O} \rightarrow \text{cy}-(\text{CH}_3\text{CH}_2\text{CH}_2)\text{CHCH}_2\cdot$

1-PENTENE + OXYGEN ATOM

REACTION ORDER: 2.

73 KER/HUI

 $\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_2\cdot$

1-PENTENE + HYDROGEN ATOM

REACTION ORDER: 2.

72 KER/PAR

NOTE: k_{ref} : $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$ k/k_{ref} : 0.89

 $\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3(\text{CH}_2)_2)\text{CHCH}_2\text{S}$

1-PENTENE + SULFUR ATOM

REACTION ORDER: 2.

72 KER/PAR

 $\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2 + \text{CH}_4$

1-PENTENE + METHYL FREE RADICAL

REACTION ORDER: 2.

76 KER/PAR

 $\text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 + \text{CHCH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$

1-PENTENE + PROPYL FREE RADICAL

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
72 KER/PAR	REACTION ORDER: 2. -----	298	-	-	3410	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{O} \rightarrow \text{Products}$ $\text{cis-2-PENTENE} + \text{OXYGEN ATOM}$ 73 HBR/HUI REACTION ORDER: 2. -----		298	1.1(+13)	-	-	0.7 1.3
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-PENTENE} + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.39$		298 300	3.8(+11) -	- -	- -	
NOTE: $k_{\text{ref}}: \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$						
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$ $\text{cis-2-PENTENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. -----		298	-	-	4060	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-PENTENE} + \text{METHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. -----		298	-	-	4125	
$\text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ $\text{cis-2-PENTENE} + \text{ETHYL FREE RADICAL}$ 72 KER/PAR REACTION ORDER: 2. -----		298	-	-	4300	
$\text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $\text{trans-2-PENTENE} + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}: 0.44$		300	-	-	-	
NOTE: $k_{\text{ref}}: \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}$						
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$ $+ \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\cdot$ $1\text{-BUTENE, 2-METHYL-}, + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. -----		298	4.1(+11)	-	-	
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{D} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{D}$ $+ \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\cdot$ $1\text{-BUTENE, 2-METHYL-}, + \text{DEUTERIUM ATOM}$ 72 KER/PAR REACTION ORDER: 2. -----		298	9.1(+11)	-	-	
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{S} \rightarrow \text{cy-(CH}_3\text{CH}_2)\text{C}(\text{CH}_3)\text{CH}_2\text{S}$ $1\text{-BUTENE, 2-METHYL-}, + \text{SULFUR ATOM}$ 72 KER/PAR REACTION ORDER: 2. -----		298	2.0(+12)	-	-	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{H} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ $1\text{-BUTENE, 3-METHYL-}, + \text{HYDROGEN ATOM}$ 72 KER/PAR REACTION ORDER: 2. -----		298	7.4(+13)	-	-	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{D} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{D} + (\text{CH}_3)_2\text{CHCHDCH}_2\cdot$ $1\text{-BUTENE, 3-METHYL-}, + \text{DEUTERIUM ATOM}$ 72 KER/PAR REACTION ORDER: 2. -----		298	7.4(+11)	-	-	
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{D} \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{D} + (\text{CH}_3)_2\text{CHCHDCH}_2\cdot$ $1\text{-BUTENE, 3-METHYL-}, + \text{DEUTERIUM ATOM}$ 72 KER/PAR REACTION ORDER: 2. -----		298	7.6(+11)	-	-	

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
403-455	1.4(±10)	0	3070	
453	-	-	-	
298	-	-	-	
762	1.0(±14)	0	18875	
340-413	1.2(±10)	0	3235	
298-650	2.9(±13)	0	2920	0.7 1.3
298-650	8.0(±13)	0	2320	0.7 1.3
350-600	4.8(±11)	0	5800±250	0.7 1.3
350-800	6.0(±11)	0	4830±250	0.7 1.3
307	8.0(±10)	-	-	0.7 1.4
350-750	9.6(±10)	0	3975±250	0.7 1.3
350-750	2.0(±11)	0	4830±250	0.7 1.3

$(CH_3)_2C(•)CH(CH_3)_2$
 2-BUTENE, 2-METHYL-, • METHYL FREE RADICAL
 72 KER/PAR
 NOTE: TENTATIVE k VALUE.

NOTE: k_{ref} : $CH_2=CH_2 + CH_3$
 k/k_{ref} : 0.4

$(CH_3)_2C=CHCH_3 + CCl_4 \rightarrow (CH_3)_2C-C-CHCH_3 + CCl_4$
 2-BUTENE, 2-METHYL-, • CARBON CHLIDE(C_2O)
 72 KER/PAR
 REACTION ORDER: 2. k/k_{ref} : 100.

NOTE: k_{ref} : $CH_2=CH_2 + CCl_4$

$(CH_3)_3CCCH_2 \rightarrow (CH_3)_2C-CH_2 + CH_3$
 PROPYL, 2,2-DIMETHYL-, FREE RADICAL
 70 BEN/G'N
 REACTION ORDER: 1.

$(CH_3)_2CHCH_2CH_2 + CH_2=CH_2 \rightarrow (CH_3)_2CH(CH_2)_3CH_2$
 BUTYL, 3-METHYL-, FREE RADICAL + ETHENE
 72 KER/PAR
 REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

$CH_3CH_2CH_2CH_2CH_3 + O \rightarrow CH_3CH_2CH_2CH_2CH_2 + OH$
 PENTANE + OXYGEN ATOM
 73 BER/HUI
 REACTION ORDER: 2.

$CH_3CH_2CH_2CH_2CH_2CH_3 + O \rightarrow CH_3CH_2CH_2CH_2CH(•)CH_3$
 $+ CH_3CH_2CH(•)CH_2CH_3 + CH$
 PENTANE + OXYGEN ATOM
 73 BER/HUI
 REACTION ORDER: 2.

$CH_3CH_2CH_2CH_2CH_2CH_3 + CH_3 \rightarrow CH_3CH_2CH_2CH_2CH_2CH_2 + CH_4$
 PENTANE + METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

$CH_3CH_2CH_2CH_2CH_2CH_3 + CH_3 \rightarrow CH_3CH_2CH_2CH(•)CH_2CH_3$
 $+ CH_3CH_2CH_2CH(•)CH_3 + CH_4$
 PENTANE + METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

$(CH_3)_2CHCH_2CH_3 + O \rightarrow [C_5H_{11}•] + OH$
 BUTANE, 2-METHYL-, • OXYGEN ATOM
 73 BER/HUI
 REACTION ORDER: 2.

$(CH_3)_2CHCH_2CH_3 + CH_3 \rightarrow (CH_3)_2C(•)CH_2CH_3 + CH_4$
 BUTANE, 2-METHYL-, • METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

$(CH_3)_2CHCH_2CH_3 + CH_3 \rightarrow (CH_3)_2CHCH(•)CH_3 + CH_4$
 BUTANE, 2-METHYL-, • METHYL FREE RADICAL
 76 KER/PAR
 REACTION ORDER: 2.

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f F
NOTE: TENTATIVE & VALUE. ----- $(CH_3)_2CHCH_2CH_3 + CH_3 \rightarrow (CH_3)_2CHCH_2CH_2 \cdot$ $\cdot CH_2CH(CH_3)CH_2CH_3 + CH_4$ BUTANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE. ----- $(CH_3)_4C \rightarrow (CH_3)_3C \cdot + CH_3$ PROPANE, 2,2-DIMETHYL- 70 BEN/C'N REACTION ORDER: 1. ----- $(CH_3)_4C + O \rightarrow (CH_3)_3CO \cdot + OH$ PROPANE, 2,2-DIMETHYL-, + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2. ----- $(CH_3)_4C + CH_3 \rightarrow (CH_3)_3CCH_2 \cdot + CH_4$ PROPANE, 2,2-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- $CH_2=CHCH_2CH=CH_2 \rightarrow CH_2=CHCH_2CH_2CH_2$ 1-PROPENE, 3-ETHENYL- 70 BEN/C'N REACTION ORDER: 1. ----- $cis-CH_3CH=CHCH_2CH_3 \rightarrow trans-CH_3CH=CHCH_2CH_3$ $cis-2-BUTENOIC ACID METHYL ESTER$ 70 BEN/C'N REACTION ORDER: 1. ----- $trans-CH_3CH=CHCH_2CH_3 \rightarrow cis-CH_3CH=CHCH_2CH_3$ $trans-2-BUTENOIC ACID METHYL ESTER$ 70 BEN/C'N REACTION ORDER: 1. ----- $CH_3C(=O)CH_2CH=CH_2 + CH_3CH_2 \cdot \rightarrow CH_3C(=O)CH_2CH_2CH_2CH_3$ $+ CH_3C(=O)CH_2CH(CH_2CH_3)CH_2 \cdot$ ACETIC ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. ----- $(CH_3C(=O))_2CH_2 \rightarrow (CH_3C(=O))_2\dot{C} + HCHO$ METHANEDICHL, DIACETATE 70 BEN/C'N REACTION ORDER: 1. ----- $(CH_3)_2CHCH=CH_2 \rightarrow CH_3CH=CH_2 + CH_3CH_2$ PROPANE, 2-(ETHENYL)- 70 BEN/C'N REACTION ORDER: 1. ----- $CH_2=CHCH_2CH(CH_3)CH_3 \rightarrow CH_3CH=CH_2 + CH_3CH_2$ 4-PENTEN-2-OL 70 BEN/C'N REACTION ORDER: 1. ----- $CH_3CH_2CH_2CH_2CH_2CH_3 + CH_3 \cdot \rightarrow CH_3CH_2CH_2CH_2CH_2C(=O) \cdot + CH_4$ PENTANAL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
803-1200		5.0(+16)	0	40465	
298-650		5.9(+13)	0	2920	0.7 1.4
400-600		8.3(+11)	0	5940±350	0.6 1.4
440-473		5.0(+11)	0	15400	
673-833		1.6(+11)	0	29090	
673-833		4.0(+12)	0	29190	
308-448		2.5(+11)	0	3900	
493-578		5.0(+10)	0	18300	
720-794		3.8(+12)	0	21920	
625-663		8.5(+11)	0	20600	
350-500		1.0(+11)	0	3000±500	0.4 1.6

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	k factors F
350-500	1.0(+11)	0	3200±500	0	2.0
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3 + \text{CH}_3^\bullet \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{CH}_3)^\bullet + \text{CH}_4$ BUTANAL, 2-METHYL-, + METHYL FREE RADICAL 76 KHE/PAR NOTE: TENTATIVE k VALUE.					
350-500	1.0(+11)	0	3070±500	0.4	1.6
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 + \text{CH}_3^\bullet \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)^\bullet + \text{CH}_4$ BUTANAL, 3-METHYL-, + METHYL FREE RADICAL 76 KHE/PAR NOTE: TENTATIVE k VALUE.					
350-500	1.0(+11)	0	3170±500	0.5	2.0
$(\text{CH}_3)_3\text{CCCH}_3 + \text{CH}_3^\bullet \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)^\bullet + \text{CH}_4$ PROPANAL, 2,2-DIMETHYL-, + METHYL FREE RADICAL 76 KHE/PAR NOTE: TENTATIVE k VALUE.					
300-450	1.9(+11)	0	3675±500	0.5	1.5
$(\text{CH}_3\text{CH}_2)_2\text{CC} + \text{CH}_3^\bullet \rightarrow \text{CH}_3\text{CH}(\text{CH}_3)\text{CCCH}_2\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CCCH}_2\text{CH}_3 + \text{CH}_4$ 3-PENTANONE + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.					
500-600	2.0(+11)	0	5535±500	0.5	2.0
$(\text{CH}_3\text{CD}_2)_2\text{CC} + \text{CH}_3^\bullet \rightarrow \text{CH}_3\text{CD}_2\text{CCD}_2\text{CH}_3 + \text{CH}_4$ 3-PENTANONE-2,2,4,4-d ₄ + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.					
500-600	1.3(+11)	0	4200±500	0.5	2.0
$(\text{CH}_3\text{CD}_2)_2\text{CC} + \text{CH}_3^\bullet \rightarrow \text{CH}_3\text{CD}_2\text{CCD}(\text{CH}_3)\text{CH}_3 + \text{CH}_4$ 3-PENTANONE-2,2,4,4-d ₄ + METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2.					
300-520	2.8(+11)	0	3986±100	0.4	2.2
$\text{HCOO}(\text{CH}_2)_3\text{CH}_3 + \text{CH}_3^\bullet \rightarrow \text{HCOO}(\text{CH}_2)_3\text{CH}_2^\bullet + \text{HCOOCH}_3 + (\text{CH}_2)_2\text{CH}_3$ $+ \text{HCOOCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{HCOOCH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$ $+ \text{HCOO}(\text{CH}_2)_3\text{CH}_2^\bullet + \text{CH}_4$ FORMIC ACID BUTYL ESTER + METHYL FREE RADICAL 76 KHE/PAR NOTE: TENTATIVE k VALUE.					
503-573	7.9(+12)	0	19730		
$\text{HCOO}(\text{CH}_2)_3\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HCOOH}$ FORMIC ACID 1,1-DIMETHYL ETHYL ESTER 70 BEN/G'N REACTION ORDER: 1.					
725-810	2.5(+12)	0	24006		
$\text{CH}_3\text{COOCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID PROPYL ESTER 70 BEN/G'N REACTION ORDER: 1.					
586-801	1.0(+13)	0	22645		
$\text{CH}_3\text{COOCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1-METHYLETHYL ESTER 70 BEN/G'N REACTION ORDER: 1.					

NOTE: RELIABILITY NO BETTER THAN AN ORDER OF MAGNITUDE.

CHEMICAL REACTIONS

T/K	A	B	E/R (ln OK)	k factors f
778-875	5.6(+12)	0	24400	
300-650	2.5(+11)	0	4125±500	0.5 1.5
725-810	1.6(+12)	0	24460	
573-648	7.9(+12)	0	21800	
757-799	3.2(+13)	0	30200	
875-925	1.4(+15)	0	35330	
420	3.0(+7)	-	-	0.5 2.0
350-550	2.0(+11)	0	3975±500	0.5 1.5
390-463	7.1(+11)	0	15050	
320-550 435	4.6(+11) -	0 -	1233 -	
320-550 435	3.4(+11) -	0 -	1102 -	

$\text{CH}_3\text{CH}_2\text{C}(\text{OCH}_2\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{OCH}_3)_2 + \text{CH}_2=\text{CH}_2$
PROPANOIC ACID ETHYL ESTER
70 BEN/6'N
REACTION ORDER: 1.

$\text{CH}_3\text{CH}_2\text{C}(\text{OCH}_2\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{C}(\text{OCH}_2\text{CH}_3)_2$
+ $\text{CH}_3\text{CH}_2\text{C}(\text{OCH}_2\text{CH}_3)_2 + \cdot\text{CH}_2\text{CH}_2\text{C}(\text{OCH}_2\text{CH}_3)_2$
+ $\text{CH}_3\text{CH}_2\text{C}(\text{OCH}_2\text{CH}_3)_2 + \text{CH}_4$
PROPANOIC ACID ETHYL ESTER + METHYL FREE RADICAL
76 KER/PAR
REACTION ORDER: 2.

$\text{CH}_3\text{C}(\text{OCH}_2\text{CH}_3)_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_3 + \text{CH}_3\text{C}(\text{OCH}_3)_2$
ACETIC ACID (2-METHOXY ETHYL) ESTER
70 BEN/6'N
REACTION ORDER: 1.

$\text{CH}_3\text{CH}_2\text{C}(\text{OCH}_2\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH} + \text{C}_2\text{H}_4 + \text{CH}_2=\text{CH}_2$
CARBOIC ACID DIETHYL ESTER
70 BEN/6'N
REACTION ORDER: 1.

$(\text{CH}_3\text{CH}_2)_2\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$
+ $\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 + \text{H}_2$
2-BUTANOL, 2-METHYL-
70 BEN/6'N
REACTION ORDER: 1.

$(\text{CH}_3)_3\text{CCN} \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CN} + \text{CH}_3\cdot$
PROPANENITRILE, 2,2-DIMETHYL-
70 BEN/6'N
REACTION ORDER: 1.

$(\text{CH}_3\text{CH}_2)_2\text{NCH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_2\text{CH}_3)_2$
+ $\cdot\text{CH}_2\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2 + (\text{CH}_3\text{CH}_2)_2\text{NCH}_2\cdot + \text{CH}_4$
ETHANAMINE, N-ETHYL-N-METHYL-, + METHYL FREE RADICAL
76 KER/PAR
REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

$(\text{CH}_3)_2\text{NCCN}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2(\text{CH}_3)\text{NCCN}(\text{CH}_3)_2 + \text{CH}_4$
UREA, TETRAMETHYL-, + METHYL FREE RADICAL
76 KER/PAR
REACTION ORDER: 2.

$\text{CH}_2=\text{CHCH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{cy-CH}_2\text{CH}=\text{CHCH}=\text{CHCH}_2$
cis-1,3,5-HEXATRIENE
70 BEN/6'N
REACTION ORDER: 1.

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} + \text{N} \rightarrow \text{products}$
1-HEXYNE + NITROGEN ATOM
72 KER/PAR
REACTION ORDER: 2.

NOTE: k_{ref} : $\text{CHCH} + \text{N}$.
 k/k_{ref} : 14.0

$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_2\text{CH}_3 + \text{N} \rightarrow \text{products}$
3-HEXYNE + NITROGEN ATOM
72 KER/PAR
REACTION ORDER: 2.

NOTE: k_{ref} : $\text{CH}\equiv\text{CH} + \text{N}$.
 k/k_{ref} : 14.0

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
474-518	6.3(+10)	0	16355	
530	1.3(+11)	0	17865	
473-510	5.2(+11)	0	18199	
318-414	1.6(+11)	0	2265	
473	1.7(+11)	0	16485	
298	3.1(+12)	-	-	0.7 1.3
338-435	3.9(+10)	0	3400	
298	-	-	4060	
298	-	-	4150	
298	-	-	3450	
298	-	-	4390	
298-400	3.4(+12)	0	-790	0.8 1.2

cis-CH₂-CH₂-CHCH-CHCH₂CH₃
cis-1,3-HEXADIENE
70 BEN/6'N
REACTION ORDER: 1.

CD₂-CHCH₂CH₂CH-CD₂ → CH₂-CHCH₂CD₂CH-CH₂
1,5-HEXADIENE-1,1,6,6-D₄
70 BEN/6'N
REACTION ORDER: 1.

(CH₃)₂C-CHCH-CH₂ → CH₂-C(CH₃)CH-CHCH₃
1,3-PENTADIENE, 4-METHYL-
70 BEN/6'N
REACTION ORDER: 1.

CH₂-C(CH₃)C(CH₃)-CH₂ + CH₃CH₂• →
+ CH₃CH₂CH₂C(•)(CH₃)C(CH₃)-CH₂
+ •CH₂C(CH₃)(CH₂CH₃)C(CH₃)-CH₂
1,3-BUTADIENE, 2,3-DIMETHYL-, + ETHYL FREE RADICAL
72 KER/PAR
REACTION ORDER: 2.

cis-CH₂-C(CH₃)CH-CHCH₃ → (CH₃)₂C-CHCH-CH₂
cis-1,3-PENTADIENE, 2-METHYL-
70 BEN/6'N
REACTION ORDER: 1.

CH₃(CH₂)₃CH-CH₂ + 6 → cy-[CH₃(CH₂)₃]CHCH₂6
1-HEXENE + OXYGEN ATOM
73 HER/HUI
REACTION ORDER: 2.

CH₃(CH₂)₃CH-CH₂ + CH₃CH₂• → CH₃(CH₂)₃CH(•)CH₂CH₂CH₃
+ CH₃(CH₂)₃CH(CH₂CH₂CH₃)CH₂•
1-HEXENE + ETHYL FREE RADICAL
72 KER/PAR
REACTION ORDER: 2.

cis-CH₃CH₂CH₂CH-CHCH₃ + CH₃• → CH₃CH₂CH₂CH(•)CH(CH₃)₂
cis-2-HEXENE + METHYL FREE RADICAL
72 KER/PAR
REACTION ORDER: 2.

cis-CH₃CH₂CH₂CH-CHCH₃ + CH₃• → CH₃CH₂CH₂CH(CH₃)CH(•)(CH₃)
cis-2-HEXENE + METHYL FREE RADICAL
72 KER/PAR
REACTION ORDER: 2.

CH₃CH₂CH₂C(CH₃)-CH₂ + CH₃• → CH₃CH₂CH₂C(•)(CH₃)CH₂CH₃
1-PENTENE, 2-METHYL-, + METHYL FREE RADICAL
72 KER/PAR
REACTION ORDER: 2.

cis-(CH₃)₂CHCH-CHCH₃ + CH₃• → (CH₃)₂CHCH(•)CH(CH₃)₂
cis-2-PENTENE, 4-METHYL-, + METHYL FREE RADICAL
72 KER/PAR
REACTION ORDER: 2.

(CH₃)₂C-C(CH₃)₂ + 6 → Products
2-BUTENE, 2,3-DIMETHYL-, + OXYGEN ATOM
73 HER/HUI
REACTION ORDER: 2.

(CH₃)₂C-C(CH₃)₂ + H → (CH₃)₂C(•)(CH₃)₂
2-BUTENE, 2,3-DIMETHYL-, + HYDROGEN ATOM

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 0.84	298	7.8(+11)	-	-	
NOTE: k _{ref} : CH ₃ -CH=CH ₂ + H		300	-	-	-	
(CH ₃) ₂ C-C(CH ₃) ₂ + S → cy-[(CH ₃) ₂ CC(CH ₃) ₂ S	-----					
2-BUTENE, 2,3-DIMETHYL-, + SULFUR ATOM						
72 KER/PAR	REACTION ORDER: 2. -----	298	8.5(+13)	-	-	
(CH ₃) ₂ C-C(CH ₃) ₂ + N → products						
2-BUTENE, 2,3-DIMETHYL-, + NITROGEN ATOM						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 3.5	320-550 435	1.7(+11)	0	690	
NOTE: k _{ref} : CH ₂ =CH ₂ + N	-----					
(CH ₃) ₂ C-C(CH ₃) ₂ + ¹ CH ₂ → products						
2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 2.16	257	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + ¹ CH ₂	-----					
(CH ₃) ₂ C-C(CH ₃) ₂ + ³ CH ₂ → products						
2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 2.74	257	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + ³ CH ₂	-----					
(CH ₃) ₂ C-C(CH ₃) ₂ + CH ₃ → (CH ₃) ₂ C-(CH ₃)CCH ₂ + 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) ₂ C-C(CH ₃) ₂ + CH ₃ → (CH ₃) ₃ CC(•)(CH ₃) ₂						
2-BUTENE, 2,3-DIMETHYL-, + METHYL FREE RADICAL						
72 KER/PAR	REACTION ORDER: 2.	403-453	1.0(+10)	0	3400	
NOTE: TENTATIVE k VALUE.						
NOTE: k _{ref} : CH ₂ =CH ₂ + CH ₃	k/k _{ref} : 0.2	453	-	-	-	
(CH ₃) ₂ C-C(CH ₃) ₂ + CCl ₄ → (CH ₃) ₂ C-C-C(CH ₃) ₂ + CCl ₃	-----					
2-BUTENE, 2,3-DIMETHYL-, + CARBON CLIDE(C ₂ Cl ₄)						
72 KER/PAR	REACTION ORDER: 2. k/k _{ref} : 250.	298	-	-	-	
NOTE: k _{ref} : CH ₂ =CH ₂ + CCl ₄	-----					
CH ₃ CH(•)(CH ₂ CH ₂ CH ₂ CH ₃ → CH ₃ CH=CH ₂ + CH ₃ CH ₂ CH ₂ •						
PENTYL, 1-METHYL-, FREE RADICAL						
70 BEN/6'N	REACTION ORDER: 1. -----	822	2.0(+14)	0	13800	
CH ₃ (CH ₂) ₄ CH ₃ + Cl → CH ₃ (CH ₂) ₄ CH ₂ • + ClH						
HEXANE + OXYGEN ATOM						
73 HBR/HUI	REACTION ORDER: 2. -----	298-650	2.9(+13)	0	2920	0.7 1.3
CH ₃ (CH ₂) ₄ CH ₃ + Cl → CH ₃ CH(•)(CH ₂ CH ₂ CH ₂ CH ₃						
+ CH ₃ CH ₂ CH(•)(CH ₂ CH ₂ CH ₃ + ClH						
HEXANE + OXYGEN ATOM						
73 HBR/HUI	REACTION ORDER: 2.	298-650	1.1(+14)	0	2250	0.7 1.3

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
350-800	4.8(+11)	0	5800±250	0.7 1.3
CH₃(CH₂)₄CH₃ + CH₃° → CH₃(CH₂)₄CH₂° + CH₄ HEXANE + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE.				
350-800	7.9(+11)	0	4830±250	0.7 1.3
1000-1200	3.2(+16)	0	39250	
1000-1200	1.0(+17)	0	41800	
298-650	5.9(+13)	0	2920	0.7 1.3
298-650	3.1(+13)	0	1650	0.7 1.3
350-750	9.5(+11)	0	5800±250	0.7 1.3
350-750	1.9(+11)	0	3975±250	0.7 1.3
300-500	5.0(+10)	0	3445	
439-566	4.7(+11)	0	4525	
416-467	5.4(+11)	0	14745	
CH₃(CH₂)₄CH₃ + CH₃° → CH₃(CH₂)₄CH₂° + CH₄ HEXANE + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE.				
CH₃(CH₂)₄CH₃ + CH₃° → CH₃CH₂CH(°)CH₂CH₂CH₃ + CH₃CH₂CH₂CH(°)CH₃ + CH₄ HEXANE + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE.				
(CH₃)₂CHCH(CH₃)₂ → (CH₃)₂CH° + (CH₃)₂CH° BUTANE, 2,3-DIMETHYL- 70 BEN/6°N REACTION ORDER: 1.				
(CH₃)₂CHCH(CH₃)₂ → (CH₃)₂CH(°)CH(CH₃)₂ + CH₃° BUTANE, 2,3-DIMETHYL- 70 BEN/6°N REACTION ORDER: 1.				
(CH₃)₂CHCH(CH₃)₂ + ° → °CH₂CH(CH₃)CH(CH₃)₂ + °H BUTANE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2.				
(CH₃)₂CHCH(CH₃)₂ + ° → (CH₃)₂C(°)CH(CH₃)₂ + °H BUTANE, 2,3-DIMETHYL-, + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2.				
(CH₃)₂CHCH(CH₃)₂ + CH₃° → °CH₂CH(CH₃)CH(CH₃)₂ + CH₄ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE.				
(CH₃)₂CHCH(CH₃)₂ + CH₃° → (CH₃)₂C(°)CH(CH₃)₂ + CH₄ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE.				
(CH₃)₂CHCH(CH₃)₂ + CH₃° → (CH₃)₂CHC(°)(CH₃)₂ + °CH₂CH(CH₃)CH(CH₃)₂ + CH₄ BUTANE, 2,3-DIMETHYL-, + METHYL FREE RADICAL 72 KEN REACTION ORDER: 2.				
(CH₃)₂CHCH(CH₃)₂ + CD₃° → (CH₃)₂C(°)CH(CH₃)₂ + °CH₂CH(CH₃)CH(CH₃)₂ + CD₃H BUTANE, 2,3-DIMETHYL-, + METHYL-d₃ FREE RADICAL 72 KEN REACTION ORDER: 2.				
CH₂=C(CH₃)CHCH=CH₂ → CH₃-C(°)CH₂CH=CH₂ 1-PROPENE, 3-(1-METHYLETHENYL)XY- 70 BEN/6°N REACTION ORDER: 1.				
CH₂=C(CH₃)CH₂CH=CH₂ → CH₂=C(CH₃)CH₂CH₂CH₂°				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
423-461	1.4(+11)	0	14645	
423-461	2.1(+11)	0	14025	
511-548	1.4(+11)	0	18400	
352-453	2.5(+11)	0	3875	
493-541	1.9(+10)	0	16560	
373-464	2.5(+14)	0	15100	
607-643	1.4(+12)	0	20500	
590-650	1.4(+11)	0	21330	
303-435	2.5(+10)	0	3070	
725-810	1.6(+12)	0	23150	
576-710	2.0(+13)	0	23450	
725-810	7.9(+11)	0	23800	

1-PROPENE, 2-METHYL-3(ETHENYLOXY)-
70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{OCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$
 1-PROPENE, 3-METHYL-3(ETHENYLOXY)-
70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_2=\text{CHC}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$
 3-BUTENOIC ACID, 2,2-DIMETHYL-
70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow$
 $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$
 PROPANE ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL
 72 KBR/PAR REACTION ORDER: 2.

 $(\text{CH}_3\text{COO})_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{COOCH}_3 + \text{CH}_3\text{CO}$
 1,1-ETHANEDICL, DIACETATE
 70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCC}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{O} + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{O}$
 PEROXIDE, BIS(1-CYCLOPENTYL)-
70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_2=\text{CHCH}_2\text{C}(\text{O})(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CO}$
 4-PENTEN-2-OL, 2-METHYL-
70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_2=\text{CHC}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_3$
 BUTANE, 1-(ETHENYLOXY)-
70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_2=\text{CHC}(\text{CH}_2)_3\text{CH}_3 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{C}(\text{CH}_3)_3$
 BUTANE, 1-(ETHENYLOXY)-
70 BEN/°N REACTION ORDER: 2.

 $\text{CH}_3\text{COO}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{COOH}$
 ACETIC ACID BUTYL ESTER
 72 KBR/PAR REACTION ORDER: 1.

 $\text{CH}_3\text{COOCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$
 + $\text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$
 ACETIC ACID 1-METHYLPEROXYL ESTER
 70 BEN/°N REACTION ORDER: 1.
 NOTE: 57% 1-BUTENE: *trans*/*cis*-2-BUTENE = 0.64.

 $\text{CH}_3\text{COOCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{COOH}$
 ACETIC ACID 2-METHYLPEROXYL ESTER
 70 BEN/°N REACTION ORDER: 1.

 $\text{CH}_3\text{COOCC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{COOH}$
 ACETIC ACID 1,1-DIMETHYLPEROXYL ESTER

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f F
514-564	1.4(+13)	0	20130	
495-528	4.3(+11)	0	16255	
650-710	1.1(+13)	0	23450	
725-810	1.2(+12)	0	24100	
696-760	4.2(+14)	0	31960	
400-600	2.1(+11)	0	4100±500	0.5 2.0
420-428	4.0(+15)	0	18700	
300-450	2.3(+11)	0	4100±500	0.5 1.5
350-500	8.9(+10)	0	3925±500	0.5 1.5
523-563	2.5(+16)	0	23900	
350-500	2.0(+11)	0	3370±750	

70 HEN/O'N
REACTION ORDER: 1.

(CH₃)₂C(OH)CH₂COCH₃ → (CH₃)₂CO + (CH₃)₂CO
2-PENTANONE, 4-HYDROXY-4-METHYL-
70 HEN/O'N
REACTION ORDER: 1.

CH₃COCH(CH₃)CH₂COCH₃ → CH₃COCH + CH₂=CHCH₂COCH₃
+ cis- and trans-CH₃CH=CHCOCH₃
2-PROPANOL, 1-METHOXY-, ACETATE
70 HEN/O'N
REACTION ORDER: 1.

NOTE: 58% PROPENE, 3-METHOXY-

CH₃COCH₂CH₂COCH₂CH₃ → CH₂=CHCOCH₂CH₃ + CH₃COCH
ETHANOL, 2-ETHOXY-, ACETATE
70 HEN/O'N
REACTION ORDER: 1.

(CH₃)₂CHCOCH(CH₃)₂ → CH₃CH=CH₂ + (CH₃)₂CHOH
PROPANE, 2,2'-OXYBIS-
70 HEN/O'N
REACTION ORDER: 1.

NOTE: SUSPECT RATE CONSTANT.

(CH₃)₂CHCOCH(CH₃)₂ + CH₃• → (CH₃)₂C(•)COCH(CH₃)₂
+ CH₂CH(CH₃)COCH(CH₃)₂ + CH₄
PROPANE, 2,2'-OXYBIS- + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

CH₃CH₂CH₂COCH₂CH₂CH₃ → CH₃CH₂CH₂CO• + CH₃CH₂CH₂COCH₂CH₂CH₃
PEROXIDE, DIPEPYL
70 HEN/O'N
REACTION ORDER: 1.

(CH₃)₂CHCOCH(CH₃)₂ + CH₃• → (CH₃)₂C(•)COCH(CH₃)₂
+ CH₂CH(CH₃)COCH(CH₃)₂ + CH₄
PEROXIDE, BIS(1-METHYLETHYL)-, + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

CH₃CH=NC(CH₃)₃ + CH₃• → CH₃C(•)=NC(CH₃)₃
+ CH₂CH=NC(CH₃)₃ + CH₃CH=NC(CH₃)₂CH₂• + CH₄
2-PROPANIMINE, N-ETHYLIDENE-2-METHYL-,
+ METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

(CH₃)₂CHN=NC(CH₃)₂ → (CH₃)₂CHN=• + (CH₃)₂CH.
DIAZENE, BIS(1-METHYLETHYL)-
70 HEN/O'N
REACTION ORDER: 1.

(CH₃)₂CHNCH(CH₃)₂ + CH₃• → (CH₃)₂CHN(•)CH(CH₃)₂
+ (CH₃)₂C(•)NCH(CH₃)₂ + CH₂CH(CH₃)NCH(CH₃)₂ + CH₄
2-PROPANAMINE, N-(1-METHYLETHYL)-, + METHYL FREE RADICAL
76 KEE/PAR
REACTION ORDER: 2.

NOTE: TENTATIVE K VALUE.

(CH₃CH₂)₃N + CH₃• → CH₃CH(•)N(CH₂CH₃)₂
+ CH₂CH₂CH₂N(CH₂CH₃)₂ + CH₄

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f
350-600	5.0(±11)	0	4000±500	0 2.0
ETHANAMINE, N,N-DIETHYL-, + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
445-491	9.3(±9)	0	14330	
$\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CH}(\cdot)\text{CH}_2\text{CH}=\text{CH}_2$ 1,2,6-HEPTADIENE 70 HEN/6'N REACTION ORDER: 1.				
451-523	3.9(±11)	0	4430	
$\text{CH}_3(\text{CH}_2)_4\text{CCH} + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{C}(\cdot)\text{CHCH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH}_2$ 1-HEPTYNE + ETHYL FREE RADICAL 72 KEE/PAR REACTION ORDER: 2.				
451-523	1.3(±11)	0	16355	
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_2\text{CH}=\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ 1,5-HEPTADIENE 70 HEN/6'N REACTION ORDER: 1.				
451-523	7.1(±10)	0	17590	
$\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$ 1,5-HEXADIENE, 3-METHYL- 70 HEN/6'N REACTION ORDER: 1.				
304	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CCl}\cdot \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CCl}$ 2,3-PHNTADIENE, 2,4-DIMETHYL-, + CARBON OXIDE(C ₂ O) 70 HEN/6'N REACTION ORDER: 2. k/k_{ref} : 113. NOTE: k_{ref} : $\text{CH}_2=\text{CH}_2 + \text{CCl}\cdot$				
355-439	6.2(±10)	0	3500	
$\text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ 1-HEPTENE + ETHYL FREE RADICAL 72 KEE/PAR REACTION ORDER: 2.				
298	1.6(±12)	-	-	
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 + \text{H}\cdot \rightarrow (\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2\cdot$ $+ (\text{CH}_3)_3\text{CC}(\cdot)(\text{CH}_3)_2$ 1-BUTENE, 2,3,3-TRIMETHYL-, + HYDROGEN ATOM 72 KEE/PAR REACTION ORDER: 2.				
322-364	7.8(±9)	0	2800	
NOTE: TENTATIVE k VALUE BASED ON REACTION $(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}\cdot$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2\cdot \rightarrow$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ 1-BUTENE, 2,3,3-TRIMETHYL-, + ETHYL FREE RADICAL 72 KEE/PAR REACTION ORDER: 2.				
298-650	2.9(±13)	0	2920	0.7 1.3
$\text{CH}_3(\text{CH}_2)_5\text{CH}_3 + \text{O}\cdot \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2\cdot + \text{OH}$ HEPTANE + OXYGEN ATOM 73 HEN/HUI REACTION ORDER: 2.				
298-650	1.2(±14)	0	2190	0.7 1.3
$\text{CH}_3(\text{CH}_2)_5\text{CH}_3 + \text{O}\cdot \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ $+ \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3 + \text{OH}$ HEPTANE + OXYGEN ATOM 73 HEN/HUI REACTION ORDER: 2.				

CHEMICAL REACTIONS

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f
$(CH_3)_3C(CH_2)_2CH_3 + \delta \rightarrow$ products PENTANE, 2,2-DIMETHYL-, + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2. -----	307	6.5(+10)	-	-	0.7 1.4
$(CH_3)_2CHCH_2CH(CH_3)_2 + e \rightarrow$ products PENTANE, 2,4-DIMETHYL-, + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2. -----	307	1.0(+11)	-	-	0.7 1.4
$(CH_3CH_2)_3CH + CH_3 \rightarrow (CH_3CH_2)_3C + CH_4$ PENTANE, 3-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$(CH_3CH_2)_3CH + CH_3 \rightarrow (CH_3CH_2)_2CHCH_2CH_3 + CH_4$ PENTANE, 3-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	6.0(+11)	0	4830±250	0.7 1.3
$(CH_3CH_2)_3CH + CH_3 \rightarrow (CH_3CH_2)_2CHCH_2CH_2 + CH_4$ PENTANE, 3-ETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
$(CH_3)_3CCH(CH_3)_2 \rightarrow (CH_3)_3C + (CH_3)_2CH$ BUTANE, 2,2,3-TRIMETHYL- 70 BEN/6'N REACTION ORDER: 1. -----	1065-1197	1.1(+16)	0	36335	
$CH_2=C(CH_3)C(CH_3)_2C_6H_5 \rightarrow (CH_3)_2C=C(CH_3)_2 + C_6H_5$ 3-BUTENOIC ACID 2,2,3-TRIMETHYL- 70 BEN/6'N REACTION ORDER: 1. -----	447-488	7.1(+10)	0	16560	
$trans-CH_3CH=CHC(CH_3)_2C_6H_5 \rightarrow CH_3CH_2CH=C(CH_3)_2 + C_6H_5$ trans-3-PENTENOIC ACID, 2,2-DIMETHYL- 70 BEN/6'N REACTION ORDER: 1. -----	526-564	5.5(+11)	0	20300	
$CH_3C_6H_4CH(CH_3)CH_2CH=CH_2 \rightarrow CH_3C_6H_5 + CH_2=CHCH_2CH=CH_2$ + cis-, and trans $CH_3CH=CHCH=CH_2$ ACETIC ACID 1-METHYL-3-BUTENYL ESTER 70 BEN/6'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	
$CH_3C_6H_4CH(CH_3)CH_2C_6H_5 \rightarrow CH_3CH=CHC_6H_5 + CH_3C_6H_5$ 2-2-PENTADIENE, 4-ACETYLXY- 70 BEN/6'N REACTION ORDER: 1. -----	525-570	7.9(+11)	0	18800	
$(CH_3CH_2C_6H_5)_2CH_2 \rightarrow (CH_3CH_2C_6H_5)_2 + HCH_3$ METHANEDIOL, DIPREFANGATE 70 BEN/6'N REACTION ORDER: 1. -----	493-578	5.0(+10)	0	18300	
$CH_3C_6H_4(CH_2)_4CH_3 \rightarrow CH_3CH_2CH_2CH=CH_2 + CH_3C_6H_5$ ACETIC ACID PENTYL ESTER 70 BEN/6'N REACTION ORDER: 1.	725-810	1.6(+12)	0	23350	

CHEMICAL REACTIONS

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f F
1-PENTENE, 2,4,4-TRIMETHYL-, + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. ----- $\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \theta \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot + \theta\text{H}$ OCTANE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----	309-364	1.9(+10)	0	2870	
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \theta \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ + θH OCTANE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----	298-650	2.9(+13)	0	2920	0.7 1.3
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot + \text{CH}_4$ OCTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	298-650	9.3(+13)	0	2030	0.7 1.3
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 + \text{CH}_3\cdot \rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ + $\text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3$ + CH_4 OCTANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-800	4.8(+11)	0	5800±250	0.7 1.3
$(\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 + \theta \rightarrow \text{products}$ PENTANE, 2,2,4-TRIMETHYL-, + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----	307	5.5(+10)	-	-	0.6 1.5
$(\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCCH}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	2.0(+11)	0	4830±250	0.7 1.3
$(\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCCH}_2\text{C}(\cdot)(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	9.5(+10)	0	3975±250	0.7 1.3
$(\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_3\text{CCCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\cdot$ + $\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_4$ PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE & VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \theta \rightarrow \text{products}$ PENTANE, 2,3,4-TRIMETHYL-, + OXYGEN ATOM 73 KER/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 & VALUE.	350-750	1.2(+12)	0	5800±250	0.7 1.3

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
$(CH_3)_2CHCH(CH_3)CH(CH_3)_2 + CH_3^{\bullet} \rightarrow (CH_3)_2CHC(\bullet)(CH_3)CH(CH_3)_2 + CH_4$ PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL 76 KEE/PAR NOTE: TENTATIVE & VALUE.	2.9(+11)	0	3975±250	0.7 1.3
$(CH_3)_2CHCH(CH_3)CH(CH_3)_2 + CH_3^{\bullet} \rightarrow [C_6H_{17}^{\bullet}] + CH_4$ PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL 72 KGN REACTION ORDER: 2.	4.7(+11)	0	4575	
$(CH_3)_3CC(CH_3)_3 \rightarrow (CH_3)_3C^{\bullet} + (CH_3)_3C^{\bullet}$ BUTANE, 2,2,3,3-TETRAMETHYL- 70 BEN/G'N REACTION ORDER: 1.	5.0(+16)	0	33800	
$(CH_3)_3CC(CH_3)_3 + \bullet \rightarrow$ Products BUTANE, 2,2,3,3-TETRAMETHYL- 73 BEN/HUI REACTION ORDER: 2.	8.0(+9)	-	-	0.6 1.5
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow \bullet CH_2C(CH_3)_2CC(CH_3)_2 + CH_4$ BUTANE, 2,2,3,3-TETRAMETHYL-, + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2.	1.4(+12)	0	5800±250	0.7 1.3
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow (CH_3)_3CC(CH_3)_2 + CH_3CH_2CH_2CH_3$ 2-BUTENE-1,1-DICL, DIACETATE 70 BEN/G'N REACTION ORDER: 1.	1.3(+11)	0	16600	
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow (CH_3)_3CC(CH_3)_2 + CH_3CH_2CH_2CH_3$ 1,1-BUTANEDICL, DIACETATE 70 BEN/G'N REACTION ORDER: 1.	3.0(+10)	0	16560	
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow (CH_3)_3CC(CH_3)_2 + CH_3CH_2CH_2CH_3$ 1,1-ETHANEDICL, DIPROFANATE 70 BEN/G'N REACTION ORDER: 1.	2.5(+10)	0	16560	
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow (CH_3)_3CC(CH_3)_2 + CH_3CH_2CH_2CH_3$ 1,1-ETHANEDICL, DIPROFANATE 70 BEN/G'N REACTION ORDER: 1.	2.0(+14)	0	14900	
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow (CH_3)_3CC(CH_3)_2 + CH_3CH_2CH_2CH_3$ 1,1-ETHANEDICL, DIPROFANATE 70 BEN/G'N REACTION ORDER: 1.	1.4(+13)	0	19400	
$(CH_3)_3CC(CH_3)_3 + CH_3^{\bullet} \rightarrow (CH_3)_3CC(CH_3)_2 + CH_3CH_2CH_2CH_3$ 1,1-ETHANEDICL, DIPROFANATE 70 BEN/G'N REACTION ORDER: 1.	7.9(+11)	0	23050	

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	F
650-710	4.0(±12)	0	21740		
* cis-, and trans-$\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,2-DIMETHYLBUTYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 76% 1-PENTENE, 3-METHYL-.					
560-610	1.5(±13)	0	19525		
$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ + $(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_3 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,1-DIMETHYLBUTYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 72% 1-PENTENE, 2-METHYL-.					
560-610	1.3(±13)	0	19075		
$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$ + $\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\text{COOH}$ ACETIC ACID 1,1,2-TRIMETHYLBUTYL ESTER 70 BEN/0'N REACTION ORDER: 1. NOTE: 90% 1-BUTENE, 2,3-DIMETHYL-.					
403-443	4.0(±15)	0	18800		
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{CH}_2 + (\text{CH}_3)_3\text{CO}$ PEROXIDE, BIS(1,1-DIMETHYLETHYL) 70 BEN/0'N REACTION ORDER: 1. NOTE: 90% 1-BUTENE, 2,3-DIMETHYL-.					
350-500	1.8(±12)	0	5900±150	0.3	3
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 + \text{CH}_3 \rightarrow \text{CH}_2\text{C}(\text{CH}_3)_2\text{COOC}(\text{CH}_3)_3 + \text{CH}_4$ PEROXIDE, BIS(1,1-DIMETHYLETHYL)-, METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2.					
472-673	3.2(±16)	0	25165		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{N}$ + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ DIAZENE, DIBUTYL- 70 BEN/0'N REACTION ORDER: 1.					
535-618	4.0(±16)	0	23500		
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{NCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{N}$ + $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)$ DIAZENE, BIS(1-METHYLPROPYL)- 70 BEN/0'N REACTION ORDER: 1.					
473-673	1.7(±16)	0	24660		
$(\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{NCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{N}$ + $(\text{CH}_3)_2\text{CHCH}_2$ DIAZENE, BIS(2-METHYLPROPYL)- 70 BEN/0'N REACTION ORDER: 1.					
473-673	1.4(±17)	0	21900		
$(\text{CH}_3)_3\text{CN}=\text{NC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{CN}=\text{N} + (\text{CH}_3)_3\text{C}$ DIAZENE, BIS(1,1-DIMETHYLETHYL)- 70 BEN/0'N REACTION ORDER: 1.					
471-508	2.5(±14)	0	17365		
$(\text{CH}_3\text{CH}_2)_2\text{NN}=\text{NN}(\text{CH}_2\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{NN}=\text{N} + (\text{CH}_3\text{CH}_2)_2\text{N}$ 2-TETRAZENE, 1,1,4,4-TETRAETHYL- 70 BEN/0'N REACTION ORDER: 1.					
374-402	2.5(±14)	0	12900		
$(\text{CH}_3)_2\text{CHCH}_2\text{N}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{N}$ + $(\text{CH}_3)_2\text{CHCH}_2$ PROPANE, 1-NITROSC-2-METHYL-, DIMERIC 70 BEN/0'N REACTION ORDER: 1.					

CHEMICAL REACTIONS

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

APPENDIX: CONVERSION TABLES
EQUIVALENT SECOND ORDER RATE CONSTANTS

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

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

Table adapted from Evaluated Kinetic Data for High Temperature Reactions, Volume 1: Homogeneous Gas Phase Reactions of the $\text{H}_2\text{-O}_2$ System, Butterworths, London, 1972.

EQUIVALENT THIRD ORDER RATE CONSTANTS

A \ B	$6 \text{ cm}^3 \text{ mol}^{-2} \text{ s}^{-1}$	$6 \text{ dm}^3 \text{ mol}^{-2} \text{ s}^{-1}$	$6 \text{ mol}^{-2} \text{ s}^{-1}$	$6 \text{ cm}^3 \text{ molecule}^{-2} \text{ s}^{-1}$	$(\text{mm Hg})^{-2} \text{ s}^{-1}$	$\text{atm}^{-2} \text{ s}^{-1}$	$\text{ppm}^{-2} \text{ min}^{-1}$	$4 \text{ kN}^{-2} \text{ s}^{-1}$
$1 \text{ cm}^3 \text{ mol}^{-2} \text{ s}^{-1} =$	1	10^{-6}	10^{-12}	2.76×10^{-48}	$2.57 \times 10^{-10} \text{ T}^{-2}$	$1.48 \times 10^{-4} \text{ T}^{-2}$	1.003×10^{-19}	$1.447 \times 10^{-8} \text{ T}^{-2}$
$1 \text{ dm}^3 \text{ mol}^{-2} \text{ s}^{-1} =$	10^6	1	10^{-6}	2.76×10^{-42}	$2.57 \times 10^{-4} \text{ T}^{-2}$	148 T^{-2}	1.003×10^{-13}	$1.447 \times 10^{-2} \text{ T}^{-2}$
$1 \text{ m}^3 \text{ mol}^{-2} \text{ s}^{-1} =$	10^{12}	10^6	1	2.76×10^{-36}	257 T^{-2}	$1.48 \times 10^8 \text{ T}^{-2}$	1.003×10^{-7}	$1.447 \times 10^4 \text{ T}^{-2}$
$1 \text{ cm}^3 \text{ molecule}^{-2} \text{ s}^{-1} =$	3.628×10^{47}	3.628×10^{41}	3.628×10^{35}	1	$9.328 \times 10^{37} \text{ T}^{-2}$	$5.388 \times 10^{43} \text{ T}^{-2}$	3.64×10^{28}	$5.248 \times 10^{39} \text{ T}^{-2}$
$1 (\text{mm Hg})^{-2} \text{ s}^{-1} =$	$3.89 \times 10^9 \text{ T}^2$	$3.89 \times 10^3 \text{ T}^2$	$3.89 \times 10^{-3} \text{ T}^2$	$1.07 \times 10^{-38} \text{ T}^2$	1	5.776×10^5	3.46×10^{-5}	56.25
$1 \text{ atm}^{-2} \text{ s}^{-1} =$	$6.733 \times 10^{32} \text{ T}^2$	$6.733 \times 10^{-3} \text{ T}^2$	$6.733 \times 10^{-9} \text{ T}^2$	$1.86 \times 10^{-44} \text{ T}^2$	1.73×10^{-6}	1	6×10^{-11}	9.74×10^{-5}
$1 \text{ ppm}^{-2} \text{ min}^{-1} =$ at 298K, 1 atm. total pressure	9.97×10^{18}	9.97×10^{12}	9.97×10^6	2.75×10^{-29}	2.89×10^4	1.667×10^{10}	1	1.623×10^6
$1 \text{ m}^3 \text{ kN}^{-2} \text{ s}^{-1} =$	$6.91 \times 10^{72} \text{ T}^2$	69.1 T^2	$6.91 \times 10^{-5} \text{ T}^2$	$1.904 \times 10^{-40} \text{ T}^2$	0.0178	1.027×10^4	6.16×10^{-7}	1

See note to Table for Second Order Rate Constants

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