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

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Washington, D.C. 20234

November 1979

Prepared for  
**Department of Energy**  
**Washington, D.C. 20545**

and

**Office of Standard Reference Data**  
**National Bureau of Standards**  
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**U.S. DEPARTMENT OF COMMERCE**

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**NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director***



Table of Recommended Rate Constants for Chemical  
Reactions Occurring in Combustion

by

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National Measurement Laboratory  
National Bureau of Standards  
Washington, DC 20234

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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	<u>1008</u>

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

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

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

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

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

#### Uncertainty expressed by factors.

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  $k_0$  is the central value of a rate constant, the statement that  $k_0$  is uncertain to a factor of  $F$  means that the uncertainty limits are defined by the relationship:

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

which shows that division and multiplication of the central value  $k_0$  by  $F$  gives respectively the lower and upper reliability limits of the rate

constant. By comparing relationships (1) and (2), it is obvious that in the case of an uncertainty expressed by a unique F the upper factor is equal to the unique factor itself, while the lower factor f is the reciprocal of F:

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

Uncertainty expressed by algebraic addends.

There are three types of uncertainty limits for rate constants expressed as algebraic addends, which are currently used by kineticists: a). Uncertainty appended to one of the Arrhenius factors (A, B, or E/R); b). Uncertainty appended to  $\log_{10} k_0$ ; and c). Uncertainty expressed as a percentage of  $k_0$ . With respect to the type a) uncertainties, the B factor uncertainties have been eliminated as being unimportant, while the uncertainties for the E/R factor may be omitted because they are of secondary importance and are included in the k factors. Therefore, the only uncertainty of type a) considered below is the one appended to the coefficient of the A factor.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

then relationship (10) becomes:

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

which can take the form:

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

or

$$k_0 / F < k < F k_0 \quad (13)$$

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

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

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

Formulas (14) and (15) are the relationships needed to transform the type b uncertainties into reliability limits expressed by k factors. A numerical example follows:

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

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:

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

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

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

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

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

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

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:  $fk_o < k < Fk_o$ .

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 reactions .....s<sup>-1</sup>
- 2 for second order reactions .....cm<sup>3</sup>mol<sup>-1</sup>s<sup>-1</sup>
- 3 for third order reactions .....cm<sup>6</sup>mol<sup>-2</sup>s<sup>-1</sup>

Following the reaction order, -on the same line-, the presence of an inert reaction partner ("third body") is indicated by the letter M: followed by its chemical formula. E.g.: M:Ar or M:CO<sub>2</sub>. No indication is given if M is undefined, or if the reaction does not include M. In all, there are 112 reactions with M specified.

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

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

E.g.:  $k/k_{\text{ref}}$ : 0.59.

The last line of column 1, placed under the line including the short reference and reaction order information, begins with the heading NOTE:. It is given only when necessary and might include information about the dependence of  $k$  factors on temperature range, or the reaction taken as reference when the ratio  $k/k_{\text{ref}}$  is given in the previous line, or other information pertinent to the reaction indicated above. The rate constant,  $k_{\text{ref}}$ , for the reference reaction indicated in the note (by the same author) can be found in the table in the proper place. For a certain number of reactions taken from Baulch, et al. (1972, 1973, and 1976) the relationship  $k_1 = K k_{-1}$  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  $\text{cal mol}^{-1}$  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

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\*) . 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, O<sub>2</sub>, O<sub>3</sub>.
- 2). H-O system: H, H<sub>2</sub>, OH, HO<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>O<sub>2</sub>.
- 3). S-O-H system: S, S<sub>2</sub>, SO, SO<sub>2</sub>, SO<sub>3</sub>, SH, SH<sub>2</sub>, SOH.
- 4). N-O-H-S system: N, N<sub>2</sub>, NO, NO<sub>2</sub>, NO<sub>3</sub>, N<sub>2</sub>O, N<sub>2</sub>O<sub>4</sub>, N<sub>2</sub>O<sub>5</sub>, NH, NH<sub>2</sub>,  
NH<sub>3</sub>, N<sub>2</sub>H<sub>4</sub>, HN<sub>3</sub>, HNO, HNO<sub>3</sub>, NS.
- 5). C-O-H-S-N system: C<sub>1</sub> compounds: C, CO, CO<sub>2</sub>, CH, CH<sub>2</sub>, CH<sub>3</sub>, CH<sub>4</sub>, CHO, HCHO, CH<sub>3</sub>O., CH<sub>3</sub>OH, CH<sub>3</sub>OOH, CS, CS<sub>2</sub>, COS, CH<sub>3</sub>S, CH<sub>3</sub>SH, CN, C(NO<sub>2</sub>)<sub>4</sub>, CHN, CH<sub>3</sub>NH<sub>2</sub>, CH=N≡N, CH<sub>3</sub>NHNH<sub>2</sub>, CH<sub>3</sub>NO, CH<sub>3</sub>NO<sub>2</sub>, CH<sub>3</sub>NO<sub>3</sub>, CH<sub>3</sub>ONH<sub>2</sub>.  
C<sub>2</sub> compounds: C<sub>2</sub>, C<sub>2</sub>O, CH≡CH, CH<sub>2</sub>=CH<sub>2</sub>, CH<sub>3</sub>CH<sub>2</sub>., CH<sub>3</sub>CH<sub>3</sub>, CH<sub>2</sub>=C=O, etc.  
C<sub>3</sub> compounds, etc., up to C<sub>10</sub> compounds follow, being ordered according to the same pattern.

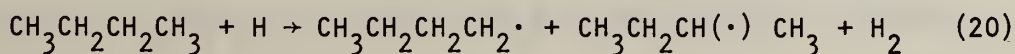
It is clear now that, for instance, the compounds included in the S-O-H system contain at least one sulfur atom, while the compounds containing only H, or O atoms, or both, are already listed in the previous two systems (O-system and H-O system). It is to be noted that for the C-O-H-S-N system the standard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

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

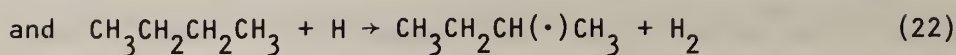
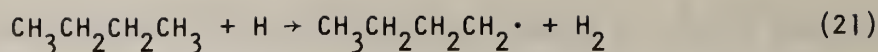


can be switched around, a number of bimolecular and termolecular reactions are inserted in the table in two - and respectively - three places. E.g.: Reaction  $\text{CH}_4 + \text{O} \rightarrow \text{CH}_3\cdot + \text{OH}$ , is inserted in the C-O-H-S-N system. This reaction may also be written as  $\text{O} + \text{CH}_4 \rightarrow \text{OH} + \text{CH}_3\cdot$  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  $\text{CH}_4$  as first reactant if he is interested in the reactions of methane, or listed with  $\text{O}$  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  $\text{M}$ . For this group of reactions,  $\text{M}$  will always be placed after all the other reactants, which means that the second order reactions with  $\text{M}$  as reactant will be inserted in the table only once, while the third order reactions with  $\text{M}$  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  $\text{O} + \text{NO} + \text{M} \rightarrow \text{NO}_2 + \text{M}$ .

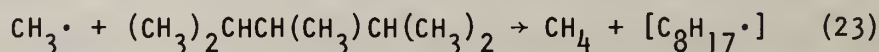
Most of the chemical reactions included in the table are balanced. A number of reactions are only apparently unbalanced. For instance, reaction



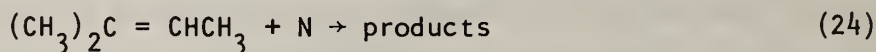
has a rate constant which in fact the sum of the rate constants for the two reactions



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:  $\text{CH}_4$ ,  $\text{CH}_3\text{CH}_3$ ,  $\text{CH}_3\text{CH}_2\text{CH}_3$ ,  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ ,  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ .

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,  $\text{CH}_2$ , are written without dot. Hydroperoxyl free radical is written  $\text{HO}_2\cdot$  (with dot).

## Sources of Recommended Rate Constants

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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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- Kondratiev, V. N., "Konstanty Skorosti Gazofaznykh Reaktsij Spravochnik," (Izdatelstvo "Nauka", Moskva, 1970); also issued as "Rate Constants of Gas Phase Reactions, Reference Book," R. M. Fristrom, Ed., Translated by L. J. Holtschlag COM-72-10014, Office of Standard Reference Data, NBS (1972) (Distributed by National Technical Information Service, Springfield, Virginia 22151).
- Lloyd, A. C., "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical," Int. J. Chem. Kinet. 6, 169-228 (1974).

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
150-4000	1.9(*13)	0	-900±175	0.8 1.2
190-400	1.0(*14)	0	-720	0.5 1.5
2000-10000	4.7(*23)	-2.5	0	0.4 2.5
AT 8000K				
1500-2500	6.3(*11)	0.5	0	0.8 1.2
200-500	2.2(*14)	-	-	0.8 1.3
1500-2500	1.5(*14)	-	-	0.8 1.2
1500-2500	2.1(*14)	-	-	0.8 1.2
200-500	5.2(*12)	0	2090±260	0.5 1.5
1500-2500	7.9(*15)	0	0	0.1 10.
400-2000	1.8(*10)	1.0	4480±150	0.7 1.3
416-968	2.0(*13)	0	5500	0.5 2.0
300	2.3(*13)	-	-	0.6 1.4
1500-2500	2.5(*13)	0	0	0.5 2.0
1500-2500	6.3(*11)	0.5	0	0.01 100.
1500-2500	1.0(*17)	0	0	0.01 100.

$O \cdot d \cdot M \rightarrow O_2 \cdot M$   
 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<sub>2</sub>  
 M: O<sub>2</sub>  
 NOTE: k<sub>1</sub> = k<sub>2</sub> - 1.0 k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 8000K.

$O \cdot d_2 \rightarrow O_2 \cdot d$   
 OXYGEN ATOM + OXYGEN MOLECULE  
 76 HEN/GGL  
 REACTION ORDER: 2.

$O \cdot d_2 \cdot M \rightarrow O_3 \cdot M$   
 OXYGEN ATOM + OXYGEN MOLECULE  
 76 HAU/DRY  
 REACTION ORDER: 3. M: O<sub>2</sub>  
 NOTE: M eff: O<sub>2</sub>(1.5)

NOTE: M eff: Ar(1.0)  
 NOTE: M eff: N<sub>2</sub>(1.4)

$O \cdot d_3 \rightarrow O_2 \cdot d_2$   
 OXYGEN ATOM + OZONE  
 76 HAU/DRY  
 REACTION ORDER: 2.  
 NOTE: k FACTORS CHANGING TO: f = 0.6; F = 3.0 AT 1000K

$O \cdot H \cdot M \rightarrow OH \cdot M$   
 OXYGEN + HYDROGEN ATOMS  
 76 ENG  
 REACTION ORDER: 3.

$O \cdot H_2 \rightarrow OH \cdot H$   
 OXYGEN ATOM + HYDROGEN MOLECULE  
 72 HAU/DRY  
 REACTION ORDER: 2.

$O \cdot D_2 \rightarrow OD \cdot D$   
 OXYGEN ATOM + DEUTERIUM MOLECULE  
 72 HAU/DRY  
 REACTION ORDER: 2.

$O \cdot OH \rightarrow O_2 \cdot H$   
 OXYGEN ATOM + HYDROXYL FREE RADICAL  
 72 HAU/DRY  
 76 ENG  
 REACTION ORDER: 2.

$O \cdot OH \rightarrow O_2 \cdot H$   
 OXYGEN ATOM + HYDROXYL FREE RADICAL  
 75 HEN/GGL  
 REACTION ORDER: 2.

$O \cdot OH \cdot M \rightarrow HO_2 \cdot M$   
 OXYGEN ATOM + HYDROXYL FREE RADICAL  
 76 ENG  
 REACTION ORDER: 3.

$O \cdot OH \rightarrow OH \cdot d$   
 OXYGEN ATOM + HYDROXYL FREE RADICAL

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
300-2000	6.3(+11)	0.5	4000	0.7 1.5
300-2000	6.8(+13)	0	9240±200	0.7 1.5
300-2000	6.3(+11)	0.5	0	0.7 1.5
2770	2.0(+11)	0.5	2770	0.7 1.3
298	6.3(+11)	0.5	0	0.7 1.3
298	6.7(+16)	-	-	0.7 1.3
440-2100	1.3(+14)	-0.5	5980	0.3 1.7
440-2100	6.3(+11)	0.5	0	0.3 1.7
200-400	6.3(+11)	0	4000	0.5 2.0
200-400	6.4(+16)	-0.5	0	0.5 2.0
2000-5000	7.6(+13)	0	38000±150	0.5 2.0
1300-2500	1.4(+13)	0	10400±1500	0.7 1.5
1000-3000	1.5(+9)	1.0	19500±150	0.7 1.3

75 BEN/GOL  
 REACTION ORDER: 2.  
 -----  
 O \* H<sub>2</sub>O → OH \* OH  
 OXYGEN ATOM \* WATER  
 72 BAU/DRY

O \* S<sub>2</sub> → SO \* S  
 OXYGEN ATOM \* SULFUR DIMER  
 75 BEN/GOL

O \* SO → O<sub>2</sub> \* S  
 OXYGEN ATOM \* SULFUR MONOXIDE  
 75 BEN/GOL

O \* SO → SO \* O  
 OXYGEN ATOM \* SULFUR MONOXIDE  
 75 BEN/GOL

O \* SO \* M → SO<sub>2</sub> \* M  
 OXYGEN ATOM \* SULFUR MONOXIDE  
 76 BAU/DRY

O \* SO<sub>2</sub> → O<sub>2</sub> \* SO  
 OXYGEN ATOM \* SULFUR DIOXIDE  
 76 BAU/DRY

NOTE: k<sub>1</sub> = k<sub>-1</sub>

O \* SH → H \* SO  
 OXYGEN ATOM \* MERCAPTO FREE RADICAL  
 75 BEN/GOL

O \* SH → OH \* S  
 OXYGEN ATOM \* MERCAPTO FREE RADICAL  
 75 BEN/GOL

O \* N \* M → NO \* M  
 OXYGEN ATOM \* NITROGEN ATOM  
 73 BAU/DRY

O \* N<sub>2</sub> → NO \* N  
 OXYGEN ATOM \* NITROGEN MOLECULE  
 73 BAU/DRY

NOTE: k<sub>1</sub> = k<sub>-1</sub>

O \* N<sub>2</sub> \* M → N<sub>2</sub>O \* M  
 OXYGEN ATOM \* NITROGEN MOLECULE  
 73 BAU/DRY

O \* NO → O<sub>2</sub> \* N  
 OXYGEN ATOM \* NITROGEN OXIDE(NO)  
 73 BAU/DRY

NOTE: k<sub>1</sub> = k<sub>-1</sub>; 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
<p> <math>\phi \cdot \text{NO} \rightarrow \text{NO} \cdot \phi</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>0</sub>)            75 BEN/GBL            REACTION ORDER: 2.         </p>			6.3(+11)	0.5	0	
<p> <math>\phi \cdot \text{NO} \cdot \text{M} \rightarrow \text{NO}_2 \cdot \text{M}</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>0</sub>)            73 BAU/DRY            REACTION ORDER: 3.            NOTE: M eff: O<sub>2</sub>(1.0) AT 297K         </p>		200-500	1.1(+15)	0	-940±50	0.8 1.2
<p>           Ar(0.1) AT 297K         </p>		200-500	1.1(+14)	0	-940±50	0.8 1.2
<p>           H<sub>2</sub>O(6.1) AT 297K         </p>		200-500	6.7(+15)	0	-940±15	0.8 1.2
<p>           D<sub>2</sub>O(5.0) AT 297K         </p>		200-500	5.5(+15)	0	-940±50	0.8 1.2
<p>           SF<sub>6</sub>(2.6) AT 297K         </p>		200-500	2.9(+15)	0	-940±50	0.8 1.2
<p>           N<sub>2</sub>(1.4) AT 297K         </p>		200-500	1.5(+15)	0	-940±50	0.8 1.2
<p>           N<sub>2</sub>O(2.1) AT 297K         </p>		200-500	2.3(+15)	0	-940±50	0.8 1.2
<p>           CO<sub>2</sub>(2.1) AT 297K         </p>		200-500	2.3(+15)	0	-940±50	0.8 1.2
<p>           CH<sub>4</sub>(2.2) AT 297K         </p>		200-500	2.4(+15)	0	-940±50	0.8 1.2
<p>           CF<sub>4</sub>(2.2) AT 297K         </p>		200-500	2.4(+15)	0	-940±50	0.8 1.2
<p> <math>\phi \cdot \text{NO}_2 \rightarrow \phi_2 \cdot \text{NO}</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>0</sub>2)            73 BAU/DRY            REACTION ORDER: 2.         </p>		300-550	1.0(+13)	0	300±100	0.8 1.3
<p> <math>\phi \cdot \text{NO}_2 \rightarrow \phi_2 \cdot \text{NO}</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>0</sub>2)            76 ENG            REACTION ORDER: 2.         </p>		1500-2500	1.0(+13)	0	500±250	0.5 2.0
<p> <math>\phi \cdot \text{NO}_2 \cdot \text{M} \rightarrow \text{NO}_3 \cdot \text{M}</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>0</sub>2)            73 BAU/DRY            NOTE: k<sub>0</sub> (LOW PRESSURE).            NOTE: LIMITING HIGH PRESSURE k<sub>∞</sub>.         </p>		295	2.3(+16)	-	-	0.4 2.5
<p> <math>\phi \cdot \text{N}_2\phi \rightarrow \phi_2 \cdot \text{N}_2</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>2</sub>φ)            73 BAU/DRY            REACTION ORDER: 2.         </p>		295	1.1(+13)	-	-	0.4 2.5
<p> <math>\phi \cdot \text{N}_2\phi \rightarrow \phi_2 \cdot \text{N}_2</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>2</sub>φ)            73 BAU/DRY            REACTION ORDER: 2.         </p>		1200-2000	1.0(+14)	0	1±100±2000	0.4 2.5
<p> <math>\phi \cdot \text{N}_2\phi \rightarrow \text{NO} \cdot \text{NO}</math>            OXYGEN ATOM + NITROGEN OXIDE(N<sub>2</sub>φ)            73 BAU/DRY            REACTION ORDER: 2.         </p>		1200-2000	1.0(+14)	0	1±100±1500	0.5 2.0
<p> <math>\phi \cdot \text{NH} \rightarrow \phi\phi \cdot \text{N}</math>            OXYGEN ATOM + IMIDGEN FREE RADICAL         </p>						



CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
75 BEN/G6L	REACTION ORDER: 2.		6.3(+11)	0.5	4000	
Ø * NH → NO * H	-----					
ØXYGEN ATOM * IMIDGGEN FREE RADICAL						
75 BEN/G6L	REACTION ORDER: 2.		6.3(+11)	0.5	0	
Ø * NH * M → HNO * M	-----					
ØXYGEN ATOM * IMIDGGEN FREE RADICAL		1500-2500	1.0(+16)	-0.5	0±2500	0.3 3.2
76 ENG	REACTION ORDER: 3.					
Ø * NH <sub>3</sub> → OH * NH <sub>2</sub>	-----					
ØXYGEN ATOM * AMMONIA		300-1000	1.5(+12)	0	3000±300	0.5 1.5
73 BAU/DRY	REACTION ORDER: 2.					
Ø * HNO → OH * NO	-----					
ØXYGEN ATOM * NITROSYL HYDRIDE		1500-2500	5.0(+11)	0.5	0±2500	0.3 3.2
76 ENG	REACTION ORDER: 2.					
Ø * HNO → O <sub>2</sub> * NH	-----					
ØXYGEN ATOM * NITROSYL HYDRIDE		1500-2500	1.0(+11)	0.5	3500±2500	0.3 3.2
76 ENG	REACTION ORDER: 2.					
Ø * HNO → NO <sub>2</sub> * H	-----					
ØXYGEN ATOM * NITROSYL HYDRIDE		1500-2500	5.0(+10)	0.5	0±2500	0.3 3.2
76 ENG	REACTION ORDER: 2.					
Ø * NS → SO * N	-----					
ØXYGEN ATOM * NITROGEN SULFIDE(NS)			6.3(+11)	0.5	4000	
75 BEN/G6L	REACTION ORDER: 2.					
Ø * NS → NO * S	-----					
ØXYGEN ATOM * NITROGEN SULFIDE(NS)			6.3(+11)	0.5	0	
75 BEN/G6L	REACTION ORDER: 2.					
Ø * C * M → CO * M	-----					
ØXYGEN ATOM * CARBON ATOM		7000-15000	3.3(+26)	-3.1	2114	0.3 1.8
76 BAU/DRY	REACTION ORDER: 3.					
NOTE: M = AT, BR CO k <sub>1</sub> = k <sub>k-1</sub>	-----					
Ø * CO → O <sub>2</sub> * C	-----					
ØXYGEN ATOM * CARBON MONOXIDE			1.0(+12)	0.5	69300	
75 BEN/G6L	REACTION ORDER: 2.					
Ø * CO → CO * Ø	-----					
ØXYGEN ATOM * CARBON MONOXIDE			6.3(+11)	0.5	0	
75 BEN/G6L	REACTION ORDER: 2.					
Ø * CO * M → CO <sub>2</sub> * M	-----					
ØXYGEN ATOM * CARBON MONOXIDE		250-500	2.4(+15)	0	2184±280	0.8 1.2
76 BAU/DRY	REACTION ORDER: 3.					
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.2 AT 500K.	-----					
Ø * CO <sub>2</sub> → O <sub>2</sub> * CO	-----					

## CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
OXYGEN ATOM + CARBON DIOXIDE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K. k <sub>1</sub> = k <sub>k-1</sub>	1500-3000	1.7(+13)	0	26500±2500	0.5 2.0
O + CH → OH + C OXYGEN ATOM + METHYLILYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	4000	
O + CH → C + H OXYGEN ATOM + METHYLILYNE FREE RADICAL 75 BEN/GOL REACTION ORDER: 2.		6.3(+11)	0.5	0	
O + CH + M → CHO + M OXYGEN ATOM + METHYLILYNE FREE RADICAL 76 ENG REACTION ORDER: 3.	1500-2500	1.0(+16)	-0.5	0±2500	0.3 3.2
O + :CH <sub>2</sub> → H + .CHO OXYGEN ATOM + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+11)	0.5	2000±2500	0.3 3.2
O + :CH <sub>2</sub> → OH + CH OXYGEN ATOM + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	2.0(+11)	0.7	13100±2500	0.3 3.2
O + CH <sub>3</sub> → H + HCHO OXYGEN ATOM + METHYL FREE RADICAL 76 ENG REACTION ORDER: 2.	1500-2500	5.0(+13)	0	0	0.5 2.0
O + CH <sub>4</sub> → CH + CH <sub>3</sub> OXYGEN ATOM + METHANE 73 BER/HUI 76 ENG REACTION ORDER: 2.	350-1000 1500-2500	2.1(+13) 2.0(+13)	0 0	4550 4530±500	0.7 1.3 0.6 1.6
O + .CHO → H + C <sub>6</sub> <sub>2</sub> OXYGEN ATOM + METHYL, CHO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	0	0±1500	
O + .CHO → OH + C OXYGEN ATOM + METHYL, CHO-, FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED.	1500-2500	3.2(+11)	1.0	250±1500	
O + HCHO → OH + .CHO OXYGEN ATOM + FORMALDEHYDE 76 ENG REACTION ORDER: 2.	1500-2500	1.0(+11)	1.0	1750±1000	0.5 1.2
O + HCHO → products OXYGEN ATOM + FORMALDEHYDE 73 BER/HUI REACTION ORDER: 2.	300	9.0(+10)	-	-	0.7 1.3
O + HCO → products OXYGEN ATOM + FORMALDEHYDE REACTION ORDER: 2.					

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
300	4.9(+10)	-	-	
1500-2500	1.0(+14)	0	0±1500	
300	1.6(+12)	0.5	28940	
300	1.3(+13) 6.3(+11)	- 0.5	- 0	0.5 1.5
302	2.2(+11)	-	-	0.5 1.5
200-1000	2.2(+13)	0	700±150	0.7 1.3
190-1200	1.6(+13)	0	2250±250	0.5 1.5
1500-2500	1.3(+12)	0.5	14545	
1500-2500	1.0(+12)	0	0±2500	0.3 3.2
200-700	6.3(+11)	0.5	0	
200-500	1.4(+13)	0	1500	0.8 1.2
200-650	3.3(+12)	0	565	0.8 1.2
298-650	2.5(+13)	0	3200	0.7 1.3

OXYGEN ATOM + FORMALDEHYDE-d  
73 BEN/HUI REACTION ORDER: 2.  
-----

O + CH<sub>3</sub>O → OH + ECHO

OXYGEN ATOM + METHOXY FREE RADICAL  
76 ENG REACTION ORDER: 2.  
-----

NOTE: k ESTIMATED

O + CS → C + SO

OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL  
75 BEN/GGL REACTION ORDER: 2.  
-----

O + CS → CO + S

OXYGEN ATOM + CARBON MONOSULFIDE FREE RADICAL  
76 BAU/DRY REACTION ORDER: 2.  
-----

75 BEN/GGL

O + CS<sub>2</sub> → S + COS

OXYGEN ATOM + CARBON DISULFIDE  
76 BAU/DRY REACTION ORDER: 2.  
-----

O + CS<sub>2</sub> → SO + CS

OXYGEN ATOM + CARBON DISULFIDE  
76 BAU/DRY REACTION ORDER: 2.  
-----

O + COS → SO + CO

OXYGEN ATOM + CARBON OXIDE SULFIDE  
76 BAU/DRY REACTION ORDER: 2.  
-----

NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 ABOVE 600K.

O + CN → C + NO

OXYGEN ATOM + CYANOGEN FREE RADICAL  
75 BEN/GGL REACTION ORDER: 2.  
-----

O + CN → CO + N

OXYGEN ATOM + CYANOGEN FREE RADICAL  
76 ENG REACTION ORDER: 2.  
-----

O + C<sub>2</sub> → CO + C

OXYGEN ATOM + CARBON DIMER  
75 BEN/GGL REACTION ORDER: 2.  
-----

O + CH=CH → Products

OXYGEN ATOM + ETHYLENE  
73 BEN/HUI REACTION ORDER: 2.  
-----

O + CH<sub>2</sub>=CH<sub>2</sub> → cy-CH<sub>2</sub>CH<sub>2</sub>O

OXYGEN ATOM + ETHENE  
73 BEN/HUI REACTION ORDER: 2.  
-----

O + CH<sub>3</sub>CH<sub>3</sub> → OE + CH<sub>2</sub>CH<sub>2</sub>O

OXYGEN ATOM + ETHANE  
73 BEN/HUI REACTION ORDER: 2.  
-----

## CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
<p>-----</p> <p>δ + CH<sub>2</sub>=C=O → products OXYGEN ATOM + ETHENE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	5.3(+11)	-	-	0.7 1.3
<p>δ + CH<sub>3</sub>CHO → products OXYGEN ATOM + ACETALDEHYDE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298-500	1.4(+13)	0	1140	0.5 2.0
<p>δ + cy-C<sub>2</sub>H<sub>2</sub>O → products OXYGEN ATOM + OXIRANE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	7.0(+8)	-	-	0.6 1.5
<p>δ + CH<sub>3</sub>CH<sub>2</sub>OH → products OXYGEN ATOM + ETHANOL 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	8.7(+10)	-	-	0.6 1.5
<p>δ + CH<sub>3</sub>COCH<sub>3</sub> → products OXYGEN ATOM + METHANE, OXYEIS- 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	200-500	5.9(+12)	0	1520	0.7 1.3
<p>δ + CH<sub>3</sub>C=CH → products OXYGEN ATOM + PROPENE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	4.0(+11)	-	-	0.5 2.0
<p>δ + CH<sub>3</sub>CH=CH<sub>2</sub> → cy-(CH<sub>3</sub>)COC<sub>2</sub>H<sub>5</sub> OXYGEN ATOM + 1-PROPENE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	200-500	2.5(+12)	0	38	0.8 1.2
<p>δ + CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub> → OH + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub> + (CH<sub>3</sub>)<sub>2</sub>CH. OXYGEN ATOM + PROPANE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	258	9.0(+9)	-	-	0.7 2
<p>δ + (CH<sub>3</sub>)<sub>2</sub>CHOH → products OXYGEN ATOM + 2-PROPANOL 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	1.3(+11)	-	-	0.6 1.5
<p>δ + (CH<sub>3</sub>)<sub>2</sub>C=CH<sub>2</sub> → cy-(CH<sub>3</sub>)<sub>2</sub>COC<sub>2</sub>H<sub>5</sub> OXYGEN ATOM + 1-PROPENE, 2-METHYL- 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	1.2(+13)	-	-	0.7 1.3
<p>δ + CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub> → products OXYGEN ATOM + 1,3-BUTADIENE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	300	9.0(+11)	-	-	0.7 1.4
<p>δ + CH<sub>2</sub>=C(CH<sub>3</sub>)CH<sub>2</sub> → products OXYGEN ATOM + 1,3-BUTADIENE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	258-400	3.4(+12)	0	-380	0.7 1.3
<p>δ + CH<sub>3</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → cy-(CH<sub>3</sub>CH<sub>2</sub>)COC<sub>2</sub>H<sub>5</sub> OXYGEN ATOM + 1-BUTENE 73 HRR/HUI</p> <p>REACTION ORDER: 2. -----</p>	298	2.3(+12)	-	-	0.8 1.2

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	F
250-500	5.9(±12)	0	-165	0.8	1.2
<p>6 • cis-CH<sub>3</sub>CF=CHCH<sub>3</sub> → products  OXYGEN ATOM • cis-2-BUTENE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298	1.4(±13)	-	-	0.7	1.3
<p>6 • trans-CH<sub>3</sub>CH=CHCH<sub>3</sub> → products  OXYGEN ATOM • trans-2-BUTENE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-650	3.0(±13)	0	2920	0.7	1.3
<p>6 • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> → 6H • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  OXYGEN ATOM • BUTANE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-650	4.3(±13)	0	2410	0.7	1.3
<p>6 • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> → 6H • CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  OXYGEN ATOM • BUTANE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298	2.8(±12)	-	-	0.7	1.3
<p>6 • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → cy-(CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>)CHCH<sub>2</sub>•  OXYGEN ATOM • 1-PENTENE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298	1.1(±13)	-	-	0.7	1.3
<p>6 • cis-CH<sub>3</sub>CH<sub>2</sub>CH=CHCH<sub>3</sub> → products  OXYGEN ATOM • cis-2-PENTENE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-400	3.9(±12)	0	-680	0.8	1.2
<p>6 • (CH<sub>3</sub>)<sub>2</sub>C=CHCH<sub>3</sub> → products  OXYGEN ATOM • 2-BUTENE, 2-METHYL-  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-650	2.9(±13)	0	2920	0.7	1.3
<p>6 • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> → 6H • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  OXYGEN ATOM • PENTANE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-650	8.0(±13)	0	2320	0.7	1.3
<p>6 • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> → 6H • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  • CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>3</sub>  OXYGEN ATOM • PENTANE  73 HRR/HUI  REACTION ORDER: 2.</p>					
307	8.0(±10)	-	-	0.7	1.4
<p>6 • (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> → 6H • (CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>  • (CH<sub>3</sub>)<sub>2</sub>CHCH(•)CH<sub>3</sub> • (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>2</sub>• • CH<sub>2</sub>CH(CH<sub>3</sub>)CH<sub>2</sub>CH<sub>3</sub>  OXYGEN ATOM • BUTANE, 2-METHYL-  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-650	5.9(±13)	0	2920	0.7	1.4
<p>6 • (CH<sub>3</sub>)<sub>3</sub>C → 6H • (CH<sub>3</sub>)<sub>3</sub>CCH<sub>2</sub>•  OXYGEN ATOM • PROPANE, 2,2-DIMETHYL-  73 HRR/HUI  REACTION ORDER: 2.</p>					
298	3.1(±12)	-	-	0.7	1.3
<p>6 • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → cy-(CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>)CHCH<sub>2</sub>•  OXYGEN ATOM • 1-HEXENE  73 HRR/HUI  REACTION ORDER: 2.</p>					
298-400	3.4(±12)	0	-790	0.8	1.2
<p>6 • (CH<sub>3</sub>)<sub>2</sub>C=C(CH<sub>3</sub>)<sub>2</sub> → products  OXYGEN ATOM • 2-BUTENE, 2,3-DIMETHYL-  73 HRR/HUI  REACTION ORDER: 2.</p>					

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
<p>-----  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_4\text{CH}_2\cdot</math>            OXYGEN ATOM + HEXANE            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	2.9(+13)	0	2920	0.7 1.3
<p>-----  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3</math>  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3</math>            OXYGEN ATOM + HEXANE            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	1.1(+14)	0	2250	0.8 1.3
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{6H} + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2</math>            OXYGEN ATOM + BUTANE, 2,3-DIMETHYL-            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	5.9(+13)	0	2920	0.7 1.3
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{6H} + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2</math>            OXYGEN ATOM + BUTANE, 2,3-DIMETHYL-            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	3.1(+13)	0	1650	0.7 1.3
<p>-----  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_5\text{CH}_2\cdot</math>            OXYGEN ATOM + HEPTANE            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	2.9(+13)	0	2920	0.7 1.3
<p>-----  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_3</math>  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_3</math>            OXYGEN ATOM + HEPTANE            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	1.2(+14)	0	2190	0.7 1.3
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_3\text{C}(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{products}</math>            OXYGEN ATOM + PENTANE, 2,2-DIMETHYL-            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	307	6.5(+10)	-	-	0.7 1.4
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}</math>            OXYGEN ATOM + PENTANE, 2,4-DIMETHYL-            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	307	1.0(+11)	-	-	0.7 1.4
<p>-----  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_6\text{CH}_2\cdot</math>            OXYGEN ATOM + OCTANE            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	2.9(+13)	0	2920	0.7 1.3
<p>-----  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_3</math>  <math>\phi \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{6H} + \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3</math>            OXYGEN ATOM + OCTANE            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	298-650	9.3(+13)	0	2030	0.7 1.3
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}</math>            OXYGEN ATOM + PENTANE, 2,2,4-TRIMETHYL-            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	307	5.5(+10)	-	-	0.6 1.5
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}</math>            OXYGEN ATOM + PENTANE, 2,3,4-TRIMETHYL-            73 HBR/HUI            REACTION ORDER: 2.            -----</p>	307	3.0(+10)	-	-	0.6 1.5
<p>-----  <math>\phi \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow \text{products}</math></p>	307	3.0(+10)	-	-	0.6 1.5

CHEMICAL REACTIONS	T/K	A	B	E/R (in OK)	k factors f
OXYGEN ATOM * BUTANE, 2,2,3,3-TETRAMETHYL- 73 HBR/HUI ----- O <sub>2</sub> * O - O * O <sub>2</sub> OXYGEN MOLECULE * OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----	307	8.0(+9)	-	-	0.6 1.5
O <sub>2</sub> * O * M - O <sub>3</sub> * M OXYGEN MOLECULE * OXYGEN ATOM 76 HAV/DRY REACTION ORDER: 3. M: O <sub>2</sub> M: Ar M: N <sub>2</sub> NOTE: M eff: O <sub>2</sub> (1.5) Ar(1.0) N <sub>2</sub> (1.4) -----	300	2.2(+14)	-	-	0.8 1.2
O <sub>2</sub> * H - O * OH OXYGEN MOLECULE * HYDROGEN ATOM 72 HAV/DRY REACTION ORDER: 2. -----	300	1.5(+14)	-	-	0.8 1.3
O <sub>2</sub> * D - O * OD OXYGEN MOLECULE * DEUTERIUM ATOM 72 HAV/DRY REACTION ORDER: 2. -----	300	2.1(+14)	-	-	0.8 1.2
O <sub>2</sub> * H * M - H <sub>2</sub> * M OXYGEN MOLECULE * HYDROGEN ATOM 72 HAV/DRY REACTION ORDER: 3. M: H <sub>2</sub> M: O <sub>2</sub> M: H <sub>2</sub> M: He M: Ar M: N <sub>2</sub> M: CO <sub>2</sub> NOTE: M eff: H <sub>2</sub> (1.0) O <sub>2</sub> (0.4) H <sub>2</sub> O(6.4) He(0.3). k <sub>1</sub> = k <sub>k-1</sub> Ar(0.3). k <sub>1</sub> = k <sub>k-1</sub> N <sub>2</sub> (0.4) CO <sub>2</sub> (1.5) -----	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 <sub>2</sub> * H * M - H <sub>2</sub> * M OXYGEN MOLECULE * HYDROGEN ATOM 72 HAV/DRY REACTION ORDER: 3. M: H <sub>2</sub> M: O <sub>2</sub> M: H <sub>2</sub> M: He M: Ar M: N <sub>2</sub> M: CO <sub>2</sub> NOTE: M eff: H <sub>2</sub> (1.0) O <sub>2</sub> (0.4) H <sub>2</sub> O(6.4) He(0.3). k <sub>1</sub> = k <sub>k-1</sub> Ar(0.3). k <sub>1</sub> = k <sub>k-1</sub> N <sub>2</sub> (0.4) CO <sub>2</sub> (1.5) -----	800-1000	8.9(+13)	-	7500	0.5 1.5
O <sub>2</sub> * H <sub>2</sub> - OH * OH OXYGEN MOLECULE * HYDROGEN MOLECULE 76 HNG REACTION ORDER: 2. -----	300-2000	1.5(+15)	0	-500*250	0.5 1.5
O <sub>2</sub> * H <sub>2</sub> - H <sub>2</sub> * H OXYGEN MOLECULE * HYDROGEN MOLECULE 72 HAV/DRY REACTION ORDER: 2. -----	300-2000	5.9(+14)	0	-500*250	0.5 1.5
O <sub>2</sub> * S - O * SO OXYGEN MOLECULE * SULFUR ATOM 76 HAV/DRY REACTION ORDER: 2. -----	300-2000	9.5(+15)	0	-500*250	0.5 1.5
O <sub>2</sub> * H <sub>2</sub> - OH * OH OXYGEN MOLECULE * HYDROGEN MOLECULE 76 HNG REACTION ORDER: 2. -----	300-2000	4.4(+14)	0	-500*250	0.5 1.5
O <sub>2</sub> * H <sub>2</sub> - H <sub>2</sub> * H OXYGEN MOLECULE * HYDROGEN MOLECULE 72 HAV/DRY REACTION ORDER: 2. -----	300-2000	4.4(+14)	0	-500*250	0.5 1.5
O <sub>2</sub> * S - O * SO OXYGEN MOLECULE * SULFUR ATOM 76 HAV/DRY REACTION ORDER: 2. -----	300-2000	5.9(+14)	0	-500*250	0.5 1.5
O <sub>2</sub> * H <sub>2</sub> - OH * OH OXYGEN MOLECULE * HYDROGEN MOLECULE 76 HNG REACTION ORDER: 2. -----	300-2000	2.2(+15)	0	-500*250	0.5 1.5
O <sub>2</sub> * H <sub>2</sub> - OH * OH OXYGEN MOLECULE * HYDROGEN MOLECULE 76 HNG REACTION ORDER: 2. -----	1500-2500	2.5(+12)	0	19630*5000	0.1 10.
O <sub>2</sub> * H <sub>2</sub> - H <sub>2</sub> * H OXYGEN MOLECULE * HYDROGEN MOLECULE 72 HAV/DRY REACTION ORDER: 2. -----	290-800	5.5(+13)	0	29100*350	0.4 2.5
O <sub>2</sub> * S - O * 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
$O_2 \cdot SO \rightarrow O \cdot SO_2$ 76 BAU/DRY	----- SULFUR MONOXIDE REACTION ORDER: 2. -----	440-2100	4.5(+11)	0	3250*590	0.3 1.7
$O_2 \cdot N \rightarrow O \cdot NO$ 73 BAU/DRY	----- NITROGEN ATOM 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
$O_2 \cdot N_2 \rightarrow O \cdot N_2O$ 73 BAU/DRY	----- NITROGEN MOLECULE REACTION ORDER: 2. NOTE: k <sub>1</sub> = k <sub>k-1</sub> -----	1200-2000	6.3(+13)	0	55200*2000	0.4 2.5
$O_2 \cdot NO \rightarrow O \cdot NO_2$ 73 BAU/DRY	----- NITROGEN MOLECULE REACTION ORDER: 2. NOTE: k <sub>1</sub> = k <sub>k-1</sub> -----	300-550	1.7(+12)	0	23400	0.8 1.3
$O_2 \cdot NO \cdot NO \rightarrow NO_2 \cdot NO_2$ 73 BAU/DRY	----- NITROGEN OXIDE(NO) REACTION ORDER: 2. NOTE: k <sub>1</sub> = k <sub>k-1</sub> -----	273-660	1.2(+9)	0	-530*100	0.5 1.5
$O_2 \cdot NO \cdot NO_2 \rightarrow NO_2 \cdot NO_3$ 73 BAU/DRY	----- NITROGEN OXIDE(NO) + NITROGEN OXIDE(NO <sub>2</sub> ) REACTION ORDER: 3. -----	300-500	2.9(+7)	0	-400*500	0.4 2.5
$O_2 \cdot C \rightarrow O \cdot CO$ 75 BEN/GOI	----- CARBON ATOM REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$O_2 \cdot CO \rightarrow O \cdot CO_2$ 76 BAU/DRY	----- CARBON MONOXIDE 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
$O_2 \cdot CH \rightarrow O \cdot CH_2$ 76 ENG	----- METHYLIDENE FREE RADICAL REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	3000*2500	0.3 3.2
$O_2 \cdot CH_2 \rightarrow O \cdot HCHO$ 76 ENG	----- METHYLENE FREE RADICAL REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	3500*2500	0.3 3.2
$O_2 \cdot CH_3 \rightarrow O \cdot CH_3O$ 76 ENG	----- METHYL FREE RADICAL REACTION ORDER: 2. NOTE: k ESTIMATED. -----	1500-2500	3.2(+12)	0	15100*1500	
$O_2 \cdot CH_3 \cdot OH \rightarrow OH \cdot HCHO$ 76 ENG	----- METHYL FREE RADICAL 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
1500-2500	3.2(+12)	0	34975±1500	
<p> <math>\phi_2 \cdot CH_3 \rightarrow H\phi_2 \cdot \cdot CH_2</math>                      OXYGEN MOLECULE + METHYL FREE RADICAL                      REACTION ORDER: 2.                      76 ENG                      NOTE: k ESTIMATED                 </p>				
1500-2500	1.6(+12)	0	3500±1500	
<p> <math>\phi_2 \cdot \cdot CH\phi \rightarrow H\phi_2 \cdot \cdot C\phi</math>                      OXYGEN MOLECULE + METHYL, OXO-, FREE RADICAL                      REACTION ORDER: 2.                      76 ENG                      NOTE: k ESTIMATED.                 </p>				
1500-2500	1.0(+12)	0	3000±1500	
<p> <math>\phi_2 \cdot CH_3\phi \rightarrow H\phi_2 \cdot \cdot HCH\phi</math>                      OXYGEN MOLECULE + METHOXY FREE RADICAL                      REACTION ORDER: 2.                      76 ENG                      NOTE: k ESTIMATED.                 </p>				
1500-2500	3.2(+11)	0	0±5000	0.3 3.2
<p> <math>\phi_2 \cdot CN \rightarrow C\phi \cdot N\phi</math>                      OXYGEN MOLECULE + CYANOGEN FREE RADICAL                      REACTION ORDER: 2.                      76 ENG                 </p>				
2500-8000 2000-10000	3.5(+25) 9.8(+24)	-2.5 -2.5	59380 59380	0.5 2.0 0.4 2.5
<p> <math>\phi_2 \cdot M \rightarrow e \cdot e \cdot M</math>                      OXYGEN MOLECULE                      76 BAU/DRY                      NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT W 8000K                      M: O2                      M: Ar                 </p>				
3000-18000	1.8(+18)	-1.0	59380±4900	0.5 2.0
200-500	5.2(+12)	0	2090±260	0.5 1.5
<p> <math>\phi_3 \cdot \phi \rightarrow \phi_2 \cdot \phi_2</math>                      OZONE + OXYGEN ATOM                      76 BAU/DRY                      NOTE: k FACTORS CHANGING TO: f = 0.3; F = 3.0 AT W 1000K                 </p>				
300	1.6(+13)	-	-	0.5 2.0
<p> <math>\phi_3 \cdot H \rightarrow \phi_2 \cdot \phi H</math>                      OZONE + HYDROGEN ATOM                      76 BAU/DRY                 </p>				
300	3.9(+10)	-	-	0.5 1.5
<p> <math>\phi_3 \cdot H\phi_2 \rightarrow \phi_2 \cdot \phi_2 \cdot \phi H</math>                      OZONE + HYDROXYL FREE RADICAL                      REACTION ORDER: 2.                      76 BAU/DRY                 </p>				
298	9.1(+ 8)	-	-	0.5 1.5
<p> <math>\phi_3 \cdot H_2S \rightarrow S\phi_2 \cdot H_2\phi</math>                      OZONE + HYDROGEN SULFIDE                      76 BAU/DRY                 </p>				
298	4.0(+ 2)	-	-	0.1 10.
<p> <math>\phi_3 \cdot N\phi \rightarrow \phi_2 \cdot N\phi_2</math>                      OZONE + NITROGEN OXIDE(NO)                      73 BAU/DRY                 </p>				
200-350	8.9(+11)	0	1230±130	0.5 1.5
<p> <math>\phi_3 \cdot N\phi_2 \rightarrow \phi_2 \cdot N\phi_3</math> </p>				

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	F
OZONE + NITROGEN OXIDE(N <sub>2</sub> ) 73 BAU/DRY O <sub>3</sub> + M → O + O <sub>2</sub> + M OZONE 76 BAU/DRY	REACTION ORDER: 2. ----- M: Ar	0	3500	0.5	2.0
H + O + M → OH + M HYDROGEN ATOM + OXYGEN ATOM 76 ENG	REACTION ORDER: 3. -----	0	0	0.8	1.3
H + O <sub>2</sub> → OH + O HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY	REACTION ORDER: 2. -----	0	8450±250	0.7	1.3
D + O <sub>2</sub> → OD + O DEUTERIUM ATOM + OXYGEN MOLECULE 72 BAU/DRY	REACTION ORDER: 2. -----	0	7500		
H + O <sub>2</sub> + M → HO <sub>2</sub> + M HYDROGEN ATOM + OXYGEN MOLECULE 72 BAU/DRY NOTE: M eff: H <sub>2</sub> (1.0)	REACTION ORDER: 3. ----- M: H <sub>2</sub>	0	-500±250	0.5	1.5
O <sub>2</sub> (0.4) H <sub>2</sub> O(6.4)	M: O <sub>2</sub>	0	-500±250	0.5	1.5
He(0.3). k <sub>1</sub> = k <sub>k-1</sub> Ar(0.3). k <sub>1</sub> = k <sub>k-1</sub> N <sub>2</sub> (0.4) CO <sub>2</sub> (1.5)	M: He M: Ar M: N <sub>2</sub> M: CO <sub>2</sub>	0	-500±250	0.5	1.5
H + O <sub>3</sub> → OH + O <sub>2</sub> HYDROGEN ATOM + OZONE 76 BAU/DRY	REACTION ORDER: 2. -----	-	-	0.5	2.0
H + H + M → H <sub>2</sub> + M HYDROGEN ATOM 72 BAU/DRY NOTE: M eff: H <sub>2</sub> (1.0)	REACTION ORDER: 3. ----- M: H <sub>2</sub>	-	-	0.5	1.5
H + H <sub>2</sub> → H <sub>2</sub> + H HYDROGEN ATOM + HYDROGEN MOLECULE 75 BEN/GEL	REACTION ORDER: 2. ----- M: Ar(0.25). k <sub>1</sub> = k <sub>k-1</sub>	-1.0	0	0.4	2.5
H + D <sub>2</sub> → DH + D	REACTION ORDER: 2. -----	0.5	4000		

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	k factors F
368-1000	3.1(*13)	0	4485±250	0.6	1.6
HYDROGEN ATOM * DEUTERIUM MOLECULE REACTION ORDER: 2. -----					
400-1000	5.0(*13)	0	3690±40	0.9	1.1
D * H <sub>2</sub> - DE * H DEUTERIUM ATOM * HYDROGEN MOLECULE REACTION ORDER: 2. -----					
400-2000	8.3(*9)	1.0	3500±150	0.7	1.3
H * OH - H <sub>2</sub> * O HYDROGEN ATOM * HYDROXYL FREE RADICAL REACTION ORDER: 2. -----					
	6.3(*11)	0.5	0		
H * OH - OH * H HYDROGEN ATOM * HYDROXYL FREE RADICAL REACTION ORDER: 2. -----					
1000-3000	1.4(*23)	-2.0	0	0.7	1.5
H * OH * M - H <sub>2</sub> O * M HYDROGEN ATOM * HYDROXYL FREE RADICAL REACTION ORDER: 3. M: H <sub>2</sub> O					
1000-3000	8.4(*21)	-2.0	0	0.5	2.0
72 BAU/DRY NOTE: M eff: H <sub>2</sub> O(1.0). k <sub>1</sub> = k <sub>k-1</sub> M: Ar					
1000-3000	2.2(*22)	-2.0	0	0.5	2.0
Ar(0.06) N <sub>2</sub> (0.16) M: N <sub>2</sub>					
300-1000	5. (*13)	0	500	0.3	3.2
H * HO <sub>2</sub> - O * H <sub>2</sub> O HYDROGEN ATOM * HYDROPEROXYL FREE RADICAL REACTION ORDER: 2. -----					
1500-2500	1.0(*13)	0	500±500	0.1	1.0
74 LIC NOTE: ESTIMATED. 76 ENG					
290-800	2.5(*13)	0	350±350	0.4	2.5
H * HO <sub>2</sub> - H <sub>2</sub> * O <sub>2</sub> HYDROGEN ATOM * HYDROPEROXYL FREE RADICAL REACTION ORDER: 2. -----					
1500-2500	2.5(*13)	0	350±350	0.5	2.0
72 BAU/DRY 76 ENG					
290-800	2.5(*14)	0	950±350	0.5	2.0
H * HO <sub>2</sub> - OH * OH HYDROGEN ATOM * HYDROPEROXYL FREE RADICAL REACTION ORDER: 2. -----					
1500-2500	2.5(*14)	0	950±500	0.5	2.0
72 BAU/DRY 76 ENG					
300-2500	9.3(*13)	0	10250±100	0.5	1.5
H * H <sub>2</sub> O - OH * H <sub>2</sub> HYDROGEN ATOM * WATER REACTION ORDER: 2. -----					
300-800	1.7(*12)	0	1900±250	0.5	2.0
NOTE: ERROR LIMITS ARE 50% FOR UPPER T'S. -----					
300-800	7.9(*12)	0.5	8355		
H * H <sub>2</sub> O <sub>2</sub> - H <sub>2</sub> * HO <sub>2</sub> HYDROGEN ATOM * HYDROGEN PEROXIDE REACTION ORDER: 2. -----					
72 BAU/DRY					
H * S <sub>2</sub> - SH * S HYDROGEN ATOM * SULFUR DIMER REACTION ORDER: 2. -----					
75 BEN/GGL					

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
	4.0(+12)	0.5	11200	
	6.3(+11)	0.5	19930	
1660-2120	5.1(+15)	-	-	0.5 1.5
298	1.5(+13)	-	-	0.5 1.5
	6.3(+11)	0.5	0	
190-470	7.8(+12)	0	860*50	0.5 1.5
1500-2500	2.5(+17)	-0.5	0*1000	0.1 10.
	2.0(+13)	0.5	75945	
	2.5(+12)	0.5	24460	
	5.0(+12)	0.5	38200	
230-700	5.4(+15)	0	-300*100	0.5 1.5
1500-2500	5.0(+15)	0	-300*150	0.5 2.0
298-630	3.5(+14)	0	740*500	0.5 1.5

H \* S6 - CH \* S  
HYDROGEN ATOM \* SULFUR MONOXIDE  
75 BEN/GGL  
REACTION ORDER: 2.

H \* S6 - SH \* G  
HYDROGEN ATOM \* SULFUR MONOXIDE  
75 BEN/GGL  
REACTION ORDER: 2.

H \* S6 \* M - HS62 \* M  
HYDROGEN ATOM \* SULFUR DIOXIDE  
76 HAU/DRY  
REACTION ORDER: 3.

H \* SH - H2 \* S  
HYDROGEN ATOM \* MERCAPTO FREE RADICAL  
76 HAU/DRY  
REACTION ORDER: 2.

H \* SH - SH \* H  
HYDROGEN ATOM \* MERCAPTO FREE RADICAL  
75 BEN/GGL  
REACTION ORDER: 2.

H \* H2S - H2 \* SH  
HYDROGEN ATOM \* HYDROGEN SULFIDE  
76 HAU/DRY  
REACTION ORDER: 2.

H \* N \* M - NH \* M  
HYDROGEN ATOM \* NITROGEN ATOM  
76 ENG  
REACTION ORDER: 3.

H \* N2 - NH \* N  
HYDROGEN ATOM \* NITROGEN MOLECULE  
75 BEN/GGL  
REACTION ORDER: 2.

H \* N6 - CH \* N  
HYDROGEN ATOM \* NITROGEN OXIDE(N6)  
75 BEN/GGL  
REACTION ORDER: 2.

H \* N6 - NH \* G  
HYDROGEN ATOM \* NITROGEN OXIDE(N6)  
75 BEN/GGL  
REACTION ORDER: 2.

H \* N6 \* M - HNG \* M  
HYDROGEN ATOM \* NITROGEN OXIDE(N6)  
73 HAU/DRY  
REACTION ORDER: 3.

H \* N6 \* M - HNG \* M  
HYDROGEN ATOM \* NITROGEN OXIDE(N6)  
76 ENG  
REACTION ORDER: 3. M: H2

H \* N62 - CH \* N6  
HYDROGEN ATOM \* NITROGEN OXIDE(N62)  
73 HAU/DRY  
REACTION ORDER: 2.

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

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f F
H + NO <sub>2</sub> → OH + NO HYDROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+14)	0	750±500	0.5 2.0
H + N <sub>2</sub> O → OH + N <sub>2</sub> HYDROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 73 BAU/DRY REACTION ORDER: 2. -----	700-2500	7.6(+13)	0	7600±500	0.5 1.5
H + N <sub>2</sub> O → NH + NO HYDROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.5	15100±2500	0.3 3.2
H + NH → H <sub>2</sub> + N HYDROGEN ATOM + 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 <sub>2</sub> + M → NH <sub>3</sub> + M HYDROGEN ATOM + AMIDGEN FREE RADICAL 73 BAU/DRY REACTION ORDER: 3. M: Ar NOTE: k <sub>1</sub> = k <sub>2</sub> -1 -----	2000-3000	4.8(+14)	0	-8300±2500	0.5 2.0
H + NH <sub>2</sub> NH <sub>2</sub> → H <sub>2</sub> + NH <sub>2</sub> NH. HYDROGEN ATOM + HYDRAZINE 73 BAU/DRY REACTION ORDER: 2. -----	250-500	1.3(+13)	0	1250±100	0.5 2.0
H + HNO → H <sub>2</sub> + NO HYDROGEN ATOM + NITROSYL HYDRIDE 73 BAU/DRY REACTION ORDER: 2. -----	2000	4.8(+12)	-	-	0.5 1.5
H + HNO → 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 + O HYDROGEN ATOM + CARBON MONOXIDE 75 BEN/GGL REACTION ORDER: 2. -----		2.0(+13)	0.5	77755	
H + CO → CH + O 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
<p>H + C6 → M → •CH6 + M HYDROGEN ATOM + CARBON MONOXIDE 76 BAU/DRY NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 773K. 76 ENG</p>	<p>298-773 1500-2500</p>	<p>6.9(+14) 1.6(+20)</p>	<p>0 -1.5</p>	<p>850±500 0</p>	<p>0.7 1.3 0.3 3.2</p>
<p>H + C6 → 2H + C6 HYDROGEN ATOM + CARBON DIOXIDE 76 BAU/DRY</p>	<p>1000-3000</p>	<p>1.5(+14)</p>	<p>0</p>	<p>13300±150</p>	<p>0.8 1.2</p>
<p>H + CH → H2 + C HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL</p>		<p>6.3(+11)</p>	<p>0.5</p>	<p>4000</p>	
<p>H + CH → CH + H HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GOL</p>		<p>6.3(+11)</p>	<p>0.5</p>	<p>0</p>	
<p>H + CH → M → CH2 + M HYDROGEN ATOM + METHYLIDYNE FREE RADICAL 76 ENG</p>	<p>1500-2500</p>	<p>1.0(+19)</p>	<p>-1.0</p>	<p>0</p>	<p>0.3 3.2</p>
<p>H + CH2 → H2 + CH HYDROGEN ATOM + METHYLENE FREE RADICAL 76 ENG</p>	<p>1500-2500</p>	<p>3.2(+11)</p>	<p>0.7</p>	<p>2500±2500</p>	<p>0.3 3.2</p>
<p>H + CH4 → H2 + CH3 HYDROGEN ATOM + METHANE 76 ENG</p>	<p>1500-2500</p>	<p>6.3(+13)</p>	<p>0</p>	<p>5990±150</p>	<p>0.5 2.0</p>
<p>D + CH4 → DH + CH3 DEUTERIUM ATOM + METHANE 72 KON</p>	<p>523-673</p>	<p>8.3(+12)</p>	<p>0</p>	<p>5100</p>	
<p>H + •CH6 → H2 + C6 HYDROGEN ATOM + METHYL, C6H5, FREE RADICAL 76 ENG</p>	<p>1500-2500</p>	<p>1.6(+12)</p>	<p>0.5</p>	<p>0±2500</p>	<p>0.3 3.2</p>
<p>H + HCH6 → H2 + •CH6 HYDROGEN ATOM + FORMALDEHYDE 76 ENG</p>	<p>1500-2500</p>	<p>1.3(+10)</p>	<p>1.0</p>	<p>1600</p>	<p>0.3 3.2</p>
<p>H + CH3O → H2 + HCO HYDROGEN ATOM + METHOXY FREE RADICAL 76 ENG</p>	<p>1500-2500</p>	<p>1.0(+14)</p>	<p>0</p>	<p>0±1500</p>	
<p>NOTE: k ESTIMATED.</p>					
<p>H + CS → C + SH HYDROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GOL</p>	<p>1500-2500</p>	<p>2.0(+13)</p>	<p>0.5</p>	<p>48870</p>	
<p>H + CS → CH + S HYDROGEN ATOM + CARBON MONOSULFIDE FREE RADICAL</p>					

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
75 HEN/GGL REACTION ORDER: 2. -----			1.3(+13)	0.5	50930	
H + C6S → HS + C6 HYDROGEN ATOM + CARBON OXIDE SULFIDE REACTION ORDER: 2. -----		298	1.3(+10)	-	-	0.8 1.3
76 HAU/DRY -----						
H + CN → C + NH HYDROGEN ATOM + CYANOGEN FREE RADICAL REACTION ORDER: 2. -----			1.0(+13)	0.5	52745	
75 HEN/GGL -----						
H + CN → CH + N HYDROGEN ATOM + CYANOGEN FREE RADICAL REACTION ORDER: 2. -----			6.3(+12)	0.5	49775	
75 HEN/GGL -----						
H + CN + M → HCN + M HYDROGEN ATOM + CYANOGEN FREE RADICAL REACTION ORDER: 2. -----		1500-2500	3.2(+16)	-0.5	0+2500	0.3 3.2
76 ENG -----						
H + C2 → CH + C HYDROGEN ATOM + CARBON DIMER REACTION ORDER: 2. -----			1.6(+13)	0.5	30450	
75 HEN/GGL -----						
H + CH2=CH2 → CH3CH2 HYDROGEN ATOM + ETHENE REACTION ORDER: 2. -----		298	9.3(+13)	0	1410	
72 IER/PAR -----						
H + CH2=CH2 + M → CH3CH2 + M HYDROGEN ATOM + ETHENE REACTION ORDER: 3. -----		298-813	5.6(+17)	0.5	495	
72 IGN -----						
H + CH3CH3 → H2 + CH3CH2 HYDROGEN ATOM + ETHANE REACTION ORDER: 2. -----		285-1440	1.0(+14)	0	4615+70	0.8 1.2
72 IGN -----						
H + CH3C≡CH → CH3C≡CH + CH3C(•)≡CH2 HYDROGEN ATOM + 1-PROPENE REACTION ORDER: 2. -----		298	0.5(+11)	-	-	
72 IER/PAR -----						
NOTE: k TAKEN AS LOWER LIMIT.						
H + CH3CH=CH2 → CH3CH2CH2 HYDROGEN ATOM + 1-PROPENE REACTION ORDER: 2. -----		298	7.2(+12)	0	1460	
72 IER/PAR -----						
NOTE: TENTATIVE k VALUE.						
H + CH3CH=CH2 → CH3CH(•)CH3 HYDROGEN ATOM + 1-PROPENE REACTION ORDER: 2. -----		298	7.2(+12)	0	605	
72 IER/PAR -----						
NOTE: ARRHENIUS PARAMETERS ARE MINIMUM VALUES OF THEIR HIGH-PRESSURE LIMITS.						
H + CH3CH2CH3 → H2 + (CH3)2CH + CH3CH2CH2 HYDROGEN ATOM + PROPANE REACTION ORDER: 2. -----		333-933	1.0(+13)	0	3130+160	0.7 1.4
72 IGN -----						

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
<p>H • (CH<sub>3</sub>)<sub>2</sub>CO → H<sub>2</sub> • CH<sub>3</sub>C(O)CH<sub>2</sub>  HYDROGEN ATOM • 2-PYRACETONE  72 KER</p> <p>REACTION ORDER: 2.</p>	298-873	4.6(+13)	0	4220±20	
<p>H • CH<sub>2</sub>-CHCH-CH<sub>2</sub> → CH<sub>2</sub>-CHCH(•)CH<sub>3</sub> • CH<sub>2</sub>-CHCH<sub>2</sub>CH<sub>2</sub>•  HYDROGEN ATOM • 1,3-BUTADIENE  72 KER/PAR</p> <p>REACTION ORDER: 2.</p> <p>NOTE: AVERAGED RATE CONSTANT.</p>	298	4.10(+13)	0	655	
<p>H • CH<sub>2</sub>-CHCH-CH<sub>2</sub> → CH<sub>2</sub>-CHCH(•)CH<sub>3</sub> • CH<sub>2</sub>-CHCH<sub>2</sub>CH<sub>2</sub>•  HYDROGEN ATOM • 1,3-BUTADIENE  72 KER/PAR</p> <p>REACTION ORDER: 2. k/k<sub>ref</sub>: 4.9</p>	300	-	-	-	
<p>H • CH<sub>3</sub>CH<sub>2</sub>CH-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub> • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  HYDROGEN ATOM • 1-BUTENE  72 KER/PAR</p> <p>REACTION ORDER: 2. k/k<sub>ref</sub>: 1.03</p>	300	-	-	-	
<p>NOTE: k<sub>ref</sub>: H • CH<sub>3</sub>CH=CH<sub>2</sub></p>	298	8.7(+11)	-	-	
<p>H • CH<sub>3</sub>CH<sub>2</sub>CH-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  HYDROGEN ATOM • 1-BUTENE  72 KER/PAR</p> <p>REACTION ORDER: 2.</p> <p>NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.</p>	298	5.0(+10)	-	-	
<p>H • CH<sub>3</sub>CH<sub>2</sub>CH-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  HYDROGEN ATOM • 1-BUTENE  72 KER/PAR</p> <p>REACTION ORDER: 2.</p> <p>NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.</p>	298	8.1(+11)	-	-	
<p>H • cis-CH<sub>3</sub>CH=CHCH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  HYDROGEN ATOM • cis-2-BUTENE  72 KER/PAR</p> <p>REACTION ORDER: 2.</p> <p>NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION.  k/k<sub>ref</sub>: 0.47</p>	298	4.6(+11)	-	-	
<p>NOTE: k<sub>ref</sub>: H • CH<sub>3</sub>CH=CH<sub>2</sub>.</p>	300	-	-	-	
<p>H • trans-CH<sub>3</sub>CH=CHCH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  HYDROGEN ATOM • trans-2-BUTENE  72 KER/PAR</p> <p>REACTION ORDER: 2.</p> <p>NOTE: AVERAGE k</p>	298	5.6(+11)	-	-	
<p>NOTE: k<sub>ref</sub>: H • CH<sub>3</sub>CH=CH<sub>2</sub>.</p>	300	-	-	-	
<p>H • (CH<sub>3</sub>)<sub>2</sub>C-CH<sub>2</sub> → (CH<sub>3</sub>)<sub>3</sub>C•  HYDROGEN ATOM • 1-PROPENE, 2-METHYL-  72 KER/PAR</p> <p>REACTION ORDER: 2.</p>	298	3.10(+13)	0	755	
<p>H • (CH<sub>3</sub>)<sub>2</sub>C-CH<sub>2</sub> → (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>•  HYDROGEN ATOM • 1-PROPENE, 2-METHYL-  72 KER/PAR</p>					



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 REACTION ORDER: 2.  
 NOTE: CALCULATED ON THE BASIS OF 0.5% NON-TERMINAL  
 ADDITION OF H TO (CH<sub>3</sub>)<sub>2</sub>C=CH<sub>2</sub>.  
 -----  
 H + (CH<sub>3</sub>)<sub>2</sub>C=CH<sub>2</sub> → (CH<sub>3</sub>)<sub>3</sub>C + (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>.  
 HYDROGEN ATOM + 1-PENTENE, 2-METHYL-  
 REACTION ORDER: 2. k/k<sub>ref</sub>: 2.52  
 72 KER/PAR  
 NOTE: k<sub>ref</sub>: H + CH<sub>3</sub>CH=CH<sub>2</sub>  
 -----  
 H + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> → H<sub>2</sub> + CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub> + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  
 HYDROGEN ATOM + BUTANE  
 72 ION REACTION ORDER: 2.  
 -----  
 H + (CH<sub>3</sub>)<sub>3</sub>CH → H<sub>2</sub> + (CH<sub>3</sub>)<sub>3</sub>C + (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>•  
 HYDROGEN ATOM + PROPANE, 2-METHYL-  
 REACTION ORDER: 2.  
 72 ION  
 -----  
 H + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  
 + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  
 HYDROGEN ATOM + 1-PENTENE  
 72 IBE/PAR REACTION ORDER: 2.  
 k/k<sub>ref</sub>: 0.89  
 -----  
 NOTE: k<sub>ref</sub>: H + CH<sub>3</sub>CH=CH<sub>2</sub>.  
 -----  
 H + cis-CH<sub>3</sub>CH<sub>2</sub>CH=CHCH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>3</sub>  
 + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  
 HYDROGEN ATOM + cis-2-PENTENE  
 REACTION ORDER: 2.  
 k/k<sub>ref</sub>: 0.39  
 72 IBE/PAR  
 NOTE: k<sub>ref</sub>: H + CH<sub>3</sub>CH=CH<sub>2</sub>.  
 -----  
 H + trans-CH<sub>3</sub>CH<sub>2</sub>CH=CHCH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>3</sub>  
 + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub>  
 HYDROGEN ATOM + trans-2-PENTENE  
 REACTION ORDER: 2.  
 k/k<sub>ref</sub>: 0.44  
 72 IBE/PAR  
 NOTE: k<sub>ref</sub>: H + CH<sub>3</sub>CH=CH<sub>2</sub>.  
 -----  
 H + CH<sub>3</sub>CH<sub>2</sub>C(CH<sub>3</sub>)-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>C(•)(CH<sub>3</sub>)<sub>2</sub>  
 + CH<sub>3</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)CH<sub>2</sub>•  
 HYDROGEN ATOM + 1-BUTENE, 2-METHYL-  
 REACTION ORDER: 2.  
 72 IBE/PAR  
 -----  
 D + CH<sub>3</sub>CH<sub>2</sub>C(CH<sub>3</sub>)-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>C(•)(CH<sub>3</sub>)CH<sub>2</sub>D  
 + CH<sub>3</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)CH<sub>2</sub>•  
 DEUTERIUM ATOM + 1-BUTENE, 2-METHYL-  
 REACTION ORDER: 2.  
 72 IBE/PAR  
 -----  
 H + (CH<sub>3</sub>)<sub>2</sub>CHCH=CH<sub>2</sub> → (CH<sub>3</sub>)<sub>2</sub>CHCH(•)CH<sub>3</sub>  
 + (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>2</sub>•  
 HYDROGEN ATOM + 1-BUTENE, 3-METHYL-  
 REACTION ORDER: 2.  
 72 IBE/PAR

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
D + (CH <sub>3</sub> ) <sub>2</sub> CHCH=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHCH(•)(CH <sub>2</sub> ) <sub>2</sub> + (CH <sub>3</sub> ) <sub>2</sub> CHCHDCH <sub>2</sub> <sup>•</sup> DEUTERIUM ATOM + 1-HUTENE, 3-METHYL- 72 KER/PAR		298	7.6(+11)	-	-	
H + (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHCH(•)(CH <sub>3</sub> ) + (CH <sub>3</sub> ) <sub>2</sub> C(•)CH <sub>2</sub> CH <sub>3</sub> HYDROGEN ATOM + 2-HUTENE, 2-METHYL- 72 KER/PAR		298 300	9.1(+11)	-	-	
NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub> k/k <sub>ref</sub> : 1.03						
H + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHC(•)(CH <sub>3</sub> ) <sub>2</sub> HYDROGEN ATOM + 2-EUTENE, 2,3-DIMETHYL- 72 KER/PAR		298 300	7.8(+11)	-	-	
NOTE: k <sub>ref</sub> : H + CH <sub>3</sub> CH=CH <sub>2</sub>						
H + (CH <sub>3</sub> ) <sub>3</sub> CC(CH <sub>3</sub> )=CH <sub>2</sub> → (CH <sub>3</sub> ) <sub>3</sub> CC(CH <sub>3</sub> )CH <sub>2</sub> <sup>•</sup> + (CH <sub>3</sub> ) <sub>3</sub> CC(•)(CH <sub>3</sub> ) <sub>2</sub> HYDROGEN ATOM + 1-HUTENE, 2,3,3-TRIMETHYL- 72 KER/PAR		298	1.6(+12)	-	-	
NOTE: TENTATIVE VALUE BASED ON REACTION: H + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub>						
H <sub>2</sub> + O → H + OH HYDROGEN MOLECULE + OXYGEN ATOM 72 BAU/DRY		400-2000	1.8(+10)	1.0	4480±150	0.7 1.3
D <sub>2</sub> + O → D + OD DEUTERIUM MOLECULE + OXYGEN ATOM 72 BAU/DRY		416-968	2.0(+13)	0	5500	0.5 2.0
H <sub>2</sub> + O <sub>2</sub> → H + HO <sub>2</sub> <sup>•</sup> HYDROGEN MOLECULE + OXYGEN MOLECULE 72 BAU/DRY		290-800	5.5(+13)	0	29100±350	0.4 2.5
H <sub>2</sub> + O <sub>2</sub> → OH + OH HYDROGEN MOLECULE + OXYGEN MOLECULE 76 ENG		1500-2500	2.5(+12)	0	19630±5000	0.1 10.
H + H → H + H <sub>2</sub> HYDROGEN MOLECULE + HYDROGEN ATOM 75 HEN/GOL			6.3(+11)	0.5	4000	
H <sub>2</sub> + D → H + HD HYDROGEN MOLECULE + DEUTERIUM ATOM 72 KON		400-1000	5.0(+13)	0	3890±40	0.9 1.1
D <sub>2</sub> + H → D + DH DEUTERIUM MOLECULE + HYDROGEN ATOM 72 KON		1000	3.1(+13)	0	4485±250	0.6 1.6

## CHEMICAL REACTIONS

T/K	A	B	E/R (in OK)	k factors f	F
300-2500	2.2(+13)	0	2590±100	0.8	1.2
<p>H<sub>2</sub> ♦ OH → H ♦ H<sub>2</sub>O  HYDROGEN MOLECULE ♦ HYDROXYL FREE RADICAL  REACTION ORDER: 2.  72 HAU/DRY  NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 FOR T : 300K  T &gt; 300K  -----</p>					
300-623	1.9(+13)	0	2904±280	0.5	2.0
<p>D<sub>2</sub> ♦ OH → D ♦ DHO  DEUTERIUM MOLECULE ♦ HYDROXYL FREE RADICAL  REACTION ORDER: 2.  72 KDN  -----</p>					
300-800	7.3(+11)	0	9400±250	0.5	2.0
<p>H<sub>2</sub> ♦ H<sub>2</sub> → H ♦ H<sub>2</sub>O<sup>2</sup>  HYDROGEN MOLECULE ♦ HYDROPEROXYL FREE RADICAL  REACTION ORDER: 2.  72 HAU/DRY  -----</p>					
298	1.3(- 1)	-	-	0.5	1.5
<p>H<sub>2</sub> ♦ S → H ♦ SH  HYDROGEN MOLECULE ♦ SULFUR ATOM  REACTION ORDER: 2.  76 HAU/DRY  NOTE: k<sub>1</sub> = Kk-1  75 BEN/GOL  -----</p>					
1500-2500	2.5(+12)	0.5	18700	0.3	3.2
<p>H<sub>2</sub> ♦ N → H ♦ NH  HYDROGEN MOLECULE ♦ NITROGEN ATOM  REACTION ORDER: 2.  75 BEN/GOL  -----</p>					
1500-2500	1.6(+12)	0.5	15700	0.5	1.5
<p>H<sub>2</sub> ♦ C → H ♦ CH  HYDROGEN MOLECULE ♦ CARBON ATOM  REACTION ORDER: 2.  75 BEN/GOL  -----</p>					
370-700	3.2(+12)	0	3525±1500	0.7	1.3
<p>H<sub>2</sub> ♦ CO<sub>2</sub> → H<sub>2</sub>O ♦ CO  HYDROGEN MOLECULE ♦ CARBON DIOXIDE  REACTION ORDER: 2.  76 ENG  -----</p>					
400-570	8.5(+11)	0	5500±500	0.6	1.7
<p>H<sub>2</sub> ♦ CH<sub>2</sub> → H ♦ CH<sub>3</sub><sup>•</sup>  HYDROGEN MOLECULE ♦ METHYLENE FREE RADICAL  REACTION ORDER: 2.  76 ENG  NOTE: k ESTIMATED.  -----</p>					
400-700	7.4(+11)	0	5250±235	0.5	1.5
<p>H<sub>2</sub> ♦ CH<sub>3</sub> → H ♦ CH<sub>4</sub>  HYDROGEN MOLECULE ♦ METHYL FREE RADICAL  REACTION ORDER: 2.  76 KER/PAR  -----</p>					
400-700	2.4(+11)	0	5635±500	0.5	1.5
<p>H<sub>2</sub> ♦ CD<sub>3</sub> → H ♦ CD<sub>3</sub>H  HYDROGEN MOLECULE ♦ METHYL-D<sub>3</sub>-FREE RADICAL  REACTION ORDER: 2.  72 KDN  -----</p>					
400-700	2.1(+11)	0	5300±500	0.5	1.5
<p>DH ♦ CH<sub>3</sub> → H ♦ CH<sub>3</sub>D  DEUTERIUM HYDRIDE ♦ METHYL FREE RADICAL  REACTION ORDER: 2.  76 KER/PAR  -----</p>					
<p>DH ♦ CH<sub>3</sub> → D ♦ CH<sub>4</sub>  DEUTERIUM HYDRIDE ♦ METHYL FREE RADICAL  REACTION ORDER: 2.  76 KER/PAR  -----</p>					

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
300-700	7.1(+11)	0	5990±250	0.7 1.3
<p>D<sub>2</sub> + CH<sub>3</sub>° → D + CH<sub>3</sub>D  DEUTERIUM MOLECULE + METHYL FREE RADICAL  76 KEY/PAR  REACTION ORDER: 2.  -----</p>				
1500-2500	3.2(+12)	0	2500±1500	
<p>H<sub>2</sub> + CN → H + HCN  HYDROGEN MOLECULE + CYANOGEN FREE RADICAL  76 ENG  REACTION ORDER: 2.  NOTE: k ESTIMATED.  -----</p>				
473-823	3.0(+11)	0	5435	
<p>H<sub>2</sub> + CH<sub>3</sub>CH<sub>2</sub>° → H + CH<sub>3</sub>CH<sub>3</sub>  HYDROGEN MOLECULE + ETHYL FREE RADICAL  72 ION  REACTION ORDER: 2.  -----</p>				
2500-5000	2.2(+14)	0	48300±2000	0.5 2.0
<p>H<sub>2</sub> + M → H + H + M  HYDROGEN MOLECULE  72 BAU/DRY  NOTE: k<sub>1</sub> = k<sub>k-1</sub>  -----</p>				
	6.3(+11)	0.5	4000	
<p>OH + O → O + OH  HYDROXYL FREE RADICAL + OXYGEN ATOM  75 BEN/GGL  REACTION ORDER: 2.  -----</p>				
300	2.3(+13)	-	-	0.6 1.4
<p>OH + O → H + O<sub>2</sub>  HYDROXYL FREE RADICAL + OXYGEN ATOM  72 BAU/DRY  NOTE: k<sub>1</sub> CALCULATED FROM k<sub>-1</sub> IS: 1.3 X 10<sup>13</sup> cc.mole<sup>-1</sup>.s<sup>-1</sup>  -----</p>				
1500-2500	2.5(+13)	0	0	0.5 2.0
<p>OH + O → H + O<sub>2</sub>  HYDROXYL FREE RADICAL + OXYGEN ATOM  76 ENG  REACTION ORDER: 2.  -----</p>				
1500-2500	1.0(+17)	0	0	0.01 100.
<p>OH + O → M → HO<sub>2</sub> + M  HYDROXYL FREE RADICAL + OXYGEN ATOM  76 ENG  REACTION ORDER: 3.  -----</p>				
300	3.9(+10)	-	-	0.5 1.5
<p>OH + O<sub>3</sub> → HO<sub>2</sub>° + O<sub>2</sub>  HYDROXYL FREE RADICAL + OZONE  76 BAU/DRY  REACTION ORDER: 2.  -----</p>				
400-2000	8.3(+9)	1.0	3500±150	0.7 1.3
<p>OH + H → O + H<sub>2</sub>  HYDROXYL FREE RADICAL + HYDROGEN ATOM  72 BAU/DRY  REACTION ORDER: 2.  -----</p>				
	6.3(+11)	0.5	0	
<p>OH + H → M → H<sub>2</sub>O + M  HYDROXYL FREE RADICAL + HYDROGEN ATOM  75 BEN/GGL  REACTION ORDER: 2.  -----</p>				
1000-3000	1.4(+23)	-2.0	0	0.7 1.5
<p>OH + H → M → H<sub>2</sub>O + M  HYDROXYL FREE RADICAL + HYDROGEN ATOM  72 BAU/DRY  NOTE: M eff: H<sub>2</sub>O(1.0), k<sub>1</sub> = k<sub>k-1</sub>  -----</p>				
1000-3000	8.4(+21)	-2.0	0	0.5 2.0
<p>Ar(0.06)  -----</p>				

Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f	k factors F
<p><math>N_2(0.16)</math></p> <p>OH + H<sub>2</sub> - H<sub>2</sub>O + H  HYDROXYL FREE RADICAL + HYDROGEN MOLECULE  72 HAU/DRY  REACTION ORDER: 2.  NOTE: k FACTORS CHANGING 10: f = 0.5; F = 1.5  FOR I &gt; 300K</p>	1000-3000	2.2(+22)	-2.0	0	0.5	2.0
<p>OH + D<sub>2</sub> - DH<sub>2</sub> + D  HYDROXYL FREE RADICAL + DEUTERIUM MOLECULE  72 HCN  REACTION ORDER: 2.</p>	300-623	1.9(+13)	0	2904±280	0.5	2.0
<p>OH + OH - H<sub>2</sub>O + H  HYDROXYL FREE RADICAL  72 HAU/DRY</p>	290-800	1.2(+13)	0	20200±350	0.5	2.0
<p>OH + OH - H<sub>2</sub>O + O  HYDROXYL FREE RADICAL  72 HAU/DRY</p>	300-2000	6.3(+12)	0	550±200	0.7	1.5
<p>OH + OH + M - H<sub>2</sub>O<sub>2</sub> + M  HYDROXYL FREE RADICAL  72 HAU/DRY  NOTE: k FACTORS CHANGING 10: f = 0.5; F = 2.0 AT 1500K.</p>	700-1500	9.1(+14)	0	2550±1000	0.8	1.3
<p>OH + H<sub>2</sub>O<sub>2</sub> - H<sub>2</sub>O + HO<sub>2</sub>  HYDROXYL FREE RADICAL + HYDROGEN PEROXIDE  72 HAU/DRY</p>	300-800	1.0(+13)	0	910±150	0.5	1.5
<p>OH + S - O + SH  HYDROXYL FREE RADICAL + SULFUR ATOM  75 HEN/GOL  REACTION ORDER: 2.</p>		1.3(+12)	0.5	12700		
<p>OH + S - H + SO  HYDROXYL FREE RADICAL + SULFUR ATOM  75 HEN/GOL  REACTION ORDER: 2.</p>		6.3(+11)	0.5	0		
<p>OH + H<sub>2</sub>S - H<sub>2</sub>O + HS  HYDROXYL FREE RADICAL + HYDROGEN SULFIDE  76 HAU/DRY  NOTE: k FACTORS INCREASING 10: f = 0.5; F = 1.5 AT 900K.</p>	258-900	6.3(+12)	0	200±150	0.7	1.3
<p>OH + N - O + NH  HYDROXYL FREE RADICAL + NITROGEN ATOM  75 HEN/GOL  REACTION ORDER: 2.</p>		1.3(+12)	0.5	17765		
<p>OH + N - H + NO  HYDROXYL FREE RADICAL + NITROGEN ATOM  75 HEN/GOL  REACTION ORDER: 2.</p>		6.3(+11)	0.5	0		
<p>OH + N + M - HNO + M  HYDROXYL FREE RADICAL + NITROGEN ATOM</p>						

CHEMICAL REACTIONS	T/K	A	B	E/R (ln OK)	k factors f
76 ENG REACTION ORDER: 3. ----- OH + NO <sub>2</sub> + M → HNO <sub>3</sub> + M HYDROXYL FREE RADICAL + NITROGEN OXIDE(NO <sub>2</sub> ) 73 HAU/DRY REACTION ORDER: 3. -----	1500-2500	1.0(+15)	-0.5	0	0.4 1.6
OH + N <sub>2</sub> O → H <sub>2</sub> O + N <sub>2</sub> HYDROXYL FREE RADICAL + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----	300	5.0(+17)	-	-	
OH + NH → H <sub>2</sub> O + N HYDROXYL FREE RADICAL AND IMIDGEN FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+13)	0	7550	
OH + HNO → H <sub>2</sub> O + NO HYDROXYL FREE RADICAL + NITROSYL HYDRIDE 73 HAU/DRY REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	1000±2500	0.3 3.2
OH + HNO <sub>3</sub> → H <sub>2</sub> O + NO <sub>3</sub> HYDROXYL FREE RADICAL + NITRIC ACID 73 HAU/DRY REACTION ORDER: 2. -----	2000	3.6(+13)	-	-	0.5 1.5
OH + C → H + CO HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. -----	300	8.0(+10)	-	-	0.5 2.0
OH + C → H + CO <sub>2</sub> HYDROXYL FREE RADICAL + CARBON ATOM 75 BEN/GOL REACTION ORDER: 2. -----	300	7.9(+11)	0.5	1±800	
OH + CO → H + CO <sub>2</sub> HYDROXYL FREE RADICAL + CARBON MONOXIDE 76 HAU/DRY REACTION ORDER: 2. NOTE: k FACTORS OVER 1000K: f = 0.5; F = 1.5. RECOMMENDED k FOR 250-2500K: log(k)ccmol <sup>-1</sup> s <sup>-1</sup> = 10.83 + 3.94 <sup>-4</sup> T -----	250-2000	1.5(+7)	1.3	- 385	0.8 1.2
OH + CH → H + CH <sub>2</sub> 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 <sub>2</sub> → H + HCHO HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	5.0(+11)	0.5	3000±2500	0.3 3.2
OH + CH <sub>2</sub> → H + HCHO HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----	1500-2500	1.0(+13)	0	2517	
OH + CH <sub>2</sub> → H <sub>2</sub> O + CH HYDROXYL FREE RADICAL AND METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+13)	0		

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
$\text{OH} + \text{CH}_3 \rightarrow \text{H} + \text{CH}_3\text{O}$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	6.3(+12)	0	0		
HYDROXYL FREE RADICAL AND METHYL FREE RADICAL							
$\text{OH} + \text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	6.3(+10)	0.7	1000±2500	0.3	3.2
HYDROXYL FREE RADICAL AND METHYL FREE RADICAL							
$\text{OH} + \text{CH}_4 \rightarrow \text{H}_2\text{O} + \text{CH}_3$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+13)	0	2500±250	0.5	2.0
HYDROXYL FREE RADICAL + METHANE							
$\text{OH} + \text{C}_2\text{H}_6 \rightarrow \text{H}_2\text{O} + \text{C}_2\text{H}_5$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+10)	1.0	0±1500		
HYDROXYL FREE RADICAL + METHYL, ETHYL, FREE RADICAL							
NOTE: k ESTIMATED.							
$\text{OH} + \text{CH}_3\text{O} \rightarrow \text{H}_2\text{O} + \text{HCHO}$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+13)	0	0±1500		
HYDROXYL FREE RADICAL + METHOXY FREE RADICAL							
NOTE: k ESTIMATED.							
$\text{OH} + \text{HCHO} \rightarrow \text{H}_2\text{O} + \text{CHO}$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+10)	1.0	0±1500	0.5	2.0
HYDROXYL FREE RADICAL + FORMALDEHYDE							
$\text{OH} + \text{HCN} \rightarrow \text{H}_2\text{O} + \text{HCN}$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	1500±1500		
HYDROXYL FREE RADICAL + CYANOGEN FREE RADICAL							
$\text{OH} + \text{HCN} \rightarrow \text{H}_2\text{O} + \text{CN}$							
76 ENG	REACTION ORDER: 2. -----	1500-2500	2.0(+11)	0.6	2500±2500	0.3	3.2
HYDROXYL FREE RADICAL + HYDROCYANIC ACID							
$\text{OH} + \text{CH}=\text{CH} \rightarrow \text{H}_2\text{O} + \text{CH}=\text{CH}$							
72 ION	REACTION ORDER: 2. -----	300-2000	7.6(+12)	0	2335±400	0.5	2.1
HYDROXYL FREE RADICAL + ETHYNE							
$\text{OH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{H}_2\text{O} + \text{CH}_2=\text{CH}$							
72 ION	REACTION ORDER: 2. -----	3500-1400	1.6(+14)	0	2831±445	0.4	2.4
HYDROXYL FREE RADICAL + ETHENE							
$\text{OH} + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2\text{CH}_2\text{OH}$							
72 ION/PAR	REACTION ORDER: 2. -----	300	1.1(+12)	-	-	0.8	1.3
HYDROXYL FREE RADICAL + ETHENE							
$\text{OH} + \text{CH}_3\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CH}_2$							
72 ION	REACTION ORDER: 2. -----	302-793	1.3(+14)	0	1598		
HYDROXYL FREE RADICAL + ETHANE							
$\text{OH} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}(\text{OH})\text{CH}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2$							

CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f
300	6.6(+12)	-	-	
298	9.1(+ 8)	-	-	0.5 1.5
290-800 1500-2500	2.5(+13) 2.5(+13)	0 0	350*350 350*500	0.4 2.5 0.5 2.0
300-1000	5. (+13)	0	500	0.3 3.2
290-800 1500-2500	2.5(+14) 2.5(+14)	0 0	950*350 956*500	0.5 2.0 0.5 2.0
1500-2500	1.0(+13)	0	500*500	0.1 10.
300-800	7.3(+11)	0	9*00*250	0.5 2.0
300-1000	1.0(+13)	0	500	0.5 2.0
300-800	2.8(+13)	0	16500*500	0.5 1.5
300	5.2(+ 8)	-	-	0.9 1.2
1500-2500	1.0(+11)	0	0*2500	0.3 3.2
700-1000	1.5(+14)	0	11900*1000	0.3 3.0

HYDROXYL FREE RADICAL + 1-PROPENE  
72 KER/PAR REACTION ORDER: 2.  
NOTE: ADDITION TO TERMINAL CARBON OF DOUBLE BOND IS PREFERABLY 95%  
H<sub>2</sub> + O<sub>3</sub> - OH + O<sub>2</sub> + O<sub>2</sub>  
HYDROPEROXYL FREE RADICAL + OZONE  
76 BAU/DRY REACTION ORDER: 2.  
-----

H<sub>2</sub> + H - O<sub>2</sub> + H<sub>2</sub>  
HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM  
72 BAU/DRY REACTION ORDER: 2.  
76 ENG  
-----

H<sub>2</sub> + H - H<sub>2</sub>O + O  
HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM  
74 LLG REACTION ORDER: 2.  
NOTE: ESTIMATED.  
-----

H<sub>2</sub> + H - OH + OH  
HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM  
72 BAU/DRY REACTION ORDER: 2.  
76 ENG  
-----

H<sub>2</sub> + H - H<sub>2</sub>O + O  
HYDROPEROXYL FREE RADICAL + HYDROGEN ATOM  
76 ENG  
-----

H<sub>2</sub> + H<sub>2</sub> - H<sub>2</sub>O<sub>2</sub> + H  
HYDROPEROXYL FREE RADICAL + HYDROGEN MOLECULE  
72 BAU/DRY REACTION ORDER: 2.  
-----

H<sub>2</sub> + H<sub>2</sub> - H<sub>2</sub>O<sub>2</sub> + O<sub>2</sub>  
HYDROPEROXYL FREE RADICAL  
74 LLG REACTION ORDER: 2.  
NOTE: ESTIMATED. K FACTORS ARE LARGER AT 1-300K.  
-----

H<sub>2</sub> + H<sub>2</sub>O - H<sub>2</sub>O<sub>2</sub> + OH  
HYDROPEROXYL FREE RADICAL + WATER  
72 BAU/DRY REACTION ORDER: 2.  
-----

H<sub>2</sub> + SO<sub>2</sub> - OH + SO<sub>3</sub>  
HYDROPEROXYL FREE RADICAL + SULFUR DIOXIDE  
74 LLG REACTION ORDER: 2.  
-----

H<sub>2</sub> + N - O<sub>2</sub> + NH  
HYDROPEROXYL FREE RADICAL + NITROGEN ATOM  
76 ENG REACTION ORDER: 2.  
-----

H<sub>2</sub> + CO - OH + CO<sub>2</sub>  
HYDROPEROXYL FREE RADICAL + CARBON MONOXIDE  
76 BAU/DRY REACTION ORDER: 2.  
-----

H<sub>2</sub> + CH - O<sub>2</sub> + CH<sub>2</sub>



Chemical Reactions	T/K	A	B	E/R (in °K)	k factors f	k factors F
<p>HYDROPEROXYL FREE RADICAL AND METHYLIDYNE FREE RADICAL REACTION ORDER: 2. -----</p> <p><math>H_2O_2 + CH_3 \rightarrow CH_3 + \cdot CH_3</math> 76 ENG</p>	1500-2500	1.0(+10)	0.5	7550±2500	0.3	3.2
<p>HYDROPEROXYL FREE RADICAL AND METHYLIDYNE FREE RADICAL REACTION ORDER: 2. -----</p> <p><math>H_2O_2 + CH_3 \rightarrow \cdot CH_3 + CH_4</math> 76 ENG</p>	1500-2500	5.0(+11)	0.5	3000±2500	0.3	3.2
<p>HYDROPEROXYL FREE RADICAL AND METHYL FREE RADICAL REACTION ORDER: 2. -----</p> <p><math>H_2O_2 + \cdot CH_3 \rightarrow \cdot CH_3 + HCHO</math> 76 ENG</p>	1500-2500	1.0(+11)	0.5	3000±2500	0.3	3.2
<p>HYDROPEROXYL FREE RADICAL + METHYL, <math>CH_3^{\cdot}</math>, FREE RADICAL REACTION ORDER: 2. -----</p> <p><math>H_2O_2 + \cdot CH_3 \rightarrow \cdot CH_3 + HCHO</math> 76 ENG</p> <p>NOTE: k ESTIMATED. -----</p>	1500-2500	1.0(+14)	0	1500±1500		
<p>HYDROPEROXYL FREE RADICAL + FORMALDEHYDE REACTION ORDER: 2. 74 IIC</p> <p>NOTE: k FACTORS ARE: f = 0.1; F = 10. AT 300 K. -----</p>	300-800	1.0(+12)	0	4000	0.7	1.5
<p>HYDROPEROXYL FREE RADICAL + ETHENE REACTION ORDER: 2. 74 IIC</p> <p>NOTE: RATIO DATA VERSUS <math>k_{ref}</math> FOR <math>H_2O_2 + C_2H_4 \rightarrow C_2H_5 + C_2H_5O_2</math>. k FACTORS MIGHT BE HIGHER. -----</p>	300	1.0(+7)	-	-	0.1	10.
<p>HYDROPEROXYL RADICAL + ETHANE REACTION ORDER: 2. 74 IIC</p> <p>NOTE: E ESTIMATED. UPPER LIMIT RECOMMENDED. <math>k_{ref}</math> IS FOR <math>H_2O_2 + C_2H_6 \rightarrow C_2H_5 + C_2H_5O_2</math>. -----</p>	300-1000	1.0(+12)	0	7000	0.1	10.
<p>HYDROPEROXYL FREE RADICAL + PROPANE REACTION ORDER: 2. 74 IIC</p> <p>NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS <math>k_{ref}</math> FOR <math>H_2O_2 + H_2O_2 \rightarrow H_2O_2 + \cdot O_2</math> -----</p>	300-1000	2.0(+11)	0	5300	0.1	10.
<p>HYDROPEROXYL FREE RADICAL + 1-PROPENE, 2-METHYL- REACTION ORDER: 2. 74 IIC</p> <p>NOTE: SUGGESTED k VALUE. -----</p>	300	1.0(+8)	-	-	0.1	10.
<p>HYDROPEROXYL FREE RADICAL + BUTANE REACTION ORDER: 2. 74 IIC</p> <p>NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS <math>k_{ref}</math> FOR <math>H_2O_2 + H_2O_2 \rightarrow H_2O_2 + \cdot O_2</math> -----</p>	300-1000	5.0(+11)	0	5285	0.1	10.
<p>HYDROPEROXYL FREE RADICAL + (CH<sub>3</sub>)<sub>3</sub>C. REACTION ORDER: 2. 74 IIC</p>	300-1000	1.0(+11)	0	3500	0.1	10.

## CHEMICAL REACTIONS

NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS  $k_{ref}$   
FOR  $H_2 + H_2 \rightarrow H_2^{\delta_2} + \delta_2$

$H_2^{\delta_2} + M \rightarrow H + \delta_2 + M$   
HYDROPEROXYL FREE RADICAL  
72 HAU/DRY REACTION ORDER: 2.  
NOTE: M = Ar, OR He.  $k_1 = k_{k-1}$

$H_2^{\delta_2} + \delta \rightarrow \delta H + \delta H$   
WATER + OXYGEN ATOM  
72 HAU/DRY REACTION ORDER: 2.

$H_2^{\delta_2} + H \rightarrow H_2 + \delta H$   
WATER + HYDROGEN ATOM  
72 HAU/DRY REACTION ORDER: 2.  
NOTE: GIVEN  $k$  FACTORS ARE FOR HIGH T'S.

$H_2^{\delta_2} + H_2^{\delta_2} \rightarrow \delta H + H_2^{\delta_2}$   
WATER + HYDROPEROXYL FREE RADICAL  
72 HAU/DRY REACTION ORDER: 2.

$H_2^{\delta_2} + NH \rightarrow H_2 + HNG$   
WATER + IMIDGEN FREE RADICAL  
76 ENG REACTION ORDER: 2.

$H_2^{\delta_2} + CH_3 \rightarrow \delta H + CH_4$   
WATER + METHYL FREE RADICAL  
76 KEI/PAR REACTION ORDER: 2.  
NOTE: TENTATIVE  $k$  VALUE.

$H_2^{\delta_2} + M \rightarrow H + \delta H + M$   
WATER  
72 HAU/DRY REACTION ORDER: 2. M:  $H_2^{\delta_2}$

NOTE: M = Ar:  $H_2^{\delta_2}(1.0)$ .  $k_1 = k_{k-1}$   
Ar(0.06) M: Ar  
 $N_2(0.16)$  M:  $N_2$

$H_2^{\delta_2} + H \rightarrow H_2 + H_2$   
HYDROGEN PEROXIDE + HYDROGEN ATOM  
72 HAU/DRY REACTION ORDER: 2.

$H_2^{\delta_2} + \delta H \rightarrow H_2 + H_2^{\delta_2}$   
HYDROGEN PEROXIDE + HYDROXYL FREE RADICAL  
72 HAU/DRY REACTION ORDER: 2.

$H_2^{\delta_2} + M \rightarrow \delta H + \delta H + M$   
HYDROGEN PEROXIDE  
72 HAU/DRY REACTION ORDER: 2. M:  $N_2$   
NOTE:  $k$  FACTORS CHANGING TO:  $f = 0.5$ ;  $F = 2.0$  AT 1500K.

$S + \delta_2 \rightarrow S\delta + \delta$

T/K	A	B	E/R (in °K)	k factors 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 °K)	k factors f	k factors 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 REACTION ORDER: 2. -----					
76 HAU/DRY					
S + H <sub>2</sub> → SH + H					
SULFUR ATOM + HYDROGEN MOLECULE REACTION ORDER: 2. -----					
76 HAU/DRY					
NOTE: k <sub>1</sub> = k <sub>k-1</sub>					
75 BEN/GOL					
S + OH → SO + H					
SULFUR ATOM + HYDROXYL FREE RADICAL REACTION ORDER: 2. -----					
75 BEN/GOL					
S + OH → SH + O					
SULFUR ATOM + HYDROXYL FREE RADICAL REACTION ORDER: 2. -----					
75 BEN/GOL					
S + S <sub>2</sub> → S <sub>2</sub> + S					
SULFUR ATOM + SULFUR DIMER REACTION ORDER: 2. -----					
75 BEN/GOL					
S + SO → S <sub>2</sub> + O					
SULFUR ATOM + SULFUR MONOXIDE REACTION ORDER: 2. -----					
75 BEN/GOL					
S + SO → SO + S					
SULFUR ATOM + SULFUR MONOXIDE REACTION ORDER: 2. -----					
75 BEN/GOL					
S + SH → S <sub>2</sub> + H					
SULFUR ATOM + MERCAPTO FREE RADICAL REACTION ORDER: 2. -----					
75 BEN/GOL					
S + SH → SH + S					
SULFUR ATOM + MERCAPTO FREE RADICAL REACTION ORDER: 2. -----					
75 BEN/GOL					
S + N <sub>2</sub> → NS + N					
SULFUR ATOM + NITROGEN MOLECULE REACTION ORDER: 2. -----					
75 BEN/GOL					
S + NO → SO + N					
SULFUR ATOM + NITROGEN OXIDE (NO) REACTION ORDER: 2. -----					
75 BEN/GOL					
S + NO → NS + O					
SULFUR ATOM + NITROGEN OXIDE (NO) REACTION ORDER: 2. -----					
75 BEN/GOL					
S + NH → SH + N					
SULFUR ATOM + IMIDGEN FREE RADICAL REACTION ORDER: 2. -----					
75 BEN/GOL					

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
S * NH ~ NS * H SULFUR ATOM * HYDROGEN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. -----		6.3(*11)	0.5	0	
S * NS ~ S <sub>2</sub> * N SULFUR ATOM * NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2. -----		2.0(*11)	0.5	10870	
S * NS ~ NS * S SULFUR ATOM * NITROGEN SULFIDE(NS) 75 BEN/GOL REACTION ORDER: 2. -----		6.3(*11)	0.5	0	
S * CG ~ SC * C SULFUR ATOM * CARBON MONOXIDE 75 BEN/GOL REACTION ORDER: 2. -----		4.0(*12)	0.5	66530	
S * CG ~ CS * G 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 <sub>2</sub> * 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 <sub>2</sub> * M SULFUR ATOM * CARBON MONOSULFIDE FREE RADICAL 76 HAU/DRY REACTION ORDER: 3. NOTE: K <sub>1</sub> = K <sub>k-1</sub>	1800-3700	8.7(*13)	0	4370	0.5 1.5
S * CS <sub>2</sub> ~ S <sub>2</sub> * CS SULFUR ATOM * CARBON DISULFIDE 76 HAU/DRY REACTION ORDER: 2. -----	298	3.9(*11)	-	-	0.5 1.5
S * CGS ~ S <sub>2</sub> * CG SULFUR ATOM * CARBON OXIDE 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
S • CN → CS • N SULFUR ATOM • CYANOGEN FREE RADICAL 75 HEN/GDL REACTION ORDER: 2. -----			6.3(+11)	0.5	0	
S • C <sub>2</sub> → CS • C SULFUR ATOM • CARBON LIMER 75 HEN/GDL REACTION ORDER: 2. -----			6.3(+11)	0.5	0	
S • CH=CH → CI-CH=CBS SULFUR ATOM • ETHYNE 72 KER/PAR REACTION ORDER: 2. -----		298	1.7(+11)	-	-	
S • CH <sub>2</sub> =CH <sub>2</sub> → cy-CH <sub>2</sub> CH <sub>2</sub> S SULFUR ATOM • ETHENE 72 KER/PAR REACTION ORDER: 2. -----		298	8.1(+11)	-	-	
S • CH <sub>3</sub> C=CH → cy-(CH <sub>3</sub> )C=CHS SULFUR ATOM • 1-PROPENE 72 KER/PAR REACTION ORDER: 2. -----		298	1.1(+12)	-	-	
S • CH <sub>3</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> )CHCH <sub>2</sub> S SULFUR ATOM • 1-PROPENE 72 KER/PAR REACTION ORDER: 2. -----		298	5.8(+12)	-	-	
NOTE: k <sub>ref</sub> : S • CH <sub>2</sub> =CH <sub>2</sub> -----		298	-	-	-	
S*(1D) • CH <sub>3</sub> CH=CH <sub>2</sub> → CY-(CH <sub>3</sub> )CHCH <sub>2</sub> S SULFUR ATOM (1D) • 1-PROPENE 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 1.7		300	-	-	-	
NOTE: k <sub>ref</sub> : S*(1D) • CH <sub>2</sub> =CH <sub>2</sub> -----						
S • CH <sub>3</sub> C≡CCH <sub>3</sub> → cy-(CH <sub>3</sub> )C≡C(CH <sub>3</sub> )S SULFUR ATOM • 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. -----		298	1.9(+13)	-	-	
S • CB <sub>2</sub> =CCH=CH <sub>2</sub> → cy-(CH <sub>2</sub> =CH)CHCH <sub>2</sub> S SULFUR ATOM • 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. -----		298	6.0(+13)	-	-	
S • CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → cy-(CH <sub>3</sub> CH <sub>2</sub> )CHCH <sub>2</sub> S SULFUR ATOM • 1-BUTENE 72 KER/PAR REACTION ORDER: 2. -----		298	9.3(+12)	-	-	
NOTE: k <sub>ref</sub> : S • CH <sub>2</sub> =CH <sub>2</sub> -----		298	-	-	-	
S • cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → cy-(CH <sub>3</sub> )CHCH(CH <sub>3</sub> )S SULFUR ATOM • cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. -----		298	1.4(+13)	-	-	
NOTE: k <sub>ref</sub> : S • CH <sub>2</sub> =CH <sub>2</sub> -----		298	-	-	-	
S • trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → cy-(CH <sub>3</sub> )CHCH(CH <sub>3</sub> )S SULFUR ATOM • trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. -----		298	-	-	-	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
SULFUR ATOM + trans-2-BUTENE 72 KEF/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 20.0 NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>	298 298	1.4(+13) -	-	-	.
S + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> S SULFUR ATOM + 1-PENTENE, 2-METHYL- 72 KEF/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 50.0 NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>	298 298	4.0(+13) -	-	-	.
S*( <sup>1</sup> D) + (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH <sub>2</sub> S SULFUR ATOM ( <sup>1</sup> D) + 1-PENTENE, 2-METHYL- 72 KEF/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5 NOTE: k <sub>ref</sub> : S*( <sup>1</sup> D) + CH <sub>2</sub> =CH <sub>2</sub>	300	-	-	-	.
S + CH <sub>3</sub> (CH <sub>2</sub> ) <sub>2</sub> CH=CH <sub>2</sub> → cy-CH <sub>3</sub> (CH <sub>2</sub> )CCH <sub>2</sub> S SULFUR ATOM + 1-PENTENE 72 KEF/PAR REACTION ORDER: 2.	298	8.1(+12)	-	-	.
S + CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> → cy-CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )CH <sub>2</sub> S SULFUR ATOM + 1-BUTENE, 2-METHYL- 72 KEF/PAR REACTION ORDER: 2.	298	7.4(+13)	-	-	.
S + (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) → cy-(CH <sub>3</sub> ) <sub>2</sub> CCH(CH <sub>3</sub> )S SULFUR ATOM + 2-BUTENE, 2-METHYL- 72 KEF/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 56. NOTE: k <sub>ref</sub> : S + CH <sub>2</sub> =CH <sub>2</sub>	298 298	6.5(+13) -	-	-	.
S <sub>2</sub> + O → S + SO SULFUR DIMER + OXYGEN ATOM 75 BEN/GCL REACTION ORDER: 2.	298	8.5(+13)	-	-	.
S <sub>2</sub> + H → S + SH SULFUR DIMER + HYDROGEN ATOM 75 BEN/GCL REACTION ORDER: 2.	0	6.3(+11)	0.5	0	.
S <sub>2</sub> + S → S + S <sub>2</sub> SULFUR DIMER + SULFUR ATOM 75 BEN/GCL REACTION ORDER: 2.	8355	7.9(+12)	0.5	0	.
S <sub>2</sub> + N → S + NS SULFUR DIMER + NITROGEN ATOM 75 BEN/GCL REACTION ORDER: 2.	4000	6.3(+11)	0.5	0	.
S <sub>2</sub> + C → S + CS SULFUR DIMER + CARBON ATOM		6.3(+11)	0.5	4000	.

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

k factors f	E/R (in °K)	B	A	T/K	CHEMICAL REACTIONS
0.5	-	-	5.1(+15)	1660-212	NOTE: k <sub>1</sub> = k <sub>k-1</sub> ----- S <sub>2</sub> + H + M → HS <sub>2</sub> + M SULFUR DICHLORIDE + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 3. -----
0.9	-	-	5.2(+8)	300	S <sub>2</sub> + H <sub>2</sub> → S <sub>2</sub> + 2H SULFUR DICHLORIDE + HYDROPEROXYL FREE RADICAL 74 LLC REACTION ORDER: 2. NOTE: RATE DATA VERSUS k <sub>ref</sub> FOR REACTION H <sub>2</sub> + H <sub>2</sub> → H <sub>2</sub> C <sub>2</sub> + C <sub>2</sub> -----
0.5	4000	0.5	6.3(+11)		SH + O → S + OH MERCAPTO FREE RADICAL + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	0	0.5	6.3(+11)		SH + O → S + H MERCAPTO FREE RADICAL + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	-	-	1.5(+13)	298	SH + H → S + H <sub>2</sub> MERCAPTO FREE RADICAL + HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----
0.5	0	0.5	6.3(+11)		SH + H → H + SH MERCAPTO FREE RADICAL + HYDROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	0	0.5	6.3(+11)		SH + S → H + S <sub>2</sub> MERCAPTO FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	4000	0.5	6.3(+11)		SH + S → S + SH MERCAPTO FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	-	-	7.8(+12)	295	SH + SH → H <sub>2</sub> S + S MERCAPTO FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. -----
0.5	403	0.5	6.3(+11)		SH + N → H + NS MERCAPTO FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	9060	0.5	6.3(+11)		SH + N → S + NH MERCAPTO FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	0	0.5	6.3(+11)		SH + C → H + CS MERCAPTO FREE RADICAL + CARBON ATOM 75 BEN/GGL REACTION ORDER: 2. -----
0.5	0	0.5	6.3(+11)		SH + C → S + CH -----



## CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
MERCAPTO FREE RADICAL * CARBON ATOM 75 BEN/GGL REACTION ORDER: 2. ----- H <sub>2</sub> S * S <sub>2</sub> ~ H <sub>2</sub> O * S <sub>2</sub> HYDROGEN SULFIDE * S <sub>2</sub> 76 BAU/DRY REACTION ORDER: 2. -----	298	4.0(+11)	0.5	6090	0.1 10.
H <sub>2</sub> S * H ~ SH * H <sub>2</sub> HYDROGEN SULFIDE * HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----	190-470	7.8(+12)	0	860*50	0.5 1.5
H <sub>2</sub> S * OH ~ SH * H <sub>2</sub> O HYDROGEN SULFIDE * HYDROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. NOTE: K FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 900K. -----	298-900	6.3(+12)	0	200*150	0.7 1.3
H <sub>2</sub> S * CH <sub>3</sub> ~ SH * CH <sub>4</sub> 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 ~ NC * M NITROGEN ATOM * OXYGEN ATOM 73 BAU/DRY REACTION ORDER: 3. M: N <sub>2</sub> -----	200-400	6.4(+16)	-0.5	0	0.5 1.5
N * O <sub>2</sub> ~ NC * 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 ~ NH * M NITROGEN ATOM * HYDROGEN ATOM 76 ENG REACTION ORDER: 3. -----	1500-2500	2.5(+17)	-0.5	0*1000	
N * H <sub>2</sub> ~ NH * H NITROGEN ATOM * HYDROGEN MOLECULE 75 BEN/GGL REACTION ORDER: 2. -----	1500-2500	2.5(+12)	0.5	18700	
N * OH ~ NC * H NITROGEN ATOM * HYDROXYL FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----	1500-2500	6.3(+11)	0.5	0	
N * OH ~ NH * O NITROGEN ATOM * HYDROXYL FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. -----	1500-2500	1.3(+12)	0.5	17765	
N * OH * M ~ HNC * M NITROGEN ATOM * HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 3. -----	1500-2500	1.00(+15)	-0.5	0	
N * HO <sub>2</sub> ~ NH * O <sub>2</sub> 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
N + S <sub>2</sub> → 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 → N <sub>2</sub> + 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 + N <sub>2</sub> → N <sub>2</sub> + N NITROGEN ATOM + NITROGEN MOLECULE 75 BEN/GGL REACTION ORDER: 2.	----- ----- ----- -----		6.3(+11)	0.5	4000	
N + NO → N <sub>2</sub> + 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 + NO <sub>2</sub> → N <sub>2</sub> + O <sub>2</sub> NITROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	----- ----- ----- -----	1500-2500	1.0(+12)	0	0±1500	
N + NO <sub>2</sub> → NO + NO NITROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	----- ----- ----- -----	1500-2500	4.0(+12)	0	0±1500	0.2 5.0
N + NO <sub>2</sub> → N <sub>2</sub> + O NITROGEN ATOM + NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG REACTION ORDER: 2.	----- ----- ----- -----	1500-2500	5.0(+12)	0	0±1500	0.5 2.0

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
NITROGEN ATOM + NITROGEN OXIDE(N <sub>2</sub> O) 76 ENG REACTION ORDER: 2. -----	1500-2500	5.0(+8)	0	5000*2500	0.3	3.2
N + NH → N <sub>2</sub> + H						
NITROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/G6L REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
N + NH → NH + N						
NITROGEN ATOM + IMIDGEN FREE RADICAL 75 BEN/G6L REACTION ORDER: 2. -----	1500-2500	6.3(+11)	0.5	4000		
N + NH → H + N <sub>2</sub> O						
NITROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2. -----	1500-2500	5.0(+10)	0.5	1500*2500		
N + NH → NH + NO						
NITROGEN ATOM + NITROSYL HYDRIDE 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.5	1000*2500		
N + NS → N <sub>2</sub> + S						
NITROGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/G6L REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
N + NS → NS + N						
NITROGEN ATOM + NITROGEN SULFIDE(NS) 75 BEN/G6L REACTION ORDER: 2. -----		6.3(+11)	0.5	4000		
N + CO → NC + C						
NITROGEN ATOM + CARBON MONOXIDE 75 BEN/G6L REACTION ORDER: 2. -----		5.0(+12)	0.5	57300		
N + CO → CN + C						
NITROGEN ATOM + CARBON MONOXIDE 75 BEN/G6L REACTION ORDER: 2. -----		3.2(+12)	0.5	38800		
N + CO <sub>2</sub> → NO + CO						
NITROGEN ATOM + CARBON DIOXIDE 76 ENG REACTION ORDER: 2. -----	1500-2500	2.00(+11)	0.5	1500*10000	0.1	10.
N + CH → NH + C						
NITROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/G6L REACTION ORDER: 2. -----		1.0(+12)	0.5	6995		
N + CH → CN + H						
NITROGEN ATOM + METHYLIDYNE FREE RADICAL 75 BEN/G6L REACTION ORDER: 2. -----		6.3(+11)	0.5	0		
N + CH <sub>2</sub> → NH + CH						
NITROGEN ATOM + METHYLIDYNE FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	6.3(+11)	0.7	20400*2500	0.3	3.2
N + .CH <sub>3</sub> → C + HCN						
NITROGEN ATOM + FORMYL FREE RADICAL						



CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
N ♦ CH <sub>3</sub> C=CCH <sub>3</sub> → products NITROGEN ATOM ♦ 2-BUTYNE 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 12.0	320-550 435	1.9(+11) -	0 -	926 -	
NOTE: k <sub>ref</sub> : N ♦ CH=CH.	-----					
N ♦ CH <sub>2</sub> -C(CH <sub>3</sub> )=CH <sub>2</sub> → products NITROGEN ATOM ♦ 1,3-BUTADIENE 72 KER/PAR	----- REACTION ORDER: 2.	340	3.5(+10)	-	-	
N ♦ CH <sub>3</sub> CH <sub>2</sub> CH=CH <sub>2</sub> → products NITROGEN ATOM ♦ 1-BUTENE 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 3.4	320-550 435	1.6(+11) -	0 -	660 -	
NOTE: k <sub>ref</sub> : N ♦ CH <sub>2</sub> =CH <sub>2</sub> .	-----					
N ♦ cis-CH <sub>3</sub> CH=CHCH <sub>3</sub> → products NITROGEN ATOM ♦ cis-2-BUTENE 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 2.4	320-550 435	2.3(+11) -	0 -	995 -	
NOTE: k <sub>ref</sub> : N ♦ CH <sub>2</sub> =CH <sub>2</sub> .	-----					
N ♦ trans-CH <sub>3</sub> CH=CHCH <sub>3</sub> → products NITROGEN ATOM ♦ trans-2-BUTENE 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 3.0	320-550 435	3.4(+11) -	0 -	1055 -	
NOTE: k <sub>ref</sub> : N ♦ CH <sub>2</sub> =CH <sub>2</sub> .	-----					
N ♦ (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> → products NITROGEN ATOM ♦ 1-PROPENE, 2-METHYL- 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 4.1	320-550 435	7.8(+10) -	0 -	277 -	
NOTE: k <sub>ref</sub> : N ♦ CH <sub>2</sub> =CH <sub>2</sub> .	-----					
N ♦ CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C≡CH → products NITROGEN ATOM ♦ 1-PENTYNE 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 14.0	320-550 435	3.0(+11) -	0 -	1047 -	
NOTE: k <sub>ref</sub> : N ♦ CH=CH.	-----					
N ♦ (CH <sub>3</sub> ) <sub>2</sub> C=CHCH <sub>3</sub> → products NITROGEN ATOM ♦ 2-BUTENE, 2-METHYL- 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5	320-550 435	5.3(+10) -	0 -	433 -	
NOTE: k <sub>ref</sub> : N ♦ CH <sub>2</sub> =CH <sub>2</sub> .	-----					
N ♦ CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> C≡CCH <sub>3</sub> → products NITROGEN ATOM ♦ 1-HEXYNE 72 KER/PAR	----- REACTION ORDER: 2. k/k <sub>ref</sub> : 14.0	320-550 435	4.6(+11) -	0 -	1233 -	
NOTE: k <sub>ref</sub> : N ♦ CH=CH.	-----					

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
N * CH <sub>3</sub> CH <sub>2</sub> C#CCH <sub>2</sub> CH <sub>3</sub> → products NITROGEN ATOM * 3-HEXYNE 72 KER/PAR  NOTE: k <sub>ref</sub> : N * CH#CH	REACTION ORDER: 2. k/k <sub>ref</sub> : 14.0	0	1102	
N * (CH <sub>3</sub> ) <sub>2</sub> C=C(CH <sub>3</sub> ) <sub>2</sub> → products NITROGEN ATOM * 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR  NOTE: k <sub>ref</sub> : N * CH <sub>2</sub> =CH <sub>2</sub>	REACTION ORDER: 2. k/k <sub>ref</sub> : 3.5	0	690	
N <sub>2</sub> * O → N * NO NITROGEN MOLECULE * OXYGEN ATOM 73 BAU/DRY  NOTE: k <sub>1</sub> = k <sub>k-1</sub>	REACTION ORDER: 2.	0	38000*150	0.5 2.0
N <sub>2</sub> * O * M → N <sub>2</sub> O * M NITROGEN MOLECULE * OXYGEN ATOM 73 BAU/DRY	REACTION ORDER: 3. M: Ar	0	10400*1500	0.7 1.5
N <sub>2</sub> * O <sub>2</sub> → N <sub>2</sub> O * O NITROGEN MOLECULE * OXYGEN MOLECULE 73 BAU/DRY  NOTE: k <sub>1</sub> = k <sub>k-1</sub>	REACTION ORDER: 2.	0	55200*2000	0.4 2.5
N <sub>2</sub> * H → N * NH NITROGEN MOLECULE * HYDROGEN ATOM 75 BEN/GEL	REACTION ORDER: 2.	0.5	75945	
N <sub>2</sub> * S → N * NS NITROGEN MOLECULE * SULFUR ATOM 75 BEN/GEL	REACTION ORDER: 2.	0.5	55200	
N <sub>2</sub> * N → N * N <sub>2</sub> NITROGEN MOLECULE * NITROGEN ATOM 75 BEN/GEL	REACTION ORDER: 2.	0.5	4000	
N <sub>2</sub> * C → N * CN NITROGEN MOLECULE * CARBON ATOM 75 BEN/GEL	REACTION ORDER: 2.	0.5	22750	
N <sub>2</sub> * CH → N * HCN NITROGEN MOLECULE * METHYLIDYNE FREE RADICAL 76 ENG  NOTE: REVISED ESTIMATE.	REACTION ORDER: 2.	0	9560	
N <sub>2</sub> * CH → NH * CN NITROGEN MOLECULE * METHYLIDYNE FREE RADICAL 76 ENG  NOTE: k ESTIMATED.	REACTION ORDER: 2.	0	46300*10000	
N <sub>2</sub> * CH <sub>2</sub> → NH * HCN	REACTION ORDER: 2.	0		

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

## CHEMICAL REACTIONS

	T/K	A	B	E/R (in °K)	k factors f
75 BEN/GEL NØ * H - N * ØH NITRØGEN ØXIDE(NØ) * HYDRØGEN ATØM 75 BEN/GEL REACTION ØRDER: 2.		5.0(*12)	0.5	38200	
75 BEN/GEL NØ * H * M - HØØ * M NITRØGEN ØXIDE(NØ) * HYDRØGEN ATØM 75 BEN/GEL REACTION ØRDER: 2.		2.5(*12)	0.5	24460	
76 ENG NØ * S - Ø * NS NITRØGEN ØXIDE(NØ) * SULFUR ATØM 76 ENG REACTION ØRDER: 2.	230-700 1500-2500	5.4(*15) 5.0(*15)	0 0	-300*100 -300*150	0.5 1.5 0.5 2.0
75 BEN/GEL NØ * S - N * SØ NITRØGEN ØXIDE(NØ) * SULFUR ATØM 75 BEN/GEL REACTION ØRDER: 2.		1.0(*12)	0.5	17465	
75 BEN/GEL NØ * N - e * N2 NITRØGEN ØXIDE(NØ) * NITRØGEN ATØM 75 BEN/GEL REACTION ØRDER: 2.		4.0(*11)	0.5	17260	
73 HAU/DRY NØ * N - N * NØ NITRØGEN ØXIDE(NØ) * NITRØGEN ATØM 73 HAU/DRY REACTION ØRDER: 2.	300-5000	1.6(*13)	-	-	0.8 1.2
72 KØN NØ * N - N2 * Ø2 NITRØGEN ØXIDE(NØ2) * ØXYGEN MØLECULE 72 KØN REACTION ØRDER: 2.	1370-4300	6.3(*11)	0.5	4000	
73 HAU/DRY NØ * NØ - N2Ø * Ø NITRØGEN ØXIDE(NØ) * ØXYGEN MØLECULE 73 HAU/DRY REACTION ØRDER: 2.	1200-2000	1.3(*12)	0	38060*720	0.7 1.5
73 HAU/DRY NØ * NØ * Ø2 - NØ2 * NØ2 NITRØGEN ØXIDE(NØ) * ØXYGEN MØLECULE 73 HAU/DRY REACTION ØRDER: 3.	273-660	1.3(*14)	0	32100*1500	0.5 2.0
76 ENG NØ * NØ2 - N2Ø * Ø2 NITRØGEN ØXIDE(NØ) * NITRØGEN ØXIDE(NØ2) 76 ENG REACTION ØRDER: 2.	1500-2500	1.2(* 9)	0	-530*100	0.5 1.5
73 HAU/DRY NØ * NØ2 * Ø2 - NØ2 * NØ3 NITRØGEN ØXIDE(NØ) * NITRØGEN ØXIDE(NØ2) * ØXYGEN MØLECULE 73 HAU/DRY REACTION ØRDER: 3.	300-500	1.0 (*12)	0	30200	0.01 100.
72 KØN NØ * NØ3 - NØ2 * NØ2 NITRØGEN ØXIDE(NØ) * NITRØGEN ØXIDE(NØ3) 72 KØN REACTION ØRDER: 2.	298-547	2.9(* 7)	0	-400*500	0.4 2.5
		1.5(*14)	0	1163*115	0.7 1.4

NOTE: k FACTORS CHANGING TO: F = 0.5; F = 2.0  
ABOVE 2000K



CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
<p>-----</p> <p><math>\text{NO} + \text{N}_2\text{O} \rightarrow \text{NO}_2 + \text{N}_2</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + NITROGEN OXIDE(<math>\text{N}_2\text{O}</math>)            76 ENG            REACTION ORDER: 2.</p> <p>-----</p>	1500-2500	2.0(+14)	0	25000	0.1 1.0
<p>-----</p> <p><math>\text{NO} + \text{HNO} \rightarrow \text{N}_2\text{O} + \text{OH}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + NITROSYL HYDROXIDE            76 ENG            REACTION ORDER: 2.</p> <p>-----</p>	1500-2500	2.0(+12)	0	13000±2500	0.5 2.0
<p>-----</p> <p><math>\text{NO} + \text{C} \rightarrow \text{CO} + \text{CN}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + CARBON ATOM            75 BEN/GOL            REACTION ORDER: 2.</p> <p>-----</p>		6.3(+11)	0.5	0	
<p>-----</p> <p><math>\text{NO} + \text{C} \rightarrow \text{N} + \text{CO}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + CARBON ATOM            75 BEN/GOL            REACTION ORDER: 2.</p> <p>-----</p>		6.3(+11)	0.5	4000	
<p>-----</p> <p><math>\text{NO} + \text{CH} \rightarrow \text{C} + \text{HCN}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + METHYLIDYNE FREE RADICAL            76 ENG            REACTION ORDER: 2.</p> <p>NOTE: ESTIMATED.</p> <p>-----</p>	1500-2500	2.0(+12)	0	0±1000	
<p>-----</p> <p><math>\text{NO} + \text{CH} \rightarrow \text{N} + \cdot\text{CHO}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + METHYLIDYNE FREE RADICAL            76 ENG            REACTION ORDER: 2.</p> <p>NOTE: ESTIMATED.</p> <p>-----</p>	1500-2500	1.6(+13)	0	5000±3000	
<p>-----</p> <p><math>\text{NO} + \text{CH}_2 \rightarrow \text{N} + \text{HCHO}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + METHYLENE FREE RADICAL            76 ENG            REACTION ORDER: 2.</p> <p>NOTE: ESTIMATED.</p> <p>-----</p>	1500-2500	2.0(+12)	0	3500±2000	
<p>-----</p> <p><math>\text{NO} + \cdot\text{CHO} \rightarrow \text{HNO} + \text{CO}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + FORMYL FREE RADICAL            76 ENG            REACTION ORDER: 2.</p> <p>-----</p>	1500-2500	2.0(+11)	0.5	1000±2500	0.3 3.2
<p>-----</p> <p><math>\text{NO} + \text{CN} \rightarrow \text{N}_2 + \text{CO}</math>            NITROGEN OXIDE(<math>\text{NO}</math>) + CYANOGEN FREE RADICAL            76 ENG            REACTION ORDER: 2.</p> <p>-----</p>	1500-2500	3.2(+11)	0	0±2500	0.3 3.2
<p>-----</p> <p><math>\text{NO} + \text{M} \rightarrow \text{N} + \text{O} + \text{M}</math>            NITROGEN OXIDE(<math>\text{NO}</math>)            76 ENG            REACTION ORDER: 2.</p> <p>NOTE: M = Ar, CR, N<sub>2</sub> OR O<sub>2</sub> GIVEN WITH CAUTION.            72 ION</p> <p>-----</p>	1500-2500	4.0(+20)	-1.5	7500±2500	0.3 3.2
<p>-----</p> <p><math>\text{NO}_2 + \text{O} \rightarrow \text{NO} + \text{O}_2</math>            NITROGEN OXIDE(<math>\text{NO}_2</math>) + OXYGEN ATOM            73 BAU/DRY            76 ENG            REACTION ORDER: 2.</p> <p>-----</p>	3000-8000	6.00(+2)	-1.5	75500	
<p>-----</p> <p><math>\text{NO}_2 + \text{O} + \text{M} \rightarrow \text{NO}_3 + \text{M}</math>            NITROGEN OXIDE(<math>\text{NO}_2</math>) + OXYGEN ATOM            76 ENG            REACTION ORDER: 2.</p> <p>-----</p>	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 HAU/DRY NOTE: LIMITING HIGH PRESSURE k REACTION ORDER: 2. M: N <sub>2</sub> REACTION ORDER: 3. k <sub>0</sub> (LOW PRESSURE).		295	1.1(+13)	-	-	0.4 2.5
N <sub>2</sub> + O <sub>3</sub> → N <sub>2</sub> O + O <sub>2</sub> NITROGEN OXIDE(N <sub>2</sub> O) + OZONE		295	2.3(+16)	-	-	0.4 2.5
73 HAU/DRY REACTION ORDER: 2.		286-302	5.9(+12)	0	3500	0.5 2.0
N <sub>2</sub> + H → N <sub>2</sub> O + OH NITROGEN OXIDE(N <sub>2</sub> O) + HYDROGEN ATOM		298-630	3.5(+14)	0	740±500	0.5 1.5
73 HAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING 10: f = 0.5; F = 2.0 AT 633K.		1500-2500	3.2(+14)	0	750±500	0.5 2.0
76 ENG		300	5.0(+17)	-	-	0.4 1.6
N <sub>2</sub> + OH + M → HN <sub>2</sub> O + M NITROGEN OXIDE(N <sub>2</sub> O) + HYDROXYL FREE RADICAL		1500-2500	5.0(+12)	0	0±1500	0.5 2.0
73 HAU/DRY REACTION ORDER: 3. M: He		1500-2500	1.0(+12)	0	0±1500	0.5 2.0
N <sub>2</sub> + N → N <sub>2</sub> O NITROGEN OXIDE(N <sub>2</sub> O) + NITROGEN ATOM		1500-2500	4.0(+12)	0	0±1500	0.2 5.0
76 ENG		1500-2500	1.0(+12)	0	30200	0.01 100
N <sub>2</sub> + N → O <sub>2</sub> + N <sub>2</sub> NITROGEN OXIDE(N <sub>2</sub> O) + NITROGEN ATOM		300-500	2.9(+7)	0	-400±500	0.4 2.5
76 ENG		600-2000	2.0(+12)	0	13500±100	0.7 1.3
N <sub>2</sub> + N <sub>2</sub> → N <sub>2</sub> O + N <sub>2</sub> O NITROGEN OXIDE(N <sub>2</sub> O) + NITROGEN OXIDE(N <sub>2</sub> O) + OXYGEN MOLECULE		250-350	1.1(+13)	0	-1040	0.7 1.3
73 HAU/DRY REACTION ORDER: 3. NOTE: k FACTORS INCREASING SLIGHTLY ABOVE 1000K.						
N <sub>2</sub> + N <sub>2</sub> + M → N <sub>2</sub> O + N <sub>2</sub> O + M NITROGEN OXIDE(N <sub>2</sub> O)						
73 HAU/DRY REACTION ORDER: 3. M: N <sub>2</sub> NOTE: CORRECTED k VALUE (PERSONAL COMMUNICATION FROM DR. FAULCHER TO DR. BAMPSON). k <sub>1</sub> = k <sub>k-1</sub>						
N <sub>2</sub> + N <sub>2</sub> → N <sub>2</sub> O + N <sub>2</sub> O + O <sub>2</sub> NITROGEN OXIDE(N <sub>2</sub> O) + NITROGEN OXIDE(N <sub>2</sub> O)						

## 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	1.0(+14)	0	14000±1500	0.5 2.0
900-2300	3.6(+13)	0	13700	

73 BAU/DRY REACTION ORDER: 2.

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 $\text{NO}_2 \cdot \text{NO}_3 \cdot \text{M} \rightarrow \text{N}_2\text{O}_5 \cdot \text{M}$ 
 $\text{NITROGEN OXIDE}(\text{NO}_2) \cdot \text{NITROGEN OXIDE}(\text{NO}_3)$ 

73 BAU/DRY

REACTION ORDER: 2.

NOTE: LIMITING HIGH PRESSURE K

M IS A  $\text{N}_2\text{O}_5 \cdot \text{NO}$  MIXTURE
 $\text{K}_0(\text{LOW PRESSURE}). \text{M IS A } \text{N}_2\text{O}_5 \cdot \text{NO MIXTURE}.$ 

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 $\text{NO}_2 \cdot \text{NH} \rightarrow \text{NO} \cdot \text{HNO}$ 
 $\text{NITROGEN OXIDE}(\text{NO}_2) \cdot \text{IMIDGEN FREE RADICAL}$ 

76 ENG

REACTION ORDER: 2.

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 $\text{NO}_2 \cdot \text{CO} \rightarrow \text{NO} \cdot \text{CO}_2$ 
 $\text{NITROGEN OXIDE}(\text{NO}_2) \cdot \text{CARBON MONOXIDE}$ 

72 ION

REACTION ORDER: 2.

76 ENG

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 $\text{NO}_2 \cdot \text{M} \rightarrow \text{NO} \cdot \text{O} \cdot \text{M}$ 
 $\text{NITROGEN OXIDE}(\text{NO}_2)$ 

73 BAU/DRY

REACTION ORDER: 2. M: Ar

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 $\text{NO}_3 \cdot \text{NO} \rightarrow \text{NO}_2 \cdot \text{NO}_2$ 
 $\text{NITROGEN OXIDE}(\text{NO}_3) \cdot \text{NITROGEN OXIDE}(\text{NO})$ 

72 ION

REACTION ORDER: 2.

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 $\text{NO}_3 \cdot \text{NO}_2 \rightarrow \text{NO}_2 \cdot \text{NO} \cdot \text{O}_2$ 
 $\text{NITROGEN OXIDE}(\text{NO}_3) \cdot \text{NITROGEN OXIDE}(\text{NO}_2)$ 

73 BAU/DRY

REACTION ORDER: 2.

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 $\text{NO}_3 \cdot \text{NO}_2 \cdot \text{M} \rightarrow \text{N}_2\text{O}_5 \cdot \text{M}$ 
 $\text{NITROGEN OXIDE}(\text{NO}_3) \cdot \text{NITROGEN OXIDE}(\text{NO}_2)$ 

72 BAU/DRY

REACTION ORDER: 2.

NOTE: LIMITING HIGH-PRESSURE K. M IS A  $\text{N}_2\text{O}_5 \cdot \text{NO}$  MIXTURE.k<sub>1</sub> = k<sub>-1</sub>

REACTION ORDER: 3.

 $\text{K}_0(\text{LOW PRESSURE}). \text{M IS A } \text{N}_2\text{O}_5 \cdot \text{NO MIXTURE}.$ 

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 $\text{NO}_3 \cdot \text{M} \rightarrow \text{NO} \cdot \text{O}_2 \cdot \text{M}$ 
 $\text{NITROGEN OXIDE}(\text{NO}_3)$ 

72 ION

REACTION ORDER: 2. M: NO<sub>2</sub>

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 $\text{N}_2\text{O} \cdot \text{O} \rightarrow \text{N}_2 \cdot \text{O}_2$ 
 $\text{NITROGEN OXIDE}(\text{N}_2\text{O}) \cdot \text{OXYGEN ATOM}$ 

73 BAU/DRY

REACTION ORDER: 2.

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 $\text{N}_2\text{O} \cdot \text{O} \rightarrow \text{NO} \cdot \text{NO}$ 
 $\text{NITROGEN OXIDE}(\text{N}_2\text{O}) \cdot \text{OXYGEN ATOM}$ 

73 BAU/DRY

REACTION ORDER: 2.

72 ION

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 $\text{N}_2\text{O} \cdot \text{H} \rightarrow \text{N}_2 \cdot \text{OH}$

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

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. -----						
NH ♦ H → N ♦ H <sub>2</sub> IMIDGEN FREE RADICAL ♦ HYDROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----						
NH ♦ OH → N ♦ H <sub>2</sub> 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 <sub>2</sub> O → HNO ♦ H <sub>2</sub> 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. -----						
NH ♦ S → N ♦ SH IMIDGEN FREE RADICAL ♦ SULFUR ATOM 75 BEN/GOL	REACTION ORDER: 2. -----						
NH ♦ N → H ♦ N <sub>2</sub> IMIDGEN FREE RADICAL ♦ NITROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----						
NH ♦ N → N ♦ NH IMIDGEN FREE RADICAL ♦ NITROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----						
NH ♦ NO <sub>2</sub> → HNO ♦ NO IMIDGEN FREE RADICAL ♦ NITROGEN OXIDE(NO <sub>2</sub> ) 76 ENG	REACTION ORDER: 2. -----	1500-2500	2.0(♦11)	0.5	2500♦2500	0.3	3.2
NH ♦ NH → H <sub>2</sub> ♦ N <sub>2</sub> 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. -----						
NH ♦ C → N ♦ CH IMIDGEN FREE RADICAL ♦ CARBON ATOM 75 BEN/GOL	REACTION ORDER: 2. -----						
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
<p>-----  <math>\text{NH}_2 \cdot \text{H} \cdot \text{M} \rightarrow \text{NH}_3 \cdot \text{M}</math>            AMIDOGEN FREE RADICAL + HYDROGEN ATOM            73 BAU/DRY            NOTE: <math>k_1 = k_{k-1}</math>            -----</p>	2000-3000	4.8(+14)	0	-8300±2500	0.5 2.0
<p>-----  <math>\text{NH}_3 \cdot \text{O} \rightarrow \text{NH}_2 \cdot \text{OH}</math>            AMMONIA + OXYGEN ATOM            73 BAU/DRY            -----</p>	300-1000	1.5(+12)	0	3020±300	0.5 1.5
<p>-----  <math>\text{NH}_3 \cdot \text{CH}_3 \cdot \rightarrow \text{NH}_2 \cdot \text{CH}_4</math>            AMMONIA + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.            -----</p>	350-650	1.0(+11)	0	5100±500	0.3 1.3
<p>-----  <math>\text{ND}_3 \cdot \text{CH}_3 \cdot \rightarrow \text{ND}_2 \cdot \text{CH}_3\text{D}</math>            AMMONIA-D<sub>3</sub> + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.            -----</p>	350-500	1.0(+11)	0	5535±500	0.3 1.3
<p>-----  <math>\text{NH}_3 \cdot \text{M} \rightarrow \text{H} \cdot \text{NH}_2 \cdot \text{M}</math>            AMMONIA            73 BAU/DRY            REACTION ORDER: 2.            M: Ar            -----</p>	2000-3000	9.2(+15)	0	42400±2500	0.5 2.0
<p>-----  <math>\text{NH}_2\text{NH}_2 \cdot \text{H} \rightarrow \text{NH}_2\text{NH} \cdot + \text{H}_2</math>            HYDRAZINE + HYDROGEN ATOM            73 BAU/DRY            REACTION ORDER: 2.            -----</p>	250-500	1.3(+13)	0	1260±100	0.5 2.0
<p>-----  <math>\text{NH}_2\text{NH}_2 \cdot \text{CH}_3 \cdot \rightarrow \text{NH}_2\text{NH} \cdot + \text{CH}_4</math>            HYDRAZINE + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.            -----</p>	350-500	1.0(+11)	0	2515±500	0.5 2.0
<p>-----  <math>\text{ND}_2\text{ND}_2 \cdot \text{CH}_3 \cdot \rightarrow \text{ND}_2\text{ND} \cdot + \text{CH}_3\text{D}</math>            HYDRAZINE-D<sub>4</sub> + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.            -----</p>	350-500	7.2(+10)	0	3200±500	0.5 2.0
<p>-----  <math>\text{NH}_2\text{NH}_2 \cdot \text{M} \rightarrow \text{NH}_2 \cdot + \text{NH}_2 \cdot + \text{M}</math>            HYDRAZINE            73 BAU/DRY            REACTION ORDER: 2.            M: Ar            NOTE: LIMITING HIGH PRESSURE k.            -----</p>	1250-1400	8.0(+13)	0	27700±1000	0.3 3.0
<p>-----  <math>\text{NH}_2\text{NH}_2 \cdot \text{M} \rightarrow \text{NH}_2 \cdot + \text{NH}_2 \cdot + \text{M}</math>            HYDRAZINE            73 BAU/DRY            REACTION ORDER: 2.            M: Ar            NOTE: <math>k_0</math> (LOW PRESSURE).            -----</p>	1250-1400	4.0(+15)	0	20600±1000	0.3 3.0
<p>-----  <math>\text{HN}_3 \cdot \text{CH}_3 \cdot \rightarrow \text{N}_3 \cdot + \text{CH}_4</math>            HYDRAZIC ACID + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.            NOTE: TENTATIVE k VALUE.            -----</p>	300-400	1.0(+11)	0	2100±500	0.5 2.0
<p>-----  <math>\text{HN}_3 \cdot \text{O} \rightarrow \text{H} \cdot + \text{NO}_2</math>            NITROSYL HYDRIDE + OXYGEN ATOM            76 ENG            REACTION ORDER: 2.            -----</p>	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
<p>HNØ * Ø -&gt; NØ * ØH                      NITROSYL HYDRIDE * OXYGEN ATØM                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	1.0(+11)	0.5	3500*2500	0.3 3.2
<p>HNØ * Ø -&gt; NØ * Ø2                      NITROSYL HYDRIDE * OXYGEN ATØM                      REACTION ØRDER: 2.                      -----</p>				
2000	4.8(+12)	-	-	0.5 1.5
<p>HNØ * H -&gt; NØ * H2                      NITROSYL HYDRIDE * HYDROGEN ATØM                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	2.0(+11)	0.5	11600*2500	0.3 3.2
<p>HNØ * H -&gt; NØ * ØH                      NITROSYL HYDRIDE * HYDROGEN ATØM                      REACTION ØRDER: 2.                      -----</p>				
2000	3.6(+13)	-	-	0.5 1.5
<p>HNØ * ØH -&gt; NØ * H2Ø                      NITROSYL HYDRIDE * HYDROXYL FREE RADICAL                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	1.0(+11)	0.5	1000*2500	0.3 3.2
<p>HNØ * N -&gt; NØ * NH                      NITROSYL HYDRIDE * NITROGEN ATØM                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	5.0(+10)	0.5	1500*2500	0.3 3.2
<p>HNØ * N -&gt; N2Ø * H                      NITROSYL HYDRIDE * NITROGEN ATØM                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	2.0(+12)	0	13100*2500	0.5 2.0
<p>HNØ * NØ -&gt; ØH * N2Ø                      NITROSYL HYDRIDE * NITROGEN OXIDE(NØ)                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	1.0(+11)	0.5	3500*2500	0.3 3.2
<p>HNØ * CØ -&gt; NH * CØ2                      NITROSYL HYDRIDE * CARBON MONOXIDE                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	6.3(+11)	0.5	0*2500	0.3 3.2
<p>HNØ * ØH -&gt; NØ * ØH2                      NITROSYL HYDRIDE * METHYLIDYNE FREE RADICAL                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	6.3(+11)	0.5	0*2500	0.3 3.2
<p>HNØ * ØH2 -&gt; NØ * ØH3Ø                      NITROSYL HYDRIDE * METHYLENE FREE RADICAL                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	5.0(+11)	0.5	0*2500	0.3 3.2
<p>HNØ * ØH3Ø -&gt; NØ * ØH4                      NITROSYL HYDRIDE * METHYL FREE RADICAL                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	3.2(+11)	0.5	0*2500	0.3 3.2
<p>HNØ * ØCHØ -&gt; NØ * ØCHØ                      NITROSYL HYDRIDE * METHYL, ØHØ-, FREE RADICAL                      REACTION ØRDER: 2.                      -----</p>				
1500-2500	3.2(+11)	0.5	0*2500	0.3 3.2
<p>HNØ * CN -&gt; NØ * HCN</p>				

## CHEMICAL REACTIONS

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



CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f F
76 HAU/DRY NOTE: M = Ar, O <sub>2</sub> C <sub>2</sub> K <sub>1</sub> = K <sub>1-1</sub> ----- C + O <sub>2</sub> → CO + O CARBON ATOM + OXYGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2. ----- C + H <sub>2</sub> → CH + H CARBON ATOM + HYDROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2. ----- C + OH → CO + H CARBON ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. ----- C + OH → CH + O CARBON ATOM + HYDROXYL FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. ----- C + S <sub>2</sub> → CS + S CARBON ATOM + SULFUR DIMER 75 BEN/GOL REACTION ORDER: 2. ----- C + SO → CO + S CARBON ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2. ----- C + SO → CS + O CARBON ATOM + SULFUR MONOXIDE 75 BEN/GOL REACTION ORDER: 2. ----- C + SH → CH + S CARBON ATOM + MERCAPTAN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. ----- C + SH → CS + H CARBON ATOM + MERCAPTAN FREE RADICAL 75 BEN/GOL REACTION ORDER: 2. ----- C + N <sub>2</sub> → CN + N CARBON ATOM + NITROGEN MOLECULE 75 BEN/GOL REACTION ORDER: 2. ----- C + NO → CO + N CARBON ATOM + NITROGEN MONOXIDE(NO) 75 BEN/GOL REACTION ORDER: 2. ----- C + NO → CN + O CARBON ATOM + NITROGEN MONOXIDE(NO) 75 BEN/GOL REACTION ORDER: 2. ----- C + NH → CH + N CARBON ATOM + NITROGEN FREE RADICAL	7000-14000	3.3(+26)  6.3(+11)  1.6(+12)  6.3(+11)  7.9(+11)  6.3(+11)  6.3(+11)  6.3(+11)  4.0(+11)  6.3(+11)  1.3(+12)  6.3(+11)  6.3(+11)	-3.1  0.5  0.5  0.5  0.5  0.5  0.5  0.5  0.5  0.5  0.5  0.5	-2114  0  15700  0  14800  0  0  6090  0  22750  4000  0	0.3 1.8

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
75 BEN/GGL REACTION ORDER: 2. ----- C + NH - CN + H CARBON ATOM + IMIDGEN FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + NS - CS + N CARBON ATOM + NITRIC SULFIDE 75 BEN/GGL REACTION ORDER: 2. ----- C + NS - CN + S CARBON ATOM + NITRIC SULFIDE 75 BEN/GGL REACTION ORDER: 2. ----- C + CO - C <sub>2</sub> + O CARBON ATOM + CARBON MONOXIDE 75 BEN/GGL REACTION ORDER: 2. ----- C + CH - CH + C CARBON ATOM + METHYLILYNE FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + CH - C <sub>2</sub> + H CARBON ATOM + METHYLIDYNE FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + CS - CS + C CARBON ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + CS - C <sub>2</sub> + S CARBON ATOM + CARBON MONOSULFIDE FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + CN - CN + C CARBON ATOM + CYANGEN FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + CN - C <sub>2</sub> + N CARBON ATOM + CYANGEN FREE RADICAL 75 BEN/GGL REACTION ORDER: 2. ----- C + C <sub>2</sub> - C <sub>2</sub> + C CARBON ATOM + CARBON DIMER 75 BEN/GGL REACTION ORDER: 2. ----- CO + O - O + CO CARBON MONOXIDE + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. ----- CO + O + M - CO <sub>2</sub> + M CARBON MONOXIDE + OXYGEN ATOM 76 HAU/DRY REACTION ORDER: 3. M: CO	250-500	6.3(+11) 6.3(+11) 6.3(+11) 6.3(+11) 1.0(+12) 6.3(+11) 6.3(+11) 6.3(+11) 5.0(+11) 6.3(+11) 2.5(+11) 6.3(+11) 6.3(+11)	0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5 0.5	4000 0 4000 0 58025 4000 0 0 20435 0 19300 0	. . . . . 0.8 1.2

T/K	A	B	E/R (in OK)	k factors f	F
CHEMICAL REACTIONS					
NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 500K. ----- C6 * O -> C * O2 CARBON MONOXIDE * OXYGEN ATOM 75 BEN/GOL REACTION ORDER: 2. -----	1.0 (*12)	0.5	69300		
C6 * O2 -> C62 * O CARBON MONOXIDE * OXYGEN MOLECULE 76 BAU/DRY REACTION ORDER: 2. NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K. -----	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 -> .CHG * M CARBON MONOXIDE * HYDROGEN ATOM 76 BAU/DRY REACTION ORDER: 3. M: H2 NOTE: k FACTORS CHANGING TO: f = 0.5; F = 2.0 AT 773K. -----	7.2 (*14)	0	850*500	0.7	1.3
C6 * H * M -> .CHG * M CARBON MONOXIDE * HYDROGEN ATOM 76 ENG REACTION ORDER: 3. -----	1.6 (*20)	-1.5	0	0.3	3.2
C6 * OH -> C62 * 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 <sup>3</sup> mole <sup>-1</sup> s <sup>-1</sup> ) = 10.83 + 3.94 x 10 <sup>-4</sup> T -----	1.5 (* 7)	1.3	-385	0.8	1.2
C6 * H2 -> C62 * OH CARBON MONOXIDE * HYDROPEROXYL FREE RADICAL 76 BAU/DRY REACTION ORDER: 2. -----	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 F
<p>75 BEN/GOL                      REACTION ORDER: 2.                      -----  <math>CO + NO_2 \rightarrow CO_2 + NO</math>                      CARBON MONOXIDE + NITROGEN                      OXIDE (NO<sub>2</sub>)                      72 KCN                      REACTION ORDER: 2.                      76 ENG                      -----</p>	500-800 1500-2500	5.0(+12)	0.5	57300	0.5 1.9 0.5 2.0
<p><math>CO + N_2O \rightarrow CO_2 + N_2</math>                      CARBON MONOXIDE + NITROGEN                      OXIDE (N<sub>2</sub>O)                      76 ENG                      -----</p>	1500-2500	1.0(+11)	0	10000+1500	0.5 2.0
<p><math>CO + HNO \rightarrow CO_2 + NH</math>                      CARBON MONOXIDE + NITROSYL                      HYDRIDE                      76 ENG                      -----</p>	1500-2500	1.0(+11)	0.5	3500+2500	0.3 3.2
<p><math>CO + C \rightarrow CO + C_2</math>                      CARBON MONOXIDE + CARBON                      ATOM                      75 BEN/GOL                      -----</p>	273-400	1.0(+12)	0.5	58025	
<p><math>CO + CH_3 \rightarrow CO_2 + CH_3C(=O)</math>                      CARBON MONOXIDE + METHYL                      FREE RADICAL                      72 KCN                      -----</p>	7000-15000	3.8(+8)	0	1965	
<p><math>CO + M \rightarrow CO + M</math>                      CARBON MONOXIDE                      76 BAU/DRY                      NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5                      OVER 10000K. M = Ar OR CO                      -----</p>	1500-3000	8.8(+29)	-3.5	128700+1800	0.3 1.8
<p><math>CO_2 + O \rightarrow CO + O_2</math>                      CARBON DIOXIDE + OXYGEN                      ATOM                      76 BAU/DRY                      NOTE: k FACTORS CHANGING TO: f = 0.5; F = 1.5 AT 3000K.  <math>k_1 = k_2 - 1</math>                      -----</p>	1000-3000	1.7(+13)	0	26500+2500	0.5 2.0
<p><math>CO_2 + E \rightarrow CO + OH</math>                      CARBON DIOXIDE + HYDROGEN                      ATOM                      76 BAU/DRY                      -----</p>	1500-2500	1.5(+14)	0	13300+150	0.8 1.2
<p><math>CO_2 + E_2 \rightarrow CO + H_2O</math>                      CARBON DIOXIDE + HYDROGEN                      MOLECULE                      76 ENG                      -----</p>	1500-2500	1.0(+9)	0.5	7550+2500	0.3 3.2
<p><math>CO_2 + N \rightarrow CO + NO</math>                      CARBON DIOXIDE + NITROGEN                      ATOM                      76 ENG                      -----</p>	1500-2500	2.0(+11)	0.5	15000+10000	0.1 1.0
<p><math>CO_2 + CH \rightarrow CO + \cdot CH_3</math>                      CARBON DIOXIDE + METHYLDIENE                      FREE RADICAL                      76 ENG                      -----</p>	1500-2500	1.0(+10)	0.5	3000+2500	0.3 3.2
<p><math>CO_2 + M \rightarrow CO + O + M</math>                      CARBON DIOXIDE                      -----</p>					

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f 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 <sub>2</sub> + M	METHYLIDYNE FREE RADICAL + OXYGEN ATOM	1500-2500	1.0(+16)	-0.5	0*2500	0.3 3.2
76 ENG	REACTION ORDER: 3.					
CH + O <sub>2</sub> → CH <sub>2</sub> + O	METHYLIDYNE FREE RADICAL + OXYGEN MOLECULE	1500-2500	5.0(+11)	0.5	3000*2500	0.3 3.2
76 ENG	REACTION ORDER: 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 <sub>2</sub>	METHYLIDYNE FREE RADICAL + HYDROGEN ATOM					
75 BEN/GGL	REACTION ORDER: 2.		6.3(+11)	0.5	4000	
CH + H + M → CH <sub>2</sub> + M	METHYLIDYNE FREE RADICAL + HYDROGEN ATOM	1500-2500	1.00(+19)	-1.0	0	0.3 3.2
76 ENG	REACTION ORDER: 3.					
CH + OH → CH <sub>2</sub> + H	METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL	1500-2500	5.0(+11)	0.5	5000*2500	0.3 3.2
76 ENG	REACTION ORDER: 2.					
CH + H <sub>2</sub> → CH <sub>2</sub> + H <sub>2</sub>	METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL	1500-2500	1.0(+10)	0.5	7550*2500	0.3 3.2
76 ENG	REACTION ORDER: 2.					
CH + H <sub>2</sub> → CH <sub>2</sub> + OH	METHYLIDYNE FREE RADICAL + HYDROPEROXYL FREE RADICAL	1500-2500	5.0(+11)	0.5	3000*2500	0.3 3.2
76 ENG	REACTION ORDER: 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 °K)	k factors f
CH * N - C * NH METHYLIDYNE FREE RADICAL * NITROGEN ATOM 75 BEN/GOL REACTION ORDER: 2.	-----		1.0(*12)	0.5	6995	
CH * N2 - CN * NH METHYLIDYNE FREE RADICAL * NITROGEN MOLECULE 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	3.2(*14)	0	46300*10000	
CH * N2 - HCN * N METHYLIDYNE FREE RADICAL * NITROGEN MOLECULE 76 ENG NOTE: REVISED ESTIMATE.	-----	1500-2500	1.0(*11)	0	9560	
CH * N6 - .CHC * N METHYLIDYNE FREE RADICAL * NITROGEN OXIDE(N6) 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	1.6(*13)	0	5000*3000	
CH * N6 - HCN * d METHYLIDYNE FREE RADICAL * NITROGEN OXIDE(N6) 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	2.0(*12)	0	0*1000	
CH * HN6 - CH2 * N6 METHYLIDYNE FREE RADICAL * NITROSYL HYDRIDE 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	6.3(*11)	0.5	0*2500	0.3 3.2
CH * C - H * C2 METHYLIDYNE FREE RADICAL * CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.	-----		6.3(*11)	0.5	0	
CH * C - C * CH METHYLIDYNE FREE RADICAL * CARBON ATOM 75 BEN/GOL REACTION ORDER: 2.	-----	1500-2500	6.3(*11)	0.5	4000	
CH * C62 - .CH6 * C6 METHYLIDYNE FREE RADICAL * CARBON DIOXIDE 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	1.0(*10)	0.5	3000*2500	0.3 3.2
CH * CH4 - CH2 * CH3 METHYLIDYNE FREE RADICAL * METHANE 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	2.5(*11)	0.7	3000*2500	0.3 3.2
CH * .CH6 - CH2 * C6 METHYLIDYNE FREE RADICAL * METHYL, C6-, FREE RADICAL 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	3.2(*10)	0.7	500*2500	0.3 3.2
CH * HCH6 - CH2 * .CH6 METHYLIDYNE FREE RADICAL * FORMALDEHYDE 76 ENG NOTE: k ESTIMATED.	-----	1500-2500	1.0(*11)	0.7	2000*2500	0.3 3.2







## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
297	-	-	-	-
297	-	-	-	-
297	-	-	-	-
297	-	-	-	-
297	-	-	-	-
297	-	-	-	-
1500-2500	5.0(+13)	0	0	0.5 2.0
1500-2500	3.2(+12)	0	34975±1500	

$^1\text{CH}_2$  + trans- $\text{CH}_3\text{CH}=\text{CHCH}_3$  → products  
 METHYLENE FREE RADICAL + trans-2-BUENE  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 1.39  
 NOTE:  $k_{\text{ref}}$ :  $^1\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^3\text{CH}_2$  + trans- $\text{CH}_3\text{CH}=\text{CHCH}_3$  → products  
 METHYLENE FREE RADICAL + trans-2-BUENE  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 0.89  
 NOTE:  $k_{\text{ref}}$ :  $^3\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^1\text{CH}_2$  +  $(\text{CH}_3)_2\text{C}=\text{CH}_2$  → products  
 METHYLENE FREE RADICAL + 1-PROPENE, 2-METHYL-  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 1.96  
 NOTE:  $k_{\text{ref}}$ :  $^1\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^3\text{CH}_2$  +  $(\text{CH}_3)_2\text{C}=\text{CH}_2$  → products  
 METHYLENE FREE RADICAL + 1-PROPENE, 2-METHYL-  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 2.86  
 NOTE:  $k_{\text{ref}}$ :  $^3\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^1\text{CH}_2$  +  $(\text{CH}_3)_2\text{C}=\text{CHCH}_3$  → products  
 METHYLENE FREE RADICAL + 2-BUTENE, 2-METHYL-  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 2.12  
 NOTE:  $k_{\text{ref}}$ :  $^1\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^3\text{CH}_2$  +  $(\text{CH}_3)_2\text{C}=\text{CHCH}_3$  → products  
 METHYLENE FREE RADICAL + 2-BUTENE, 2-METHYL-  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 1.83  
 NOTE:  $k_{\text{ref}}$ :  $^3\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^1\text{CH}_2$  +  $(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$  → products  
 METHYLENE FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL-  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 2.16  
 NOTE:  $k_{\text{ref}}$ :  $^1\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$^3\text{CH}_2$  +  $(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$  → products  
 METHYLENE FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL-  
 72 KEE/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 2.74  
 NOTE:  $k_{\text{ref}}$ :  $^3\text{CH}_2$  +  $\text{CH}_2=\text{CH}_2$  -----

$\text{CH}_3$  + O → HCHO + H  
 METHYL FREE RADICAL + OXYGEN ATOM  
 76 ENG REACTION ORDER: 2.  
 -----

$\text{CH}_3$  + O<sub>2</sub> → CH<sub>2</sub> + HO<sub>2</sub>  
 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 REACTION ORDER: 2. ----- 76 ENG	1500-2500	3.2(+13)	0	10000±5000	0.3 3.2
$\text{CH}_3 \cdot + \text{O}_2 \rightarrow \text{CH}_3\text{O}_2 \cdot + \text{O}$ METHYL FREE RADICAL + OXYGEN MOLECULE REACTION ORDER: 2. ----- 76 ENG NOTE: k ESTIMATED.	1500-2500	3.2(+12)	0	15100±1500	0.7 1.3
$\text{CH}_3 \cdot + \text{H}_2 \rightarrow \text{CH}_4 + \text{H} \cdot$ METHYL FREE RADICAL + HYDROGEN MOLECULE REACTION ORDER: 2. ----- 72 KER/PAR	370-700	8.5(+11)	0	5500±500	0.5 1.5
$\text{CH}_3 \cdot + \text{HD} \rightarrow \text{CH}_3\text{D} + \text{H} \cdot$ METHYL FREE RADICAL + DEUTERIUM HYDRIDE REACTION ORDER: 2. ----- 76 KER/PAR	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 REACTION ORDER: 2. ----- 76 KER/PAR	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 REACTION ORDER: 2. ----- 76 KER/PAR	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 <sub>3</sub> FREE RADICAL + HYDROGEN MOLECULE REACTION ORDER: 2. ----- 72 KGN	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 REACTION ORDER: 2. ----- 76 ENG	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 REACTION ORDER: 2. ----- 76 ENG NOTE: k ESTIMATED.	1500-2500	6.3(+12)	0	0	0.3 3.2
$\text{CH}_3 \cdot + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{O}_2$ METHYL FREE RADICAL + HYDROPEROXYL FREE RADICAL REACTION ORDER: 2. ----- 76 ENG	1500-2500	1.0(+11)	0.5	3000±2500	0.3 3.2
$\text{CH}_3 \cdot + \text{H}_2\text{O} \rightarrow \text{CH}_4 + \text{OH}$ METHYL FREE RADICAL + WATER REACTION ORDER: 2. ----- 76 KER/PAR 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 REACTION ORDER: 2. ----- 76 KER/PAR 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
350-650	1.0(+11)	0	5100±500	0.3	1.8
METHYL FREE RADICAL * AMMONIA REACTION ORDER: 2. ----- 76 KER/PAR					
350-500	1.0(+11)	0	5535±500	0.3	1.8
CH <sub>3</sub> * ND <sub>3</sub> - CH <sub>3</sub> D * ND <sub>2</sub> METHYL FREE RADICAL * AMMONIA-d <sub>3</sub> REACTION ORDER: 2. ----- 76 KER/PAR					
350-500	1.0(+11)	0	2500±500	0.5	2.0
CH <sub>3</sub> * NB <sub>2</sub> NH <sub>2</sub> - CH <sub>4</sub> * NB <sub>2</sub> NH. METHYL FREE RADICAL * HYDRAZINE REACTION ORDER: 2. ----- 76 KER/PAR					
350-500	7.2(+10)	0	3200±500	0.5	2.0
CH <sub>3</sub> * ND <sub>2</sub> ND <sub>2</sub> - CH <sub>3</sub> D * ND <sub>2</sub> ND. METHYL FREE RADICAL * HYDRAZINE-d <sub>4</sub> REACTION ORDER: 2. ----- 76 KER/PAR					
300-400	1.0(+11)	0	2100±500	0.5	2.0
CH <sub>3</sub> * HN <sub>3</sub> - CH <sub>4</sub> * N <sub>3</sub> METHYL FREE RADICAL * HYDRAZIC ACID REACTION ORDER: 2. ----- 76 KER/PAR					
1500-2500	5.0(+11)	0.5	0±2500	0.3	3.2
NOTE: TENTATIVE k VALUE. ----- 72 KEN					
273-400	3.8(+8)	0	1968		
CH <sub>3</sub> * CH <sub>0</sub> - CH <sub>3</sub> C(0). METHYL FREE RADICAL * CARBON MONOXIDE REACTION ORDER: 2. ----- 76 KER/PAR					
450-800	4.0(+11)	0	7045±250	0.7	1.3
CH <sub>3</sub> * CH <sub>4</sub> - CH <sub>4</sub> * CH <sub>3</sub> . METHYL FREE RADICAL * METHANE REACTION ORDER: 2. ----- 76 KER/PAR					
400-650	1.1(+11)	0	6995±250	0.7	1.3
CH <sub>3</sub> * CHD <sub>3</sub> - CH <sub>4</sub> * CD <sub>3</sub> . METHYL FREE RADICAL * METHANE-d <sub>3</sub> REACTION ORDER: 2. ----- 76 KER/PAR					
400-650	2.5(+11)	0	7700±500	0.5	1.5
CH <sub>3</sub> * CD <sub>4</sub> - CH <sub>3</sub> D * CD <sub>3</sub> . METHYL FREE RADICAL * METHANE-d <sub>4</sub> REACTION ORDER: 2. ----- 76 KER/PAR					
400-650	5.0(+10)	0	7200±500	0.5	1.5
CD <sub>3</sub> * CH <sub>3</sub> D - CD <sub>4</sub> * CH <sub>3</sub> . METHYL-d <sub>3</sub> -FREE RADICAL * METHANE-d REACTION ORDER: 2. ----- 76 KER/PAR					
473-623	4.1(+12)	0	8960±250		
NOTE: TENTATIVE k VALUE. ----- 72 KEN					
1500-2500	3.2(+11)	0.5	0±2500	0.3	3.2
CH <sub>3</sub> * CD <sub>4</sub> - CD <sub>4</sub> * CD <sub>3</sub> . METHYL-d <sub>3</sub> -FREE RADICAL * METHANE-d <sub>4</sub> REACTION ORDER: 2. ----- 76 KEN					
CH <sub>3</sub> * .CH <sub>0</sub> - CH <sub>4</sub> * C <sub>0</sub> METHYL FREE RADICAL * METHYL, CH <sub>0</sub> , FREE RADICAL REACTION ORDER: 2. ----- 76 ENG					

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
300-500	1.1(+11)	0	3070*500	0.5 1.5
1500-2500	1.0(+10)	0.5	3000*2500	0.3 3.2
300-500	1.4(+11)	0	3975*500	0.5 1.5
350-550	6.2(+10)	0	4900*500	0.6 1.4
350-500	1.9(+11)	0	5035*500	0.6 1.4
350-550	2.3(+11)	0	4900*500	0.6 1.4
370-550	2.0(+11)	0	5940*500	0.6 1.4
370-550	6.2(+10)	0	4900*500	0.6 1.4
400-500	1.9(+11)	0	5000*500	0.5 2.0
400-500	3.2(+10)	0	5700*1000	0.5 2.0
303	1.2(+8)	-	-	0.5 2.0
400-500	1.1(+11)	0	2050*500	0.5 2.0
400-500	7.6(+10)	0	4200*250	0.5 2.0

$\text{CH}_3 \cdot + \text{HCHO} \rightarrow \text{CH}_4 + \cdot\text{CHO}$   
 METHYL FREE RADICAL + FORMALDEHYDE  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{HCHO} \rightarrow \text{CH}_4 + \cdot\text{CHO}$   
 METHYL FREE RADICAL + FORMALDEHYDE  
 76 ENG REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{DCDO} \rightarrow \text{CH}_3\text{D} + \cdot\text{CDO}$   
 METHYL FREE RADICAL + FORMALDEHYDE-d<sub>2</sub>  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_2\text{OH}$   
 METHYL FREE RADICAL + METHANOL  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{OH}$   
 METHYL FREE RADICAL + METHANOL  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_2\text{OH}$   
 METHYL FREE RADICAL + METHANOL  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CH}_3\text{OH} \rightarrow \text{CH}_4 + \text{CH}_2\text{OH}$   
 METHYL FREE RADICAL + METHANOL  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CD}_3\text{OH} \rightarrow \text{CH}_4 + \cdot\text{CD}_2\text{OH}$   
 METHYL FREE RADICAL + METHANOL-d<sub>1</sub>  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CD}_3\text{OH} \rightarrow \text{CH}_4 + \text{CD}_2\text{OH}$   
 METHYL FREE RADICAL + METHANOL-d<sub>1</sub>  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CD}_3 \cdot + \text{CH}_3\text{OH} \rightarrow \text{CD}_3\text{H} + \cdot\text{CH}_2\text{OH}$   
 METHYL-d<sub>3</sub> FREE RADICAL + METHANOL-d  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CD}_3 \cdot + \text{CH}_3\text{OH} \rightarrow \text{CD}_4 + \text{CH}_2\text{OH}$   
 METHYL-d<sub>3</sub> FREE RADICAL + METHANOL-d  
 76 KEE/PAR REACTION ORDER: 2.

NOTE: GIVEN WITH CAUTION

$\text{CH}_3 \cdot + \text{CH}_3\text{SH} \rightarrow \text{CH}_4 + \text{CH}_3\text{S}$   
 METHYL FREE RADICAL + METHANETHIOL  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CD}_3\text{SH} \rightarrow \text{CH}_4 + \text{CD}_3\text{S}$   
 METHYL FREE RADICAL + METHANE-d<sub>3</sub>-THIOL  
 76 KEE/PAR REACTION ORDER: 2.

$\text{CH}_3 \cdot + \text{CD}_3\text{SH} \rightarrow \text{CH}_3\text{D} + \cdot\text{CD}_2\text{SH}$   
 METHYL FREE RADICAL + METHANE-d<sub>3</sub>-THIOL  
 76 KEE/PAR REACTION ORDER: 2.

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
----- CH <sub>3</sub> • CN → CH <sub>2</sub> • HCN METHYL FREE RADICAL • CYANOGEN FREE RADICAL REACTION ORDER: 2. 76 ENG -----	1500-2500	1.0(•11)	0.7	1500•2500	0.3 3.2
CH <sub>3</sub> • CH <sub>3</sub> NH <sub>2</sub> → CH <sub>4</sub> • •CH <sub>2</sub> NH <sub>2</sub> METHYL FREE RADICAL • METHANAMINE REACTION ORDER: 2. 72 KON -----	388-617	5.4(•11)	0	5020•500	0.3 3.0
CH <sub>3</sub> • CH <sub>3</sub> NH <sub>2</sub> → CH <sub>4</sub> • CH <sub>3</sub> NH <sub>2</sub> • •CH <sub>2</sub> NH <sub>2</sub> METHYL FREE RADICAL • METHANAMINE REACTION ORDER: 2. 76 KER/PAR -----	350-650	2.1(•11)	0	4330•500	0.7 1.3
CH <sub>3</sub> • CH <sub>3</sub> ND <sub>2</sub> → CH <sub>4</sub> • •CH <sub>2</sub> ND <sub>2</sub> METHYL FREE RADICAL • METHANAMINE-d <sub>2</sub> REACTION ORDER: 2. 76 KER/PAR -----	350-450	1.4(•11)	0	4530•500	0.7 1.3
CH <sub>3</sub> • CH <sub>3</sub> ND <sub>2</sub> → CH <sub>3</sub> <sup>D</sup> • CH <sub>3</sub> ND METHYL FREE RADICAL • METHANAMINE-d <sub>2</sub> REACTION ORDER: 2. 76 KER/PAR NOTE: TENTATIVE k VALUE. -----	350-450	2.0(•11)	0	5135•1000	0.5 1.5
CH <sub>3</sub> • CD <sub>3</sub> NE <sub>2</sub> → CH <sub>4</sub> • CD <sub>3</sub> NE. METHYL FREE RADICAL • METHAN-d <sub>3</sub> -AMINE REACTION ORDER: 2. 76 KER/PAR NOTE: TENTATIVE k VALUE. -----	400-500	2.0(•11)	0	4530•750	0.5 2.0
CH <sub>3</sub> • CD <sub>3</sub> NH <sub>2</sub> → CH <sub>3</sub> <sup>I</sup> • •CD <sub>2</sub> NH <sub>2</sub> METHYL FREE RADICAL • METHAN-d <sub>3</sub> -AMINE REACTION ORDER: 2. 76 KER/PAR -----	400-500	7.2(•10)	0	5100•500	0.5 1.5
CH <sub>3</sub> • CH <sub>3</sub> NHNH <sub>2</sub> → CH <sub>4</sub> • CH <sub>3</sub> N(•)NH <sub>2</sub> • CH <sub>3</sub> NHNH <sub>2</sub> • •CH <sub>2</sub> NHNH <sub>2</sub> METHYL FREE RADICAL • HYDRAZINE, METHYL- REACTION ORDER: 2. 76 KER/PAR NOTE: TENTATIVE k VALUE. -----	420	6.3(• 8)	-	-	-
CH <sub>3</sub> • HCONH <sub>2</sub> → CH <sub>4</sub> • HCONH <sub>2</sub> • •CONH <sub>2</sub> METHYL FREE RADICAL • FORMAMIDE REACTION ORDER: 2. 76 KER/PAR -----	350-500	3.6(•10)	0	3300•500	0.5 1.5
CH <sub>3</sub> • HCOND <sub>2</sub> → CH <sub>4</sub> • •COND <sub>2</sub> METHYL FREE RADICAL • FORMAMIDE-N, N-d <sub>2</sub> REACTION ORDER: 2. 76 KER/PAR -----	350-500	5.5(•10)	0	3575•500	0.5 2.0
CH <sub>3</sub> • HCOND <sub>2</sub> → CH <sub>3</sub> <sup>D</sup> • HCOND METHYL FREE RADICAL • FORMAMIDE-N, N-d <sub>2</sub> REACTION ORDER: 2. 76 KER/PAR NOTE: TENTATIVE k VALUE. -----	350-500	2.0(•11)	0	4900•500	0.5 2.0
CH <sub>3</sub> • CH <sub>3</sub> NO <sub>2</sub> → CH <sub>4</sub> • •CH <sub>2</sub> NO <sub>2</sub> METHYL FREE RADICAL • METHANE, NITRO- REACTION ORDER: 2. 76 KER/PAR -----	300-500	1.0(•11)	0	5100•750	0.5 2.5

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
NOTE: TENTATIVE k VALUE.				
-----				
CH <sub>3</sub> • CH <sub>3</sub> GNH <sub>2</sub> → CH <sub>4</sub> • CH <sub>3</sub> GNH.				
METHYL FREE RADICAL • HYDROXYLAMINE, 6-METHYL- 76 KER/PAR REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CH <sub>3</sub> GNH <sub>2</sub> → CH <sub>3</sub> D • CH <sub>3</sub> GNH.				
METHYL FREE RADICAL • HYDROXYLAMINE-N, N-d <sub>2</sub> , 6-METHYL- 76 KER/PAR REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CH=CH → CH <sub>4</sub> • CH=C.				
METHYL FREE RADICAL • ETHYLENE 76 KER/PAR REACTION ORDER: 2.				
NOTE: GIVEN WITH CAUTION.				
-----				
CH <sub>3</sub> • CH=CH → CH <sub>3</sub> CH=CH.				
METHYL FREE RADICAL • ETHYLENE 72 KER/PAR REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CH <sub>2</sub> =CH <sub>2</sub> → CH <sub>4</sub> • CH <sub>2</sub> =CH.				
METHYL FREE RADICAL • ETHYLENE 76 KER/PAR REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CH <sub>2</sub> =CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> .				
METHYL FREE RADICAL • ETHYLENE 72 KER/PAR REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CH <sub>2</sub> =CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> • (CH <sub>3</sub> ) <sub>2</sub> CH.				
METHYL FREE RADICAL • ETHYLENE 72 KCN REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CH <sub>3</sub> CH <sub>3</sub> → CH <sub>4</sub> • CH <sub>3</sub> CH <sub>2</sub> .				
METHYL FREE RADICAL • ETHANE 76 KER/PAR REACTION ORDER: 2.				
-----				
CH <sub>3</sub> • CD <sub>3</sub> CD <sub>3</sub> → CH <sub>3</sub> D • CD <sub>3</sub> CD <sub>2</sub> .				
METHYL FREE RADICAL • ETHANE-d <sub>6</sub> 76 KER/PAR REACTION ORDER: 2.				
-----				
CD <sub>3</sub> • CH <sub>3</sub> CH <sub>3</sub> → CD <sub>3</sub> H • CH <sub>3</sub> CH <sub>2</sub> .				
METHYL-d <sub>3</sub> FREE RADICAL • ETHANE 72 KCN REACTION ORDER: 2.				
-----				
CD <sub>3</sub> • CH <sub>3</sub> CD <sub>3</sub> → CD <sub>3</sub> H • CD <sub>3</sub> CH <sub>2</sub> .				
METHYL-d <sub>3</sub> FREE RADICAL • ETHANE-1,1,1-d <sub>3</sub> 76 KER/PAR REACTION ORDER: 2.				
-----				
CD <sub>3</sub> • CH <sub>3</sub> CD <sub>3</sub> → CD <sub>4</sub> • CH <sub>3</sub> CD <sub>2</sub> .				
METHYL-d <sub>3</sub> FREE RADICAL • ETHANE-1,1,1-d <sub>3</sub> 76 KER/PAR REACTION ORDER: 2.				
-----				
CD <sub>3</sub> • CD <sub>3</sub> CD <sub>3</sub> → CD <sub>4</sub> • CD <sub>3</sub> CD <sub>2</sub> .				
METHYL-d <sub>3</sub> FREE RADICAL • ETHANE-d <sub>6</sub> 76 KER/PAR REACTION ORDER: 2.				
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 (ln °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 KN	REACTION ORDER: 2. -----			
CH <sub>3</sub> + CH <sub>3</sub> CHO → CH <sub>4</sub> + CH <sub>3</sub> C(O).				
METHYL FREE RADICAL + ACETALDEHYDE				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + CH <sub>3</sub> COO → CH <sub>3</sub> D + CH <sub>3</sub> C(O).				
METHYL FREE RADICAL + ACETALDEHYDE-1-d				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + cy-CH <sub>2</sub> CH <sub>2</sub> O → CH <sub>4</sub> + cy-CH <sub>2</sub> CH(O).				
METHYL FREE RADICAL + OXIRANE				
76 KEE/PAR	REACTION ORDER: 2. -----			
NOTE: TENTATIVE k VALUE.	-----			
CH <sub>3</sub> + HCOCCH <sub>3</sub> → CH <sub>4</sub> + COCCH <sub>3</sub>				
METHYL FREE RADICAL + FORMIC ACID METHYL ESTER				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + HCOCCH <sub>3</sub> → CH <sub>4</sub> + HCOCCH <sub>2</sub> .				
METHYL FREE RADICAL + FORMIC ACID METHYL ESTER				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + HCOCCH <sub>3</sub> → CH <sub>4</sub> + COCCH <sub>3</sub> + HCOCCH <sub>2</sub>				
METHYL FREE RADICAL + FORMIC ACID METHYL ESTER				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + DCOCCH <sub>3</sub> → CH <sub>3</sub> D + COCCH <sub>3</sub>				
METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + DCOCCH <sub>3</sub> → CH <sub>4</sub> + COCCH <sub>2</sub> .				
METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER				
76 KEE/PAR	REACTION ORDER: 2. -----			
NOTE: TENTATIVE k VALUE.	-----			
CH <sub>3</sub> + CH <sub>3</sub> COO → CH <sub>4</sub> + CH <sub>2</sub> COO				
METHYL FREE RADICAL + FORMIC-d ACID METHYL ESTER				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> O → CH <sub>4</sub> + CH <sub>3</sub> CH <sub>2</sub> O.				
METHYL FREE RADICAL + ETHANOL				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> O → CH <sub>4</sub> + CH <sub>3</sub> CH(O)O				
METHYL FREE RADICAL + ETHANOL				
76 KEE/PAR	REACTION ORDER: 2. -----			
CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> O → CH <sub>4</sub> + CH <sub>3</sub> CH <sub>2</sub> O + CH <sub>3</sub> CH(O)O				
METHYL FREE RADICAL + ETHANOL				
76 KEE/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
$\text{CH}_3 \cdot + \text{CH}_3\text{CD}_2\text{OH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{O} \cdot + \cdot\text{CH}_2\text{CD}_2\text{OH}$ METHYL FREE RADICAL + ETHAN-1,1-d <sub>2</sub> -OL REACTION ORDER: 2.				
400-550	4.1(+11)	0	5735*500	0.6 1.4
$\text{CH}_3 \cdot + \text{CH}_3\text{CD}_2\text{OH} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CD}(\cdot)\text{OH}$ METHYL FREE RADICAL + ETHAN-1,1-d <sub>2</sub> -OL REACTION ORDER: 2.				
400-525	4.4(+11)	0	4900*500	0.6 1.4
$\text{CD}_3 \cdot + \text{CH}_3\text{CB}_2\text{OD} \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CH}(\cdot)\text{OD} + \cdot\text{CH}_2\text{CH}_2\text{OD}$ METHYL-d <sub>3</sub> FREE RADICAL + ETHANGL-d REACTION ORDER: 2.				
400-525	6.2(+10)	0	5135*500	0.5 2.0
$\text{CD}_3 \cdot + \text{CH}_3\text{CH}_2\text{OD} \rightarrow \text{CD}_4 + \text{CH}_3\text{CH}_2\text{O} \cdot$ METHYL-d <sub>3</sub> FREE RADICAL + ETHANGL-d REACTION ORDER: 2.				
300-550	4.2(+11)	0	5035*500	0.5 1.5
$\text{CH}_3 \cdot + \text{CH}_3\text{OCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{OCH}_2 \cdot$ METHYL FREE RADICAL + METHANE. OXYMIS- REACTION ORDER: 2.				
350-500	4.2(+11)	0	5000*1000	0.3 3.0
$\text{CH}_3 \cdot + \text{CH}_3\text{OCH}_2\text{H} \rightarrow \text{CH}_4 + \text{CH}_3\text{OCH}_2 \cdot$ METHYL FREE RADICAL + PEROXIDE, DIMETHYL- REACTION ORDER: 2.				
NOTE: TENTATIVE k VALUE.				
300-500	2.2(+11)	0	4800*500	0.5 2.0
$\text{CD}_3 \cdot + \text{cy-CH}_2\text{CH}_2\text{S} \rightarrow \text{CD}_3\text{H} + \text{cy-CH}_2\text{CH}(\cdot)\text{S}$ METHYL-d <sub>3</sub> FREE RADICAL + THIRANE REACTION ORDER: 2.				
303	3.5(+7)	-	-	0.5 2.0
$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{SH} \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{S} \cdot + \text{CH}_3\text{CH}(\cdot)\text{SH}$ METHYL FREE RADICAL + ETHANETHIOL REACTION ORDER: 2.				
NOTE: TENTATIVE k VALUE.				
350-600	5.4(+11)	0	5100*500	0.5 1.5
$\text{CH}_3 \cdot + \text{CH}_3\text{CN} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CN}$ METHYL FREE RADICAL + ACETONITRILE REACTION ORDER: 2.				
350-500	2.9(+11)	0	4200*500	0.5 2.0
$\text{CH}_3 \cdot + \text{CH}_3\text{CB}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CB}_2\text{NH} \cdot + \text{CH}_3\text{CH}(\cdot)\text{NH}_2$ METHYL FREE RADICAL + ETHANAMINE REACTION ORDER: 2.				
350-500	2.0(+11)	0	4600*500	0.5 2.0
$\text{CH}_3 \cdot + \text{CH}_3\text{CB}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CB}_2\text{NH} \cdot$ METHYL FREE RADICAL + ETHANAMINE REACTION ORDER: 2.				
NOTE: TENTATIVE k VALUE.				
350-500	2.9(+11)	0	4200*500	0.5 2.0
$\text{CH}_3 \cdot + \text{CD}_3\text{CH}_2\text{NH}_2 \rightarrow \text{CH}_4 + \text{CD}_3\text{CH}(\cdot)\text{NH}_2 + \cdot\text{CD}_2\text{CH}_2\text{NH}_2$ METHYL FREE RADICAL + ETHAN-2,2,2-d <sub>3</sub> -AMINE REACTION ORDER: 2.				



CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
$\text{CH}_3 \cdot + \text{CD}_3\text{CH}_2\text{NE}_2 \rightarrow \text{CH}_4 + \text{CD}_3\text{CH}_2\text{NE}$ METHYL FREE RADICAL + ETHAN-2,2,2-d <sub>3</sub> -AMINE 76 KHR/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	423	4.0(+5)	-		
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NH} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N} \cdot + \cdot\text{CH}_2\text{NHCH}_3$ METHYL FREE RADICAL + METHANAMINE, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.	350-650	1.6(+11)	0	3500±500	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NE} \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{N} \cdot$ METHYL FREE RADICAL + METHANAMINE, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.	350-650	6.5(+10)	0	3200±500	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{ND} \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{NDCH}_3$ METHYL FREE RADICAL + METHANAMINE-D, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.	350-500	2.9(+11)	0	4400±500	0.5 1.5
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{ND} \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{N} \cdot$ METHYL FREE RADICAL + METHANAMINE-D, N-METHYL- 76 KHR/PAR REACTION ORDER: 2.	350-500	1.0(+11)	0	4300±500	0.5 1.5
$\text{CH}_3 \cdot + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}=\text{NCH}_3$ METHYL FREE RADICAL + DIAZENE, DIMETHYL- 76 KHR/PAR REACTION ORDER: 2.	300-500	1.1(+11)	0	3975±250	0.7 1.3
$\text{CD}_3 \cdot + \text{CD}_3\text{N}=\text{NCD}_3 \rightarrow \text{CD}_4 + \text{CD}_2\text{N}=\text{NCD}_3$ METHYL-d <sub>3</sub> FREE RADICAL + DIAZENE, DI(METHYL-d <sub>3</sub> )- 76 KHR/PAR REACTION ORDER: 2.	300-450	5.0(+10)	0	3040±355	0.4 2.6
$\text{CH}_3 \cdot + \text{NE}_2\text{CH}_2\text{CH}_2\text{NE}_2 \rightarrow \text{CH}_4 + \cdot\text{NHC}_2\text{CH}_2\text{NE}_2$ METHYL FREE RADICAL + 1,2-ETHANEDIAMINE 76 KHR/PAR REACTION ORDER: 2.	300-500	6.6(+10)	0	4125±500	0.5 1.5
$\text{CH}_3 \cdot + \text{NE}_2\text{CH}_2\text{CH}_2\text{NE}_2 \rightarrow \text{CH}_4 + \cdot\text{NHC}_2\text{CH}_2\text{NE}_2$ METHYL FREE RADICAL + 1,2-ETHANEDIAMINE 76 KHR/PAR REACTION ORDER: 2.	350-500	3.8(+11)	0	4200±500	0.5 2.0
$\text{CH}_3 \cdot + \text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 \rightarrow \text{CH}_4 + \cdot\text{NHC}_2\text{CH}_2\text{ND}_2$ METHYL FREE RADICAL + 1,2-ETHANEDIAMINE-d <sub>2</sub> 76 KHR/PAR REACTION ORDER: 2.	350-500	2.0(+11)	0	4430±500	0.5 2.0
$\text{CH}_3 \cdot + \text{ND}_2\text{CH}_2\text{CH}_2\text{ND}_2 \rightarrow \text{CH}_3\text{D} + \cdot\text{NDCH}_2\text{CH}_2\text{ND}_2$ METHYL FREE RADICAL + 1,2-ETHANEDIAMINE-d <sub>2</sub> 76 KHR/PAR REACTION ORDER: 2.	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
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{NND}$ METHYL FREE RADICAL + HYDRAZINE, 1,1-DIMETHYL- REACTION ORDER: 2.				
350-500	2.4(+11)	0	2970*500	0.5 1.5
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{NND} + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{NH}_2$ METHYL FREE RADICAL + HYDRAZINE, 1,1-DIMETHYL- REACTION ORDER: 2.				
350-500	3.2(+11)	0	4125*750	0.5 2.0
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{N}(\text{CH}_3)\text{ND}$ METHYL FREE RADICAL + HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL- REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
350-500	2.1(+11)	0	3400*500	0.5 1.5
$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NND}_2 \rightarrow \text{CH}_3\text{D} + (\text{CH}_3)_2\text{NND}$ METHYL FREE RADICAL + HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL- REACTION ORDER: 2.				
350-500	2.5(+11)	0	2400*250	0.5 2.0
$\text{CH}_3 \cdot + \text{CH}_3\text{NHNHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{N}(\cdot)\text{NHCH}_3 + \cdot\text{CH}_2\text{NHNHCH}_3$ METHYL FREE RADICAL + HYDRAZINE, 1,2-DIMETHYL- REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
350-500	2.0(+11)	0	2700*500	0.5 2.0
$\text{CH}_3 \cdot + \text{CH}_3\text{NDNDCH}_3 \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{N}(\cdot)\text{NDCH}_3$ METHYL FREE RADICAL + HYDRAZINE-1,2-d <sub>2</sub> , 1,2-DIMETHYL- REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.				
400-600	7.9(+10)	0	3800*500	0.5 1.5
$\text{CH}_3 \cdot + \text{HCNCH}_3 \rightarrow \text{CH}_4 + \cdot\text{CNCH}_3 + \text{HCN}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + FORMAMIDE, N-METHYL- REACTION ORDER: 2.				
350-600	2.1(+11)	0	5235*500	0.5 1.5
$\text{CH}_3 \cdot + \text{CH}_3\text{CONH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CONH}\cdot + \cdot\text{CH}_2\text{CONH}_2$ METHYL FREE RADICAL + ACETAMIDE REACTION ORDER: 2.				
350-600	1.0(+11)	0	5200*500	0.5 1.5
$\text{CH}_3 \cdot + \text{CH}_3\text{CONH}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CONH}_2$ METHYL FREE RADICAL + ACETAMIDE REACTION ORDER: 2.				
350-600	1.1(+11)	0	5235*500	0.5 1.5
$\text{CD}_3 \cdot + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_3\text{H} + \text{CD}_3\text{CONH}\cdot$ METHYL FREE RADICAL + ACETAMIDE-2,2,2-d <sub>3</sub> REACTION ORDER: 2.				
350-600	1.4(+11)	0	5800*500	0.5 1.5
$\text{CD}_3 \cdot + \text{CD}_3\text{CONH}_2 \rightarrow \text{CD}_4 + \cdot\text{CD}_2\text{CONH}_2$ METHYL FREE RADICAL + ACETAMIDE-2,2,2-d <sub>3</sub> REACTION ORDER: 2.				
379-465	5.0(+11)	0	4400	0.5 1.5
$\text{CH}_3 \cdot + \text{CH}_3\text{C}\equiv\text{CH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}\cdot + \text{CH}_3\text{C}(\cdot)=\text{CHCH}_3$ METHYL FREE RADICAL + 1-PROPENE REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. $\text{CH}_3$ ADDITION OCCURS PREDOMINANTLY AT TERMINAL C ATOM.				

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f 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

CH<sub>3</sub> + CH<sub>2</sub>-C-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>C(•)-CH<sub>2</sub>  
METHYL FREE RADICAL + 1,2-PROPADIENE  
REACTION ORDER: 2.  
72 KER/PAR

CH<sub>3</sub> + CH<sub>3</sub>CH=CH<sub>2</sub> → CH<sub>4</sub> + CH<sub>3</sub>C(•)-CH<sub>2</sub>  
METHYL FREE RADICAL + 1-PROPENE  
REACTION ORDER: 2.  
76 KER/PAR

CH<sub>3</sub> + CH<sub>3</sub>CH=CH<sub>2</sub> → CH<sub>4</sub> + [C<sub>3</sub>H<sub>5</sub>•]  
METHYL FREE RADICAL + 1-PROPENE  
REACTION ORDER: 2.  
72 ICN

CH<sub>3</sub> + CH<sub>3</sub>CH=CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub> + (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>•  
METHYL FREE RADICAL + 1-PROPENE  
REACTION ORDER: 2.  
72 KER/PAR

NOTE: k<sub>ref</sub>: CH<sub>3</sub> + CH<sub>2</sub>=CH<sub>2</sub>  
k/k<sub>ref</sub>: 0.72

CH<sub>3</sub> + CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub> → CH<sub>4</sub> + (CH<sub>3</sub>)<sub>2</sub>CH•  
METHYL FREE RADICAL + PROPANE  
REACTION ORDER: 2.  
76 KER/PAR

CD<sub>3</sub> + CH<sub>3</sub>CD<sub>2</sub>CH<sub>3</sub> → CD<sub>3</sub>H + CH<sub>3</sub>CD<sub>2</sub>CH<sub>2</sub>•  
METHYL-d<sub>3</sub> FREE RADICAL + PROPANE-2,2-d<sub>2</sub>  
REACTION ORDER: 2.  
76 KER/PAR

CD<sub>3</sub> + CH<sub>3</sub>CD<sub>2</sub>CH<sub>3</sub> → CD<sub>4</sub> + (CH<sub>3</sub>)<sub>2</sub>CD•  
METHYL-d<sub>3</sub> FREE RADICAL + PROPANE-2,2-d<sub>2</sub>  
REACTION ORDER: 2.  
76 KER/PAR

CH<sub>3</sub> + CH<sub>3</sub>CH<sub>2</sub>CHO → CH<sub>4</sub> + CH<sub>3</sub>CH<sub>2</sub>C(•)O  
METHYL FREE RADICAL + PROPANAL  
REACTION ORDER: 2.  
76 KER/PAR

NOTE: TENTATIVE k VALUE.

CH<sub>3</sub> + (CH<sub>3</sub>)<sub>2</sub>CO → CH<sub>4</sub> + CH<sub>3</sub>C(•)OCH<sub>3</sub>  
METHYL FREE RADICAL + 2-PROPANONE  
REACTION ORDER: 2.  
76 KER/PAR

CD<sub>3</sub> + (CD<sub>3</sub>)<sub>2</sub>CO → CD<sub>4</sub> + CD<sub>3</sub>C(•)OCD<sub>3</sub>  
METHYL-d<sub>3</sub> FREE RADICAL + 2-PROPANONE-1,1,1,3,3,3-d<sub>6</sub>  
REACTION ORDER: 2.  
76 KER/PAR

CH<sub>3</sub> + HCOOCH<sub>2</sub>CH<sub>3</sub> → CH<sub>4</sub> + •COOCH<sub>2</sub>CH<sub>3</sub> + HCOOCH(•)CH<sub>3</sub>  
METHYL FREE RADICAL + FORMIC ACID ETHYL ESTER  
REACTION ORDER: 2.  
76 KER/PAR

NOTE: TENTATIVE k VALUE.

CH<sub>3</sub> + CH<sub>3</sub>COOCH<sub>3</sub> → CH<sub>4</sub> + •CH<sub>2</sub>COOCH<sub>3</sub> + CH<sub>3</sub>COOCH<sub>2</sub>•  
METHYL FREE RADICAL + ACETIC ACID METHYL ESTER  
REACTION ORDER: 2.  
76 KER/PAR

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f	k factors F
CH <sub>3</sub> • CH <sub>3</sub> COCD <sub>3</sub> → CH <sub>4</sub> • •CH <sub>2</sub> COCD <sub>3</sub> METHYL FREE RADICAL • ACETIC ACID METHYL-d <sub>3</sub> ESTER 76 KER/PAR		350-650	1.9(+11)	0	5035*500	0.4	1.6
CH <sub>3</sub> • CD <sub>3</sub> COCH <sub>3</sub> → CH <sub>4</sub> • •CD <sub>3</sub> COCH <sub>3</sub> METHYL FREE RADICAL • ACETIC-d <sub>3</sub> ACID METHYL ESTER 76 KER/PAR		400-600	1.7(+11)	0	5990*500	0.5	1.5
CH <sub>3</sub> • CH <sub>3</sub> COCH <sub>3</sub> → CH <sub>4</sub> • •CH <sub>2</sub> COCH <sub>3</sub> METHYL FREE RADICAL • CARBONIC ACID DIMETHYL ESTER 76 KER/PAR		350-500	3.2(+11)	0	5800*750	0.5	2.0
NOTE: TENTATIVE k VALUE.							
CH <sub>3</sub> • (CH <sub>3</sub> ) <sub>2</sub> CD <sub>2</sub> H → CH <sub>3</sub> D • (CH <sub>3</sub> ) <sub>2</sub> C(•)OH METHYL FREE RADICAL • 2-PROPAN-2-d-OL 76 KER/PAR		400-525	1.9(+11)	0	4900*500	0.6	1.4
CH <sub>3</sub> • (CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> D → CD <sub>3</sub> H • (CH <sub>3</sub> ) <sub>2</sub> C(•)HD • •CH <sub>2</sub> CH(CH <sub>3</sub> )HD METHYL-d <sub>3</sub> FREE RADICAL • 2-PROPANOL-d 76 KER/PAR		400-525	1.5(+11)	0	3975*500	0.6	1.4
CH <sub>3</sub> • cy-CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> S → CH <sub>4</sub> • cy-CH <sub>2</sub> CH(•)CH <sub>2</sub> S METHYL FREE RADICAL • THIEPANE 76 KER/PAR		300-450	3.2(+11)	0	4630*750	0.5	2.0
NOTE: TENTATIVE k VALUE.							
CH <sub>3</sub> • (CH <sub>3</sub> ) <sub>2</sub> CHSH → CH <sub>4</sub> • (CH <sub>3</sub> ) <sub>2</sub> CHS • (CH <sub>3</sub> ) <sub>2</sub> C(•)SH • •CH <sub>2</sub> CH(CH <sub>3</sub> )SH METHYL FREE RADICAL • 2-PROPANETHIOL 76 KER/PAR		303	4.1(+7)	-	-	0.5	2.0
NOTE: TENTATIVE k VALUE.							
CD <sub>3</sub> • CH <sub>3</sub> CH <sub>2</sub> CN → CD <sub>3</sub> H • CH <sub>3</sub> CH(•)CN • •CH <sub>2</sub> CH <sub>2</sub> CN METHYL-d <sub>3</sub> FREE RADICAL • PROPANENITRILE 76 KER/PAR		400-600	3.6(+11)	0	4330*500	0.5	1.5
CH <sub>3</sub> • (CH <sub>3</sub> ) <sub>2</sub> N → CH <sub>4</sub> • •CH <sub>2</sub> N(CH <sub>3</sub> ) <sub>2</sub> METHYL FREE RADICAL • METHANAMINE, N,N-DIMETHYL- 76 KER/PAR		350-600	4.7(+11)	0	4600*500	0.7	1.3
CH <sub>3</sub> • HC≡N(CH <sub>3</sub> ) <sub>2</sub> → CH <sub>4</sub> • •C≡N(CH <sub>3</sub> ) <sub>2</sub> • HC≡(CH <sub>3</sub> )NCH <sub>2</sub> METHYL FREE RADICAL • FORMAMIDE, N,N-DIMETHYL- 76 KER/PAR		400-600	6.3(+10)	0	3600*500	0.5	1.5
NOTE: TENTATIVE k VALUE.							
CH <sub>3</sub> • CH <sub>3</sub> CH <sub>2</sub> C≡CH → CH <sub>4</sub> • CH <sub>3</sub> CH(•)C≡CH • •CH <sub>2</sub> CH <sub>2</sub> C≡CH • CH <sub>3</sub> CH <sub>2</sub> C≡C• METHYL FREE RADICAL • 1-BUTYNE 76 KER/PAR		456-620	1.9(+12)	0	5135*500	0.6	1.4
NOTE: TENTATIVE k VALUE.							
CH <sub>3</sub> • CH <sub>3</sub> C≡CCH <sub>3</sub> → CH <sub>4</sub> • CH <sub>3</sub> C≡CCH <sub>2</sub> METHYL FREE RADICAL • 2-BUTYNE							

CHEMICAL REACTIONS

76 KER/PAR REACTION ORDER: 2.  
 NOTE: TENTATIVE k VALUE.  
 $\text{CH}_3 \cdot + \text{CH}_3\text{-CHCH-CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH-CH}_2$   
 METHYL FREE RADICAL + 1,3-BUTADIENE  
 72 KER/PAR REACTION ORDER: 2.  
 $\text{CH}_3 \cdot + \text{CH}_2\text{-CHCH-CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH-CH}_2$   
 $\cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH-CH}_2$   
 METHYL FREE RADICAL + 1,3-BUTADIENE  
 72 KER/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}: 12.0$   
 NOTE:  $k_{\text{ref}}: \text{CH}_3 \cdot + \text{CH}_2\text{-CH}_2$   
 $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH-CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{CH-CH}_2$   
 METHYL FREE RADICAL + 1-BUTENE  
 76 KER/PAR REACTION ORDER: 2.  
 $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH-CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CHCH}_3$   
 $\cdot\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$   
 METHYL FREE RADICAL + 1-BUTENE  
 72 KER/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}: 0.7$   
 NOTE:  $k_{\text{ref}}: \text{CH}_3 \cdot + \text{CH}_2\text{-CH}_2$   
 $\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH-CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH-CHCH}_2$   
 METHYL FREE RADICAL + cis-2-PENTENE  
 76 KER/PAR REACTION ORDER: 2.  
 $\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH-CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$   
 METHYL FREE RADICAL + cis-2-PENTENE  
 72 KER/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}: 0.2$   
 NOTE:  $k_{\text{ref}}: \text{CH}_3 \cdot + \text{CH}_2\text{-CH}_2$   
 $\text{CH}_3 \cdot + \text{trans-CH}_3\text{CH-CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH-CHCH}_2$   
 METHYL FREE RADICAL + trans-2-PENTENE  
 76 KER/PAR REACTION ORDER: 2.  
 $\text{CH}_3 \cdot + \text{trans-CH}_3\text{CH-CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$   
 METHYL FREE RADICAL + trans-2-PENTENE  
 72 KER/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}: 0.4$   
 NOTE:  $k_{\text{ref}}: \text{CH}_3 \cdot + \text{CH}_2\text{-CH}_2$   
 $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C-CH}_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{C}(\text{CH}_3)\text{-CH}_2$   
 METHYL FREE RADICAL + 1-PROPENE, 2-METHYL-  
 76 KER/PAR REACTION ORDER: 2.  
 $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C-CH}_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2 \cdot + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$   
 METHYL FREE RADICAL + 1-PROPENE, 2-METHYL-  
 72 KER/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}: 1.1$   
 NOTE:  $k_{\text{ref}}: \text{CH}_3 \cdot + \text{CH}_2\text{-CH}_2$

T/K	A	B	E/R (in OK)	k factors f
486-619	1.1(+12)	0	4900*500	0.6 1.4
353-453	8.1(+10)	0	2065	
453	-	-	-	
350-650	2.5(+11)	0	4200*500	0.6 1.4
353-453	1.0(+11)	0	3600	
453	-	-	-	
350-650	1.8(+11)	0	4100*500	0.6 1.4
353-453	4.5(+10)	0	3675	
453	-	-	-	
350-500	1.0(+12)	0	4830*500	0.6 1.4
353-453	1.4(+11)	0	4075	
453	-	-	-	
350-600	3.0(+11)	0	4500*500	0.6 1.4
353-453	1.4(+11)	0	3475	
453	-	-	-	

CHEMICAL REACTIONS	T/K	A	B	E/R (ln OK)	k factors f
<p>-----</p> $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + BUTANE 76 KBR/PAR REACTION ORDER: 2. -----	350-750	4.0(+11)	0	4830*250	0.7 1.3
<p>-----</p> $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + BUTANE 72 KBN REACTION ORDER: 2. -----	350-500	1.6(+11)	0	4540*150	0.7 1.4
<p>-----</p> $\text{CD}_3 \cdot + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_3\text{H} + \text{CH}_3\text{CF}_2\text{CD}_2\text{CH}_2\cdot$ METHYL-d <sub>3</sub> FREE RADICAL + BUTANE-2,2,3,3-d <sub>4</sub> 76 KBR/PAR REACTION ORDER: 2. -----	600-750	4.8(+11)	0	5735*250	0.7 1.3
<p>-----</p> $\text{CD}_3 \cdot + \text{CH}_3\text{CD}_2\text{CD}_2\text{CH}_3 \rightarrow \text{CD}_4 + \text{CH}_3\text{CD}_2\text{CD}(\cdot)\text{CH}_3$ METHYL-d <sub>3</sub> FREE RADICAL + BUTANE-2,2,3,3-d <sub>4</sub> 76 KBR/PAR REACTION ORDER: 2. -----	600-750	4.5(+11)	0	5735*250	0.7 1.3
<p>-----</p> $\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C} \cdot + (\text{CH}_3)_2\text{CHCH}_2\cdot$ METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2. -----	300-500	8.3(+10)	0	4000*500	0.5 2.0
<p>-----</p> $\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{C} \cdot$ METHYL FREE RADICAL + PROPANE, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2. -----	550-750	9.6(+10)	0	3975*250	0.7 1.3
<p>-----</p> $\text{CD}_3 \cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_3\text{H} + (\text{CH}_3)_2\text{CDCH}_2\cdot$ METHYL-d <sub>3</sub> FREE RADICAL + PROPANE-2-d, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2. -----	550-750	6.0(+11)	0	5735*250	0.7 1.3
<p>-----</p> $\text{CD}_3 \cdot + (\text{CH}_3)_3\text{CD} \rightarrow \text{CD}_4 + (\text{CH}_3)_3\text{C} \cdot$ METHYL-d <sub>3</sub> FREE RADICAL + PROPANE-2-d, 2-METHYL- 76 KBR/PAR REACTION ORDER: 2. -----	550-750	1.2(+11)	0	4800*250	0.7 1.3
<p>-----</p> $\text{CH}_3 \cdot + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3) \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{C}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + 2-BUTENAL 76 KBR/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----	350-500	1.0(+11)	0	3400*500	0.4 2.5
<p>-----</p> $\text{CH}_3 \cdot + \text{CH}_3\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{CH}_3)\text{CH}_2\cdot$ METHYL FREE RADICAL + 2,3-EUTANEDIONE 76 KBR/PAR REACTION ORDER: 2. -----	300-800	2.2(+11)	0	4300*500	0.5 1.5
<p>-----</p> $\text{CH}_3 \cdot + (\text{CH}_3\text{C}(\text{CH}_3)_2) \rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + ACETIC ACID ANHYDRIDE 76 KBR/PAR REACTION ORDER: 2. -----	300-500	1.8(+11)	0	4830*500	0.6 1.4
<p>-----</p> $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)_2$ METHYL FREE RADICAL + BUTANAL 76 KBR/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----	350-500	1.0(+11)	0	2970*500	0.4 1.6
<p>-----</p> $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHC}(\cdot)(\text{CH}_3)_2$ -----					

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
350-500	1.0(+11)	0	2970±500	0.4 1.6
<p>METHYL FREE RADICAL + PROPANAL, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p> <p>-----  <math>CH_3 \cdot + CH_3CH_2C\dot{O}CH_3 \rightarrow CH_4 + CH_3CH(\cdot)C\dot{O}CH_3 + \cdot CH_2CH_2C\dot{O}CH_3</math>  <math>\cdot CH_3CH_2C\dot{O}CH_2</math></p> <p>METHYL FREE RADICAL + 2-BUTANONE 76 KER/PAR REACTION ORDER: 2. -----  <math>CH_3 \cdot + HC\dot{O}CCH_2CH_2CH_3 \rightarrow CH_4 + \cdot C\dot{O}CCH_2CH_2CH_3</math>  METHYL FREE RADICAL + FORMIC ACID PROPYL ESTER 72 KDN REACTION ORDER: 2. -----  <math>CH_3 \cdot + HC\dot{O}CCH_2CH_2CH_3 \rightarrow CH_4 + \cdot C\dot{O}CCH_2CH_2CH_3</math>  <math>\cdot HC\dot{O}CCH(\cdot)CH_2CH_3 + HC\dot{O}CCH_2CH(\cdot)CH_3</math>  <math>\cdot HC\dot{O}CCH_2CH_2CH_2</math>  METHYL FREE RADICAL + FORMIC ACID PROPYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p> <p>-----  <math>CH_3 \cdot + HC\dot{O}CCH(CH_3)_2 \rightarrow CH_4 + \cdot C\dot{O}CCH(CH_3)_2</math>  <math>\cdot HC\dot{O}C(\cdot)(CH_3)_2 + HC\dot{O}CCH(CH_3)CH_2</math>  METHYL FREE RADICAL + FORMIC ACID 1-METHYLETHYL ESTER 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p> <p>-----  <math>CH_3 \cdot + CH_3CH_2\dot{O}CH_2CH_3 \rightarrow CH_4 + CH_3CH_2\dot{O}CH(\cdot)CH_3</math>  <math>\cdot CH_3CH_2\dot{O}CH_2CH_2</math>  METHYL FREE RADICAL + ETHANE, 1,1'-DIYHIS- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p> <p>-----  <math>CH_3 \cdot + (CH_3)_3C\dot{S}H \rightarrow CH_4 + (CH_3)_3C\dot{S} + \cdot CH_2C(CH_3)_2SH</math>  METHYL FREE RADICAL + 2-PROPANETHIOL, 2-METHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p> <p>-----  <math>CH_3 \cdot + CH_3CH=NN\cdot CHCH_3 \rightarrow CH_4 + CH_3C(\cdot)=NN\cdot CHCH_3</math>  <math>\cdot CH_2CH=NN\cdot CHCH_3</math>  METHYL FREE RADICAL + ACETALDEHYDE ETHYLIDENETHYDRAZONE 76 KER/PAR REACTION ORDER: 2. -----  <math>CH_3 \cdot + CH_3CH_2CH_2CH_2NH_2 \rightarrow CH_4 + CH_3CH_2CH_2CH_2\dot{N}H</math>  <math>\cdot CH_3CH_2CH_2CH(\cdot)NH_2 + \cdot CH_2CH_2CH_2CH_2NH_2</math>  METHYL FREE RADICAL + 1-BUTANAMINE 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p> <p>-----  <math>CH_3 \cdot + (CH_3CH_2)_2NH \rightarrow CH_4 + (CH_3CH_2)_2\dot{N}</math>  <math>\cdot CH_3CH(\cdot)NHCH_2CH_3 + \cdot CH_2CH_2NHCH_2CH_3</math>  METHYL FREE RADICAL + ETHANAMINE, N-ETHYL- 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.</p>				
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	

$\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{N}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{N}(\text{CH}_3)_2$   
 $\text{CH}_2\text{CH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_3\text{CE}_2\text{N}(\text{CH}_3)\text{CH}_2$   
 METHYL FREE RADICAL + ETHANAMINE, N,N-DIMETHYL-  
 76 KER/PAR  
 NOTE: TENTATIVE k VALUE.

$\text{CH}_3 + \text{CH}_3\text{CON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{CH}_2\text{CON}(\text{CH}_3)_2$   
 $\text{CH}_3\text{CON}(\text{CH}_3)_2$   
 METHYL FREE RADICAL + ACETAMIDE, N,N-DIMETHYL-  
 76 KER/PAR

$\text{CH}_3 \cdot + \text{CH}_3\text{CON}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CON}(\text{CH}_3)\text{CH}_2\cdot$   
 METHYL FREE RADICAL + ACETAMIDE, N,N-DIMETHYL-  
 76 KER/PAR  
 NOTE: TENTATIVE k VALUE.

$\text{CH}_3 \cdot + \text{CH}_3(\text{CH}_2)_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}=\text{CH}_2$   
 METHYL FREE RADICAL + 1-PENTENE  
 76 KER/PAR

$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2$   
 METHYL FREE RADICAL + cis-2-PENTENE  
 72 KER/PAR

$\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$   
 METHYL FREE RADICAL + cis-2-PENTENE  
 72 KER/PAR

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2$   
 METHYL FREE RADICAL + 1-BUTENE, 3-METHYL-  
 72 KER/PAR

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}=\text{CH}_2$   
 METHYL FREE RADICAL + 1-BUTENE, 3-METHYL-  
 76 KER/PAR

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2$   
 $\cdot\text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3$   
 METHYL FREE RADICAL + 2-BUTENE, 2-METHYL-  
 76 KER/PAR  
 NOTE: TENTATIVE k VALUE.

$\text{CH}_3 \cdot + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}_3$   
 $(\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2$   
 METHYL FREE RADICAL + 2-BUTENE, 2-METHYL-  
 72 KER/PAR  
 NOTE: k<sub>ref</sub>:  $\text{CH}_3 \cdot + \text{CH}_2=\text{CH}_2$

TENTATIVE k VALUE.  
 $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\cdot$   
 METHYL FREE RADICAL + PENTANE



CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
76 KER/PAR NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + PENTANE 76 KER/PAR	350-800	4.8(+11)	0	5800*250	0.7 1.3
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{C}(\cdot)\text{CH}_2\text{CH}_3$ METHYL FREE RADICAL + BUTANE, 2-METHYL- 76 KER/PAR	350-800	6.0(+11)	0	4830*250	0.7 1.3
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + BUTANE, 2-METHYL- 76 KER/PAR	350-750	9.6(+10)	0	3975*250	0.7 1.3
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\cdot$ METHYL FREE RADICAL + BUTANE, 2-METHYL- 76 KER/PAR	350-750	2.0(+11)	0	4830*250	0.7 1.3
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_4\text{C} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2\cdot$ METHYL FREE RADICAL + PROPANE, 2,2-DIMETHYL- 76 KER/PAR	350-750	7.1(+11)	0	5800*250	0.7 1.3
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)\text{C}(\cdot)$ METHYL FREE RADICAL + PENTANAL 76 KER/PAR	400-600	8.3(+11)	0	5940*350	0.6 1.4
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\cdot)$ METHYL FREE RADICAL + BUTANAL, 2-METHYL- 76 KER/PAR	350-500	1.0(+11)	0	3000*500	0.4 1.6
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CCH}_2\text{C}(\cdot)$ METHYL FREE RADICAL + BUTANAL, 3-METHYL- 76 KER/PAR	350-500	1.0(+11)	0	3200*500	0.5 2.0
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_3\text{CCH}_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CC}(\cdot)$ METHYL FREE RADICAL + PROPANE, 2,2-DIMETHYL- 76 KER/PAR	350-500	1.0(+11)	0	3070*500	0.4 1.6
NOTE: TENTATIVE k VALUE.	REACTION ORDER: 2. ----- $\text{CH}_3 \cdot + (\text{CH}_3)_2\text{CH}_2\text{C}(\cdot) \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{C}(\cdot)\text{CH}_3$ METHYL FREE RADICAL + 3-PENTANONE 76 KER/PAR	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
<p>-----  <math>\text{CH}_3 \cdot + (\text{CH}_3\text{CD}_2)_2\text{C}\ddot{\text{O}} \rightarrow \text{CH}_4 + \text{CH}_3\text{CD}_2\text{C}\ddot{\text{O}}\text{CD}_2\text{CH}_2 \cdot</math>  METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d<sub>4</sub>  REACTION ORDER: 2.  76 IER/PAR  -----</p>	500-600	2.0(+11)	0	5535*500	0.5 2.0
<p>-----  <math>\text{CH}_3 \cdot + (\text{CH}_3\text{CD}_2)_2\text{C}\ddot{\text{O}} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CD}_2\text{C}\ddot{\text{O}}\text{CD}(\cdot)\text{CH}_3</math>  METHYL FREE RADICAL + 3-PENTANONE-2,2,4,4-d<sub>4</sub>  REACTION ORDER: 2.  76 IER/PAR  -----</p>	500-600	1.3(+11)	0	4200*500	0.5 2.0
<p>-----  <math>\text{CH}_3 \cdot + \text{HC}\ddot{\text{O}}\text{C}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_4 + \cdot\text{C}\ddot{\text{O}}\text{C}(\text{CH}_2)_3\text{CH}_3</math>  <math>\text{HC}\ddot{\text{O}}\text{C}(\text{CH}_2)_3\text{CH}_3 + \text{HC}\ddot{\text{O}}\text{C}(\text{CH}_2)_3\text{CH}_3</math>  <math>\text{HC}\ddot{\text{O}}\text{C}(\text{CH}_2)_3\text{CH}_3 + \text{HC}\ddot{\text{O}}\text{C}(\text{CH}_2)_3\text{CH}_3</math>  METHYL FREE RADICAL + FORMALIC ACID BUTYL ESTER  76 IER/PAR  NOTE: TENTATIVE k VALUE.  -----</p>	350-500	2.5(+11)	0	4980*500	0.5 2.0
<p>-----  <math>\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{C}\ddot{\text{O}}\text{C}(\text{CH}_2)_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}(\cdot)\text{C}\ddot{\text{O}}\text{C}(\text{CH}_2)_2\text{CH}_3</math>  <math>\text{CH}_3\text{CH}_2\text{C}\ddot{\text{O}}\text{C}(\text{CH}_2)_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{C}\ddot{\text{O}}\text{C}(\text{CH}_2)_2\text{CH}_3</math>  <math>\text{CH}_3\text{CH}_2\text{C}\ddot{\text{O}}\text{C}(\text{CH}_2)_2\text{CH}_3</math>  METHYL FREE RADICAL + PROPANOIC ACID ETHYL ESTER  76 IER/PAR  -----</p>	300-650	2.5(+11)	0	4125*500	0.5 1.5
<p>-----  <math>\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)_2</math>  <math>\text{CH}_3\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2 + \text{CH}_3\text{CH}_2\text{N}(\text{CH}_2\text{CH}_3)_2</math>  METHYL FREE RADICAL + ETHANAMINE, N-ETHYL-N-METHYL-  76 IER/PAR  NOTE: TENTATIVE k VALUE.  -----</p>	420	3.0(+7)	-	-	0.5 2.0
<p>-----  <math>\text{CH}_3 \cdot + (\text{CH}_3)_2\text{NCO}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \cdot\text{C}(\text{CH}_3)_2\text{CON}(\text{CH}_3)_2</math>  METHYL FREE RADICAL + UREA TETRAMETHYL-  76 IER/PAR  -----</p>	350-550	2.0(+11)	0	3975*500	0.5 1.5
<p>-----  <math>\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}(\text{CH}_3)_2</math>  METHYL FREE RADICAL + cis-2-HEXENE  72 IER/PAR  -----</p>	298	-	-	4060	
<p>-----  <math>\text{CH}_3 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\cdot)\text{CH}_3</math>  METHYL FREE RADICAL + cis-2-HEXENE  72 IER/PAR  -----</p>	298	-	-	4150	
<p>-----  <math>\text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_3</math>  METHYL FREE RADICAL + 1-PENTENE, 2-METHYL-  72 IER/PAR  -----</p>	298	-	-	3450	
<p>-----  <math>\text{CH}_3 \cdot + \text{cis-}(\text{CH}_3)_2\text{CHCH}=\text{CHCH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}(\text{CH}_3)_2</math>  METHYL FREE RADICAL + cis-2-PENTENE, 4-METHYL-  72 IER/PAR  -----</p>	298	-	-	4390	
<p>-----  <math>\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}(\cdot)(\text{CH}_3)\text{CCH}_3</math>  METHYL FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL-  76 IER/PAR  -----</p>	403-614	7.8(+11)	0	4400*500	0.6 1.4

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
403-453	1.0(+10)	0	3400	
453	-	-	-	
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
<p>METHYL FREE RADICAL + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p> <p>NOTE: <math>k_{ref}: CH_3 + CH_2=CH_2</math> ----- <math>k/k_{ref}: 0.2</math></p> <p><math>CH_3 + CH_3(CH_2)_4CH_3 \rightarrow CH_4 + CH_3(CH_2)_4CH_2</math> METHYL FREE RADICAL + HEXANE 76 KER/PAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p> <p><math>CH_3 + CH_3(CH_2)_4CH_3 \rightarrow CH_4 + CH_3CH_2CH_2CH_2CH_2CH_3</math> <math>+ CH_3CH_2CH_2CH_2CH_2CH_2CH_3</math> METHYL FREE RADICAL + HEXANE 76 KER/PAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p> <p><math>CH_3 + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + \cdot CH_2CH(CH_3)CH(CH_3)_2</math> METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p> <p><math>CH_3 + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2C(\cdot)CH(CH_3)_2</math> METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 76 KER/PAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p> <p><math>CH_3 + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2CHC(\cdot)(CH_3)_2</math> <math>+ \cdot CH_3CH(CH_3)CH(CH_3)_2</math> METHYL FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p> <p><math>CD_3 + (CH_3)_2CHCH(CH_3)_2 \rightarrow CD_3H + (CH_3)_2C(\cdot)CH(CH_3)_2</math> <math>+ \cdot CH_2CH(CH_3)CH(CH_3)_2</math> METHYL-d<sub>3</sub> FREE RADICAL + BUTANE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2.</p> <p><math>CH_3 + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2C(\cdot)CH(CH_3)_2</math> <math>+ \cdot CH_2CH(CH_3)CH(CH_3)_2</math> METHYL FREE RADICAL + PROPANE, 2,2'-DIYBIS- 76 KER/PAR REACTION ORDER: 2.</p> <p><math>CH_3 + (CH_3)_2CHCH(CH_3)_2 \rightarrow CH_4 + (CH_3)_2C(\cdot)CH(CH_3)_2</math> <math>+ \cdot CH_2CH(CH_3)CH(CH_3)_2</math> METHYL FREE RADICAL + PEROXIDE, BIS(1-METHYLETHYL)- 76 KER/PAR REACTION ORDER: 2.</p> <p><math>CH_3 + CH_3CH=NC(CH_3)_3 \rightarrow CH_4 + CH_3C(\cdot)=NC(CH_3)_3</math> <math>+ \cdot CH_2CH=NC(CH_3)_3 + CH_3CH=NC(CH_3)_2CH_2</math> METHYL FREE RADICAL + PROPANIMINE, N-ETHYLIDENE-2-METHYL- 76 KER/PAR REACTION ORDER: 2.</p>				

## CHEMICAL REACTIONS

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

## CHEMICAL REACTIONS

T/K	A	B	E/R (in oK)	k factors f	k factors F
350-750	1.0(♦12)	0	5800*250	0.7	1.3
<p>CH<sub>3</sub> ♦ (CH<sub>3</sub>)<sub>2</sub>CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub> → CH<sub>4</sub>            ♦ CH<sub>2</sub>CH(CF<sub>3</sub>)CH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>            METHYL FREE RADICAL ♦ PENTANE, 2,3,4-TRIMETHYL-            REACTION ORDER: 2.            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
350-750	2.0(♦11)	0	3975*250	0.7	1.3
<p>CH<sub>3</sub> ♦ (CH<sub>3</sub>)<sub>2</sub>CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub> → CH<sub>4</sub>            ♦ (CH<sub>3</sub>)<sub>2</sub>CHC(O)(CH<sub>3</sub>)C(O)CH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>            METHYL FREE RADICAL ♦ PENTANE, 2,3,4-TRIMETHYL-            REACTION ORDER: 2.            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
414-605	4.7(♦11)	0	4575		
<p>CH<sub>3</sub> ♦ (CH<sub>3</sub>)<sub>2</sub>CHCH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub> → CH<sub>4</sub> ♦ [C<sub>8</sub>H<sub>17</sub>•]            METHYL FREE RADICAL ♦ PENTANE, 2,3,4-TRIMETHYL-            REACTION ORDER: 2.            72 KEN</p>					
350-800	1.0(♦12)	0	5800*250	0.7	1.3
<p>CH<sub>3</sub> ♦ (CH<sub>3</sub>)<sub>3</sub>CC(CH<sub>3</sub>)<sub>3</sub> → CH<sub>4</sub> ♦ CH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>C(CH<sub>3</sub>)<sub>3</sub>            METHYL FREE RADICAL ♦ BUTANE, 2,2,3,3-TETRAMETHYL-            REACTION ORDER: 2.            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
350-500	1.0(♦12)	0	5900*750	0.3	3.0
<p>CH<sub>3</sub> ♦ (CH<sub>3</sub>)<sub>3</sub>COOC(CH<sub>3</sub>)<sub>3</sub> → CH<sub>4</sub> ♦ CH<sub>2</sub>C(CH<sub>3</sub>)<sub>2</sub>COOC(CH<sub>3</sub>)<sub>3</sub>            METHYL FREE RADICAL ♦ PEROXIDE, BIS(1,1-DIMETHYLETHYL)-            REACTION ORDER: 2.            76 KER/PAR</p>					
1200-1800	2.0(♦15)	0	52340		
<p>CH<sub>4</sub> → CH<sub>3</sub> ♦ H            METHANE            REACTION ORDER: 1.            70 BEN/θ'N</p>					
350-1000	2.0(♦13)	0	4550	0.7	1.3
<p>CH<sub>4</sub> ♦ θ → CH<sub>3</sub> ♦ θH            METHANE ♦ OXYGEN ATOM            REACTION ORDER: 2.            73 BER/HUI</p>					
1500-2500	2.0(♦13)	0	4530*500	0.6	1.6
<p>CH<sub>4</sub> ♦ θ → CH<sub>3</sub> ♦ θH            METHANE ♦ OXYGEN ATOM            REACTION ORDER: 2.            76 ENG</p>					
1500-2500	6.0(♦13)	0	5990*150	0.5	2.0
<p>CH<sub>4</sub> ♦ H → CH<sub>3</sub> ♦ H<sub>2</sub>            METHANE ♦ HYDROGEN ATOM            REACTION ORDER: 2.            76 ENG</p>					
523-673	8.0(♦12)	0	5100		
<p>CH<sub>4</sub> ♦ D → CH<sub>3</sub> ♦ HD            METHANE ♦ DEUTERIUM ATOM            REACTION ORDER: 2.            72 KEN</p>					
1500-2500	3.0(♦13)	0	2500*250	0.5	2.0
<p>CH<sub>4</sub> ♦ θH → CH<sub>3</sub> ♦ H<sub>2</sub>θ            METHANE ♦ HYDROXYL FREE RADICAL            REACTION ORDER: 2.            76 ENG</p>					
1500-2500	2.5(♦11)	0.7	3000*2500	0.3	3.2
<p>CH<sub>4</sub> ♦ CH → CH<sub>3</sub> ♦ :CH<sub>2</sub>            METHANE ♦ METHYLLYLENE FREE RADICAL            REACTION ORDER: 2.            76 ENG</p>					

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
<p>-----  <math>\text{CH}_4 + \text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_3</math>            METHANE + METHYLENE FREE RADICAL            REACTION ORDER: 2.            76 ENG            -----</p>	1500-2500	1.3(+12)	0.7	10000±2500	0.3 3.2
<p>-----  <math>\text{CH}_4 + \text{CH}_3 \rightarrow \text{CH}_3 + \text{CH}_4</math>            METHANE + METHYL FREE RADICAL            REACTION ORDER: 2.            76 KBI/PAR            -----</p>	450-800	4.0(+11)	0	7045±250	0.7 1.3
<p>-----  <math>\text{CH}_3\text{D} + \text{CD}_3 \rightarrow \text{CH}_3 + \text{CD}_4</math>            METHANE-d + METHYL-d<sub>3</sub> FREE RADICAL            REACTION ORDER: 2.            76 KER/PAR            NOTE: TENTATIVE k VALUE.            -----</p>	400-650	5.0(+10)	0	7200±500	0.5 1.5
<p>-----  <math>\text{CHD}_3 + \text{CH}_3 \rightarrow \text{CD}_3 + \text{CH}_4</math>            METHANE-d<sub>3</sub> + METHYL FREE RADICAL            REACTION ORDER: 2.            76 KER/PAR            NOTE: TENTATIVE k VALUE.            -----</p>	400-650	1.1(+11)	0	6995±250	0.7 1.3
<p>-----  <math>\text{CD}_4 + \text{CH}_3 \rightarrow \text{CD}_3 + \text{CDH}_3</math>            METHANE-d<sub>4</sub> + METHYL FREE RADICAL            REACTION ORDER: 2.            76 KER/PAR            -----</p>	370-550	2.5(+11)	0	7700±500	0.5 1.5
<p>-----  <math>\text{CD}_4 + \text{CD}_3 \rightarrow \text{CD}_3 + \text{CD}_4</math>            METHANE-d<sub>4</sub> + METHYL-d<sub>3</sub> FREE RADICAL            REACTION ORDER: 2.            72 ION            -----</p>	473-623	4.1(+12)	0	8950±250	
<p>-----  <math>\text{CH}_4 + \text{CN} \rightarrow \text{HCN} + \text{CH}_3</math>            METHANE + CYANOGEN FREE RADICAL            REACTION ORDER: 2.            76 ENG            -----</p>	1500-2500	3.2(+11)	0.7	2500±2500	0.3 3.2
<p>-----  <math>\text{CH}_4 + \text{M} \rightarrow \text{CH}_3 + \text{H} + \text{M}</math>            METHANE            REACTION ORDER: 2.            76 ENG            -----</p>	1500-2500	2.0(+17)	0	44035±1000	0.5 2.0
<p>-----  <math>\cdot\text{CH}_3 + \text{C}_6 \rightarrow \text{C}_6 + \text{H}</math>            METHYL, C<sub>6</sub>-, FREE RADICAL            REACTION ORDER: 1.            70 BBN/G*N            -----</p>	298	5.0(+13)	0	9560	
<p>-----  <math>\cdot\text{CH}_3 + \text{O} \rightarrow \text{CO}_2 + \text{H}</math>            METHYL, C<sub>1</sub>-, FREE RADICAL + OXYGEN ATOM            REACTION ORDER: 2.            76 ENG            NOTE: k ESTIMATED.            -----</p>	1500-2500	3.2(+11)	0	0±1500	
<p>-----  <math>\cdot\text{CH}_3 + \text{O} \rightarrow \text{CO} + \text{OH}</math>            METHYL, C<sub>1</sub>-, FREE RADICAL + OXYGEN ATOM            REACTION ORDER: 2.            76 ENG            NOTE: k ESTIMATED.            -----</p>	1500-2500	3.2(+11)	1.0	250±1500	
<p>-----  <math>\cdot\text{CH}_3 + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2</math>            METHYL, C<sub>1</sub>-, FREE RADICAL + OXYGEN MOLECULE            REACTION ORDER: 2.            76 ENG            NOTE: k ESTIMATED.            -----</p>	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

.CH<sub>3</sub> + H → C<sub>2</sub> + H<sub>2</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + HYDROGEN ATOM  
 REACTION ORDER: 2.  
 -----  
 .CH<sub>3</sub> + OH → C<sub>2</sub> + H<sub>2</sub>O  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + HYDROXYL FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 NOTE: k ESTIMATED.  
 -----  
 .CH<sub>3</sub> + H<sub>2</sub>O → HCHO + H<sub>2</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + HYDROPEROXYL FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 NOTE: k ESTIMATED.  
 -----  
 .CH<sub>3</sub> + N → HCN + H  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + NITROGEN ATOM  
 REACTION ORDER: 2.  
 76 ENG  
 NOTE: k ESTIMATED.  
 -----  
 .CH<sub>3</sub> + N → C<sub>2</sub> + NH  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + NITROGEN ATOM  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + NO → C<sub>2</sub> + HNO  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + NITROGEN OXIDE(N<sub>2</sub>)  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + HNO → HCHO + NO  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + NITROSYL HYDRIDE  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + CH → C<sub>2</sub> + CH<sub>2</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + METHYLIDENE FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + CH<sub>2</sub> → C<sub>2</sub> + CH<sub>3</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + METHYLENE FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + CH<sub>3</sub> → C<sub>2</sub> + CH<sub>4</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + METHYL FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + .CH<sub>3</sub> → HCHO + C<sub>2</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + METHYL FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 .CH<sub>3</sub> + CN → HCN + C<sub>2</sub>  
 METHYL, CH<sub>3</sub>°, FREE RADICAL + CYANOGEN FREE RADICAL  
 REACTION ORDER: 2.  
 76 ENG  
 -----  
 HCHO + H → .CH<sub>3</sub> + OH

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f	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 BEE/HUI REACTION ORDER: 2. -----	300	9.0(+10)	-	-	0.7	1.3
HCHO + H → products FORMALDEHYDE-d + OXYGEN ATOM 73 BEE/HUI REACTION ORDER: 2. -----	300	4.9(+10)	-	-	0.7	1.3
HCHO + H → .CHO + H <sub>2</sub> FORMALDEHYDE + HYDROGEN ATOM 76 ENG REACTION ORDER: 2. -----	1500-2500	1.3(+10)	1.0	1600	0.3	3.2
HCHO + OH → .CHO + H <sub>2</sub> O FORMALDEHYDE + HYDROXYL FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	3.2(+10)	1.0	0±1500	0.5	2.0
HCHO + H <sub>2</sub> → .CHO + H <sub>2</sub> O <sub>2</sub> FORMALDEHYDE + HYDROPEROXYL FREE RADICAL 74 LIC REACTION ORDER: 2. NOTE: k FACTORS ARE: f = 0.1; F = 10. AT 300K. -----	300-800	1.0(+12)	0	4000	0.7	1.5
HCHO + CH → .CHO + CH <sub>2</sub> FORMALDEHYDE + METHYLIDENE FREE RADICAL 76 ENG REACTION ORDER: 2. -----	1500-2500	1.0(+11)	0.7	2000±2500	0.3	3.2
HCHO + CH <sub>2</sub> → .CHO + CH <sub>3</sub> FORMALDEHYDE + METHYLENE FREE RADICAL 76 ENG REACTION ORDER: 2. NOTE: k ESTIMATED. -----	1500-2500	2.0(+11)	0	3270±1500	-	-
HCHO + CH <sub>3</sub> → .CHO + CH <sub>4</sub> FORMALDEHYDE + METHYL FREE RADICAL 76 BEE/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 <sub>3</sub> → .CDO + CH <sub>3</sub> D FORMALDEHYDE-d + METHYL FREE RADICAL 76 BEE/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	4300±2500	0.3	3.2
.CH <sub>2</sub> 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 °K)	k factors f
CH <sub>3</sub> O • O → HCHO • OH METHOXY FREE RADICAL • OXYGEN ATOM 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	1500-2500	1.0(•14)	0	0±1500	
CH <sub>3</sub> O • O <sub>2</sub> → HCOO • HO <sub>2</sub> METHOXY FREE RADICAL • OXYGEN MOLECULE 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	1500-2500	1.0(•12)	0	3000±1500	
CH <sub>3</sub> O • H → HCO • H <sub>2</sub> METHOXY FREE RADICAL • HYDROGEN ATOM 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	1500-2500	1.0(•14)	0	0±1500	
CH <sub>3</sub> O • OH → HCO • H <sub>2</sub> O METHOXY FREE RADICAL • HYDROXY FREE RADICAL 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	1500-2500	3.2(•13)	0	0±1500	
CH <sub>3</sub> O • N → HCO • NH METHOXY FREE RADICAL • NITROGEN ATOM 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	1500-2500	1.0(•14)	0	0±1500	
CH <sub>3</sub> O • M → HCO • H • M METHOXY FREE RADICAL 76 ENG NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	1500-2500	4.0(•40)	-1.5	11375±1500	
CH <sub>3</sub> OH + CH <sub>3</sub> • → •CH <sub>2</sub> OH + CH <sub>4</sub> METHANOL • METHYL FREE RADICAL 76 IHR/PAR NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	350-500	1.9(•11)	0	5035±500	0.6 1.4
CH <sub>3</sub> OH + CH <sub>3</sub> • → CH <sub>3</sub> O • + CH <sub>4</sub> METHANOL • METHYL FREE RADICAL 76 IHR/PAR NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	350-550	6.2(•10)	0	4900±500	0.6 1.4
CH <sub>3</sub> OD + CD <sub>3</sub> • → •CH <sub>2</sub> OD + CD <sub>3</sub> H METHANOL-d • METHYL-d <sub>3</sub> FREE RADICAL 76 IHR/PAR NOTE: k ESTIMATED.	----- REACTION ORDER: 2.	400-500	1.9(•11)	0	5000±500	0.5 2.0
CH <sub>3</sub> OD + CD <sub>3</sub> • → CH <sub>3</sub> O • + CD <sub>4</sub> METHANOL-d • METHYL-d <sub>3</sub> FREE RADICAL 76 IHR/PAR NOTE: GIVEN WITH CAUTION.	----- REACTION ORDER: 2.	400-500	3.2(•10)	0	5700±1000	0.5 2.0
CD <sub>3</sub> OH + CH <sub>3</sub> • → •CD <sub>2</sub> OH + CH <sub>3</sub> D METHAN-d <sub>3</sub> -OL • METHYL FREE RADICAL 76 IHR/PAR NOTE: GIVEN WITH CAUTION.	----- REACTION ORDER: 2.	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 REACTION ORDER: 2. ----- $CD_3OH + CH_3 \rightarrow CD_3O + CH_4$ METHAN- $d_3$ -OL + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. -----	370-550	2.0(+11)	0	5540+500	0.6
$CH_3OOH \rightarrow CH_3O + OH$ HYDROPEROXIDE, METHYL 70 BEN/C*N REACTION ORDER: 1. NOTE: RATE CONSTANTS MAY BE SLIGHTLY LOW. -----	370-550	6.2(+10)	0	4900+500	1.4
$CS + O \rightarrow S + CO$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN ATOM 76 BAU/DRY REACTION ORDER: 2. -----	565-651	7.9(+14)	0	21640	0.5
$CS + O \rightarrow S + CO$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----	300	1.3(+13)	-	-	1.5
$CS + O \rightarrow SC + C$ CARBON MONOSULFIDE FREE RADICAL + OXYGEN 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$CS + H \rightarrow S + CH$ CARBON MONOSULFIDE FREE RADICAL + HYDROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----		1.6(+12)	0.5	28940	
$CS + H \rightarrow SH + C$ CARBON MONOSULFIDE FREE RADICAL + HYDROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----		1.3(+13)	0.5	50530	
$CS + S \rightarrow S + CS$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. -----		2.0(+13)	0.5	48870	
$CS + S \rightarrow C + S_2$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 75 BEN/GGL REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
$CS + S + M \rightarrow CS_2 + M$ CARBON MONOSULFIDE FREE RADICAL + SULFUR ATOM 76 BAU/DRY REACTION ORDER: 3. NOTE: $k_1 = k_{-1}$ -----	1800-3700	1.6(+12)	0.5	40463	0.5
$CS + N \rightarrow S + CN$ CARBON MONOSULFIDE FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----		8.7(+13)	0	4370	1.5
$CS + N \rightarrow C + NS$ CARBON MONOSULFIDE FREE RADICAL + NITROGEN ATOM 75 BEN/GGL REACTION ORDER: 2. -----		1.3(+12)	0.5	1160	
$CS + C \rightarrow S + C_2$ -----		4.0(+12)	0.5	37200	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
CARBON MONOSULFIDE FREE RADICAL + CARBON ATOM REACTION ORDER: 2. ----- CS + C → C + CS CARBON MONOSULFIDE FREE RADICAL + CARBON ATOM REACTION ORDER: 2. -----		5.0(+11)	0.5	20435	
CARBON DISULFIDE + OXYGEN ATOM REACTION ORDER: 2. ----- CS <sub>2</sub> + O → CS + SO CARBON DISULFIDE + OXYGEN ATOM REACTION ORDER: 2. -----	200-1000	2.2(+13)	0	700	0.7 1.3
CARBON DISULFIDE + OXYGEN ATOM REACTION ORDER: 2. ----- CS <sub>2</sub> + O → COS + S CARBON DISULFIDE + OXYGEN ATOM REACTION ORDER: 2. -----	302	2.2(+11)	-	-	0.5 1.5
CARBON DISULFIDE + SULFUR ATOM REACTION ORDER: 2. ----- CS <sub>2</sub> + S → CS + S <sub>2</sub> CARBON DISULFIDE + SULFUR ATOM REACTION ORDER: 2. -----	298	3.9(+11)	-	-	0.5 1.5
CARBON DISULFIDE + M REACTION ORDER: 2. M: AR ----- CS <sub>2</sub> + M → CS + S + M CARBON DISULFIDE REACTION ORDER: 2. -----	1800-3700	2.6(+15)	0	38960±9000	0.5 1.5
CARBON DIOXIDE SULFIDE + OXYGEN ATOM REACTION ORDER: 2. ----- COS + O → CO + SO CARBON DIOXIDE SULFIDE + OXYGEN ATOM 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 300K. ----- COS + H → CO + HS CARBON DIOXIDE SULFIDE REACTION ORDER: 2. -----	298	1.3(+10)	-	-	0.8 1.3
CARBON DIOXIDE SULFIDE + SULFUR ATOM REACTION ORDER: 2. ----- COS + S → CO + S <sub>2</sub> CARBON DIOXIDE SULFIDE + SULFUR ATOM REACTION ORDER: 2. -----	230-2600	1.7(+12)	0	2050±230	0.3 3.0
CH <sub>3</sub> S + CR=CH → CH <sub>3</sub> SCH=CH. METHYLTHIO FREE RADICAL + ETHYLENE REACTION ORDER: 2. ----- CH <sub>3</sub> S + CH <sub>2</sub> -CH <sub>2</sub> → CH <sub>3</sub> SCH <sub>2</sub> CH <sub>2</sub> . METHYLTHIO FREE RADICAL + ETHYLENE REACTION ORDER: 2. -----	298-333	7.9(+7)	-	-	
CH <sub>3</sub> S + CH <sub>3</sub> CE-CHCH <sub>3</sub> → CH <sub>3</sub> CH(SCH <sub>3</sub> )C(CH <sub>3</sub> )CH <sub>3</sub> METHYLTHIO FREE RADICAL + 2-BUTENE REACTION ORDER: 2. ----- NOTE: cis-trans EQUILIBRIUM - WEIGHTED k. -----	298	4.8(+8)	-	-	
CH <sub>3</sub> SH → CH <sub>3</sub> + SH METHANETHIOL REACTION ORDER: 1. ----- 70 BEN/6'N	1005-1102	3.2(+15)	0	38550	

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
CH <sub>3</sub> SH + CH <sub>3</sub> - CH <sub>3</sub> S. + CH <sub>2</sub> SH + CH <sub>4</sub> METHANETHIOL + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----	303	1.2(+8)	-	-	0.5 2.0
CD <sub>3</sub> SH + CH <sub>3</sub> - CD <sub>3</sub> S. + CD <sub>2</sub> SH + CH <sub>4</sub> METHANE-d <sub>3</sub> -THIOL + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----	400-500	1.1(+11)	0	2065*500	0.5 2.0
CD <sub>3</sub> SH + CH <sub>3</sub> - CD <sub>2</sub> SH + CH <sub>3</sub> D METHANE-d <sub>3</sub> -THIOL + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----	400-500	7.6(+10)	0	4200*250	0.5 2.0
CN + O - N + CO CYANOGEN FREE RADICAL + OXYGEN ATOM 76 ENG	REACTION ORDER: 2. -----	1500-2500	1.0(+12)	0	0*2500	0.3 3.2
CN + O - N + C CYANOGEN FREE RADICAL + OXYGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		1.3(+12)	0.5	14545	
CN + O <sub>2</sub> - N + CO CYANOGEN FREE RADICAL + OXYGEN MOLECULE 76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+11)	0	0*5000	0.3 3.2
CN + H - N + CH CYANOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+12)	0.5	49775	
CN + H - N + C CYANOGEN FREE RADICAL + HYDROGEN ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		1.0(+13)	0.5	52745	
CN + H + M - HCN + M CYANOGEN FREE RADICAL + HYDROGEN ATOM 76 ENG	REACTION ORDER: 3. -----	1500-2500	3.2(+16)	-0.5	0*2500	0.3 3.2
CN + H <sub>2</sub> - HCN + H CYANOGEN FREE RADICAL + HYDROGEN MOLECULE 76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	2500*1500	
CN + OH - HCN + O CYANOGEN FREE RADICAL + HYDROXYL FREE RADICAL 76 ENG	REACTION ORDER: 2. -----	1500-2500	3.2(+12)	0	1500*1500	
CN + S - N + CS CYANOGEN FREE RADICAL + SULFUR ATOM 75 BEN/GOL	REACTION ORDER: 2. -----		6.3(+11)	0.5	0	
CN + S - C + 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 <sub>2</sub> CYANOGEN FREE RADICAL + NITROGEN ATOM REACTION ORDER: 2. 75 BEN/GGL -----		6.3(+11)	0.5	0	
CN + N <sub>2</sub> → C <sub>2</sub> + N <sub>2</sub> CYANOGEN FREE RADICAL + NITROGEN OXIDE(N <sub>2</sub> ) REACTION ORDER: 2. 76 ENG -----	1500-2500	3.2(+11)	0	0 ± 2500	0.3 3.2
CN + NH → HCN + N CYANOGEN FREE RADICAL + IMIDGEN FREE RADICAL REACTION ORDER: 2. 76 ENG -----	1500-2500	1.0(+11)	0.5	1000 ± 2500	0.3 3.2
CN + HNO → HCN + NO CYANOGEN FREE RADICAL + NITROSYL HYDRIDE REACTION ORDER: 2. 76 ENG -----	1500-2500	4.0(+11)	0.5	0 ± 2500	0.3 3.2
CN + C → N + C <sub>2</sub> CYANOGEN FREE RADICAL + CARBON ATOM REACTION ORDER: 2. 75 BEN/GGL -----		2.5(+11)	0.5	19300	
CN + C → C + CN CYANOGEN FREE RADICAL + CARBON ATOM REACTION ORDER: 2. 75 BEN/GGL -----		6.3(+11)	0.5	0	
CN + CH <sub>2</sub> → HCN + CH CYANOGEN FREE RADICAL + METHYLENE FREE RADICAL REACTION ORDER: 2. 76 ENG NOTE: k ESTIMATED. -----	1500-2500	3.2(+12)	0	2500 ± 1500	
CN + CH <sub>3</sub> → HCN + CH <sub>2</sub> CYANOGEN FREE RADICAL + METHYL FREE RADICAL REACTION ORDER: 2. 76 ENG -----	1500-2500	1.0(+11)	0.7	1500 ± 2500	0.3 3.2
CN + CH <sub>4</sub> → HCN + CH <sub>3</sub> CYANOGEN FREE RADICAL + METHANE REACTION ORDER: 2. 76 ENG -----	1500-2500	3.2(+11)	0.7	2500 ± 2500	0.3 3.2
CN + C <sub>2</sub> H <sub>4</sub> → C <sub>2</sub> + HCN CYANOGEN FREE RADICAL + METHYL, ETHYL, FREE RADICAL REACTION ORDER: 2. 76 ENG -----	1500-2500	2.0(+11)	0.5	0 ± 2500	0.3 3.2
CN + HCHO → HCN + CH <sub>2</sub> CYANOGEN FREE RADICAL + FORMALDEHYDE REACTION ORDER: 2. 76 ENG -----	1500-2500	1.3(+11)	0.7	1500 ± 2500	0.3 3.2
C(N <sub>2</sub> ) <sub>4</sub> → C(N <sub>2</sub> ) <sub>3</sub> + N <sub>2</sub> METHANE, TETRAMETHYL- 70 BEN/d'n REACTION ORDER: 1. -----	443-506	3.4(+17)	0	20575	
HCN + OH → CN + H <sub>2</sub> O HYDROCYANIC ACID + HYDROXYL FREE RADICAL REACTION ORDER: 2. 76 ENG -----	1500-2500	2.0(+11)	0.6	2500 ± 2500	0.3 3.2

## CHEMICAL REACTIONS

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

CH<sub>3</sub>NH<sub>2</sub> + CH<sub>3</sub> → CH<sub>3</sub>NH + •CH<sub>2</sub>NH<sub>2</sub> + CH<sub>4</sub>  
 METHANAMINE + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.

CH<sub>3</sub>NH<sub>2</sub> + CH<sub>3</sub> → •CH<sub>2</sub>NH<sub>2</sub> + CH<sub>4</sub>  
 METHANAMINE + METHYL FREE RADICAL  
 72 ICN  
 REACTION ORDER: 2.

CH<sub>3</sub>ND<sub>2</sub> + CH<sub>3</sub> → CH<sub>3</sub>ND + CH<sub>3</sub>D  
 METHANAMINE-d<sub>2</sub> + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: TENTATIVE k VALUE.

CH<sub>3</sub>ND<sub>2</sub> + CH<sub>3</sub> → •CH<sub>2</sub>ND<sub>2</sub> + CH<sub>4</sub>  
 METHANAMINE-d<sub>2</sub> + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.

CD<sub>3</sub>NH<sub>2</sub> + CH<sub>3</sub> → •CD<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub>D  
 METHAN-d<sub>3</sub>-AMINE + METHYL FREE RADICAL  
 72 KER/PAR  
 REACTION ORDER: 2.

CD<sub>3</sub>NH<sub>2</sub> + CH<sub>3</sub> → CD<sub>3</sub>NH + •CH<sub>4</sub>  
 METHAN-d<sub>3</sub>-AMINE + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: TENTATIVE k VALUE.

CH<sub>2</sub>-N=N → CH<sub>2</sub> + N<sub>2</sub>  
 METHANE, DIAZO-  
 70 HEN/G'N  
 REACTION ORDER: 1.

CH<sub>3</sub>NHNH<sub>2</sub> → CH<sub>3</sub>NH + NH<sub>2</sub>  
 HYDRAZINE, METHYL-  
 70 HEN/G'N  
 REACTION ORDER: 1.  
 NOTE: SUSPECT ARRHENIUS FACTORS.

CH<sub>3</sub>NHNH<sub>2</sub> + CH<sub>3</sub> → CH<sub>3</sub>N(•)NH<sub>2</sub> + CH<sub>3</sub>NHNH.  
 •CH<sub>2</sub>NHNH<sub>2</sub> + CH<sub>4</sub>  
 HYDRAZINE, METHYL-, + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: TENTATIVE k VALUE.

CH<sub>3</sub>NO → CH<sub>2</sub>-NOH  
 METHANE, NITROSO-  
 70 HEN/G'N  
 REACTION ORDER: 1.

HC≡NH<sub>2</sub> + CH<sub>3</sub> → HCCNH + •C≡NH<sub>2</sub> + CH<sub>4</sub>  
 FORMAMIDE + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.

HC≡ND<sub>2</sub> + CH<sub>3</sub> → HCCND + CH<sub>3</sub>D  
 FORMAMIDE-N<sub>2</sub>-d<sub>2</sub> + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.

CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	F
350-500	5.5(+10)	0	3575±500	0.5	2.0
453-513	4.0(+15)	0	20700		
660	4.0(+15)	0	29700		
300-500	1.0(+11)	0	5100±750	0.4	2.5
483-513	3.2(+15)	0	20030		
300-500	5.0(+10)	0	2265±500	0.5	1.5
300-500	3.5(+10)	0	2970±500	0.5	1.5
	6.3(+11)	0.5	0		
	1.6(+13)	0.5	30450		
	6.3(+11)	0.5	0		
	6.3(+11)	0.5	0		
	6.3(+11)	0.5	0		

NOTE: TENTATIVE k VALUE.

HCND<sub>2</sub> + CH<sub>3</sub> → •CND<sub>2</sub> + CH<sub>4</sub>  
 FORMAMIDE-N,N-d<sub>2</sub> + METHYL FREE RADICAL  
 REACTION ORDER: 2.

CH<sub>3</sub>NO → CH<sub>3</sub>• + NO  
 NITROUS ACID METHYL ESTER  
 REACTION ORDER: 1.

CH<sub>3</sub>NO<sub>2</sub> → CH<sub>3</sub>• + NO<sub>2</sub>  
 METHANE, NITRO-  
 REACTION ORDER: 1.

CH<sub>3</sub>NO<sub>2</sub> + CH<sub>3</sub>• → CH<sub>2</sub>NO<sub>2</sub> + CH<sub>4</sub>  
 METHANE, NITRO- + METHYL FREE RADICAL  
 REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

CH<sub>3</sub>NO<sub>2</sub> → CH<sub>3</sub>• + NO<sub>2</sub>  
 NITRIC ACID METHYL ESTER  
 REACTION ORDER: 1.

CH<sub>3</sub>ONH<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>ONH• + CH<sub>4</sub>  
 HYDROXYLAMINE, O-METHYL-, + METHYL FREE RADICAL  
 REACTION ORDER: 2.

CH<sub>3</sub>OND<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>ND• + CH<sub>3</sub>D  
 HYDROXYLAMINE-N,N-d<sub>2</sub>, O-METHYL-, + METHYL FREE RADICAL  
 REACTION ORDER: 2.

C<sub>2</sub> + O → C + CO  
 CARBON DIMER + OXYGEN ATOM  
 REACTION ORDER: 2.

C<sub>2</sub> + H → C + CH  
 CARBON DIMER + HYDROGEN ATOM  
 REACTION ORDER: 2.

C<sub>2</sub> + S → C + CS  
 CARBON DIMER + SULFUR ATOM  
 REACTION ORDER: 2.

C<sub>2</sub> + N → C + CN  
 CARBON DIMER + NITROGEN ATOM  
 REACTION ORDER: 2.

C<sub>2</sub> + C → C + C<sub>2</sub>  
 CARBON DIMER + CARBON ATOM  
 REACTION ORDER: 2.

COO + CH=CH → products  
 CARBON OXIDE(C<sub>2</sub>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: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	304	-	-	-	
$CC_2 \cdot CH_2 \cdot CH_2 \rightarrow C_6 \cdot CH_2 \cdot C \cdot CH_2$ CARBON OXIDE(C <sub>2</sub> O) + 1-FRIPPENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 5.7 NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	297	-	-	-	
$CC_2 \cdot CH_2 \cdot C \cdot CCH_3 \rightarrow$ Products CARBON OXIDE(C <sub>2</sub> O) + 2-BUTYNE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 8.5 NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	304	-	-	-	
$CC_2 \cdot CH_2 \cdot CHCH=CH_2 \rightarrow C_6 \cdot CH_2 \cdot C \cdot CHCH=CH_2$ CARBON OXIDE(C <sub>2</sub> O) + 1,3-BUTADIENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 210. NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	298	-	-	-	
$CC_2 \cdot CH_2 \cdot CH_2 \cdot CH=CH_2 \rightarrow CH_3 \cdot CH_2 \cdot CH \cdot C \cdot CH_2 \cdot C_6$ CARBON OXIDE(C <sub>2</sub> O) + 1-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 7.0 NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	298	-	-	-	
$CC_2 \cdot cis-CH_3 \cdot CH=CHCH_3 \rightarrow C_6 \cdot cis-CH_3 \cdot CH=C \cdot CHCH_3$ CARBON OXIDE(C <sub>2</sub> O) + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 9.1 NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	297	-	-	-	
$CC_2 \cdot trans-CH_3 \cdot CH=CHCH_3 \rightarrow C_6 \cdot trans-CH_3 \cdot CH=C \cdot CHCH_3$ CARBON OXIDE(C <sub>2</sub> O) + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 10.6 NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	297	-	-	-	
$CC_2 \cdot (CH_3)_2 \cdot C \cdot CH_2 \rightarrow C_6 \cdot (CH_3)_2 \cdot C \cdot C \cdot CH_2$ CARBON OXIDE(C <sub>2</sub> O) + 1-FRIPPENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 50.0 NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	297	-	-	-	
$CC_2 \cdot (CH_3)_2 \cdot C \cdot CHCH_3 \rightarrow C_6 \cdot (CH_3)_2 \cdot C \cdot C \cdot CHCH_3$ CARBON OXIDE(C <sub>2</sub> O) + 2-BUTENE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 100. NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	298	-	-	-	
$CC_2 \cdot (CH_3)_2 \cdot C \cdot C \cdot (CH_3)_2 \rightarrow C_6 \cdot (CH_3)_2 \cdot C \cdot C \cdot C \cdot (CH_3)_2$ CARBON OXIDE(C <sub>2</sub> O) + 2-BUTENE, 2,3-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 250. NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	298	-	-	-	
$CC_2 \cdot (CH_3)_2 \cdot C \cdot C \cdot C \cdot (CH_3)_2 \rightarrow C_6 \cdot (CH_3)_2 \cdot C \cdot C \cdot C \cdot (CH_3)_2$ CARBON OXIDE(C <sub>2</sub> O) + 2,3-PENTADIENE, 2,4-DIMETHYL- 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}$ : 113. NOTE: $k_{ref}$ : $CC_2 \cdot CH_2 \cdot CH_2$	304	-	-	-	



CHEMICAL REACTIONS	T/K	A	B	E/R (in OK)	k factors f
CH <sub>3</sub> CH + d → products ETHYNE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. -----	200-700	1.4(+13)	0	1500	0.8 1.2
CH <sub>3</sub> CH + OH → CH <sub>3</sub> C. + H <sub>2</sub> O ETHYNE + HYDROXYL FREE RADICAL 72 KER REACTION ORDER: 2. -----	300-2000	7.6(+12)	0	2335+400	0.5 2.1
CH <sub>3</sub> CH + S → cy-CH=CHS ETHYNE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. -----	298	1.7(+11)	-	-	-
CH <sub>3</sub> CH + N → C <sub>2</sub> H <sub>2</sub> N ETHYNE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. ----- NOTE: UPPER LIMIT.	440	2.0(+9)	-	-	-
CH <sub>3</sub> CH + CH <sub>3</sub> → CH <sub>3</sub> C. + CH <sub>4</sub> ETHYNE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- NOTE: GIVEN WITH CAUTION.	473-773	-	-	7100	-
CH <sub>3</sub> CH + CH <sub>3</sub> → CH <sub>3</sub> CH=CH. ETHYNE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	371-479	2.5(+11)	0	3900	-
CH <sub>3</sub> CH + CH <sub>3</sub> S → CH <sub>3</sub> SCH=CH. ETHYNE + METHYLTHIO FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	298-333	7.9(+7)	-	-	-
CH <sub>3</sub> CH + CCO → products ETHYNE + CARBON OXIDE(C <sub>2</sub> O) 72 KER/PAR REACTION ORDER: 2. k/k <sub>ref</sub> : 0.3 NOTE: k <sub>ref</sub> : CH <sub>2</sub> =CH <sub>2</sub> + CCO -----	304	-	-	-	-
CH <sub>3</sub> CH + CH <sub>3</sub> CH <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> CH=CH. ETHYNE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. -----	373-473	5.0(+10)	0	3500	-
CH <sub>3</sub> CH + (CH <sub>3</sub> ) <sub>2</sub> CH. → (CH <sub>3</sub> ) <sub>2</sub> CHCH=CH. ETHYNE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----	3475	5.0(+10)	0	3475	-
CH <sub>3</sub> CH + (CH <sub>3</sub> ) <sub>3</sub> C. → (CH <sub>3</sub> ) <sub>3</sub> CCH=CH. ETHYNE + ETHYL, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. -----	363-577	1.0(+11)	0	3675	-
cis-CDH=CDH → trans-CDH=CHD cis-ETHENE-1,2-d <sub>2</sub> 70 HEN/6'N REACTION ORDER: 1. -----	723-823	1.0(+13)	0	32700	-

CHEMICAL REACTIONS	T/K	A	B	E/R (ln OK)	k factors f
$\text{CH}_2=\text{CH}_2 + \text{O} \rightarrow \text{cy-CH}_2\text{CH}_2\text{O}$ 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	
$\text{CH}_2=\text{CH}_2 + \text{H} + \text{M} \rightarrow \text{CH}_2\text{CH}_2\cdot + \text{M}$ ETHENE + HYDROGEN ATOM 72 ION REACTION ORDER: 3. M: H <sub>2</sub> -----	298-813	5.6(+17)	0.5	495	
$\text{CH}_2=\text{CH}_2 + \text{OH} \rightarrow \text{CH}_2=\text{CH}\cdot + \text{H}_2\text{O}$ 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 + HYDROXYL FREE RADICAL 74 LIQ REACTION ORDER: 2. NOTE: RATIO DATA VERSUS kref. FOR H <sub>2</sub> + C <sub>6</sub> → C <sub>6</sub> H <sub>2</sub> + OH K FACTORS MIGHT BE HIGH. -----	300	1.0(+7)	-	-	0.1 10.
$\text{CH}_2=\text{CH}_2 + \text{S} \rightarrow \text{cy-CH}_2\text{CH}_2\text{S}$ 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
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{S}\cdot \rightarrow \text{CH}_2\text{SCH}_2\text{CH}_2\cdot$ 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	
$\text{CH}_3\text{CH}_2\cdot + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_3 + \text{H}$ 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		
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$ ETHYL FREE RADICAL + ETHENE 72 KER/PAR REACTION ORDER: 2.	348-482	1.6(+11)	0	3675		
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{C}(\text{CH}_3)-\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)\cdot$ ETHYL FREE RADICAL + 1,2-PROPADIENE 72 KER/PAR REACTION ORDER: 2.	373-465	3.2(+11)	0	4630		
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHCH}_2\text{CH}_2\cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\cdot$ ETHYL FREE RADICAL + 2-PROPEN-1-OL 72 KER/PAR REACTION ORDER: 2.	323-415	1.9(+11)	0	3901		
$\text{CH}_3\text{CH}_2\cdot + \text{CH}_2=\text{CHCN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CN} + \cdot\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ 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	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ ETHYL FREE RADICAL + 1-BUTENE 72 KER/PAR REACTION ORDER: 2.				
298	-	-	4265	
$\text{CH}_3\text{CH}_2 \cdot + \text{cis-CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + cis-2-BUTENE 72 KER/PAR REACTION ORDER: 2.				
298	-	-	4350	
$\text{CH}_3\text{CH}_2 \cdot + \text{trans-CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + trans-2-BUTENE 72 KER/PAR REACTION ORDER: 2.				
303-417	7.8(+10)	0	3475	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{COCCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COCCH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COCCH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + ACETIC ACID ETHENYL ESTER 72 KER/PAR REACTION ORDER: 2.				
323-454	1.5(+10)	0	2500	
$\text{CH}_3\text{CH}_2 \cdot + \text{cis-CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ $+ \text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + cis-2-BUTENENITRILE 72 KER/PAR REACTION ORDER: 2.				
323-754	3.1(+10)	0	2600	
$\text{CH}_3\text{CH}_2 \cdot + \text{trans-CH}_3\text{CH}=\text{CHCN} \rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CN}$ $+ \text{CH}_3\text{CH}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + trans-2-BUTENENITRILE 72 KER/PAR REACTION ORDER: 2.				
312-400	2.5(+11)	0	2300	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_2=\text{C}(\text{CH}_3)\text{CN} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{CN}$ $+ \text{CH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CN}$ ETHYL FREE RADICAL + 2-PHENYLNITRILE, 2-METHYL- 72 KER/PAR REACTION ORDER: 2.				
298	-	-	4300	
$\text{CH}_3\text{CH}_2 \cdot + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}_3$ ETHYL FREE RADICAL + cis-2-PENTENE 72 KER/PAR REACTION ORDER: 2. NOTE: CRITICAL ENERGY OF REACTION.				
298	-	-	3620	
$\text{CH}_3\text{CH}_2 \cdot + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCH}(\cdot)\text{CH}_2\text{CH}_3$ ETHYL FREE RADICAL + 1-BUTENE, 3-METHYL- 72 KER/PAR REACTION ORDER: 2. NOTE: CRITICAL ENERGY OF REACTION.				
308-448	2.5(+11)	0	3900	
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{COCCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COCCH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_3$ $+ \text{CH}_3\text{COCCH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\cdot$ ETHYL FREE RADICAL + ACETIC ACID 2-PHENYLNITRILE ESTER 72 KER/PAR REACTION ORDER: 2.				
300-520	2.8(+11)	0	3986+100	0.4 2.2
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{CH}_2\text{COCCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 \cdot + \text{CH}_2\text{COCCH}_2\text{CH}_3$ ETHYL FREE RADICAL + 3-PENTANONE 72 KEN REACTION ORDER: 2.				
$\text{CH}_3\text{CH}_2 \cdot + \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\cdot)(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2$				

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
$\cdot \text{CH}_2\text{C}(\text{CH}_2)(\text{CH}_2\text{CH}_2)\text{C}(\text{CH}_3)=\text{CH}_2$ ETHYL FREE RADICAL $\cdot$ 1,3-BUTADIENE, 2,3-DIMETHYL- REACTION ORDER: 2. 72 KBR/PAR	318-414	1.6(+11)	0	2265	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot \text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2$ $\rightarrow$ $\text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ETHYL FREE RADICAL $\cdot$ 1-HEXENE REACTION ORDER: 2. 72 KBR/PAR	338-435	3.9(+10)	0	3400	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot \text{CH}_3\text{CH}_2\text{C}(\text{CH}_2)_3\text{CH}=\text{CH}_2$ $\rightarrow$ $\text{CH}_3\text{CH}_2\text{C}(\text{CH}_2)_3\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3\text{CH}_2\text{C}(\text{CH}_2)_3\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ETHYL FREE RADICAL $\cdot$ PROPANOIC ACID 2-PROPENYL ESTER REACTION ORDER: 2. 72 KBR/PAR	352-435	2.5(+11)	0	3875	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot \text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3$ $\rightarrow$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{C}(\text{CH}_2)_3\text{CH}_3$ $\cdot \text{CH}_2\text{CH}(\text{CH}_2)_3\text{C}(\text{CH}_2)_3\text{CH}_3$ ETHYL FREE RADICAL $\cdot$ BUTANE, 1-ETHENYLOXY- REACTION ORDER: 2. 72 KBR/PAR	303-435	2.5(+10)	0	3070	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{C}=\text{CH} \rightarrow$ $\text{CH}_3((\text{CH}_2)_4\text{C}(\cdot))-\text{CHCH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3)=\text{CH} \cdot$ ETHYL FREE RADICAL $\cdot$ 1-HEPTYNE REACTION ORDER: 2. 72 KBR/PAR	300-455	3.9(+11)	0	4430	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2$ $\rightarrow$ $\text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ETHYL FREE RADICAL $\cdot$ 1-HEPTENE REACTION ORDER: 2. 72 KBR/PAR	359-439	6.2(+10)	0	3500	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot (\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2$ $\rightarrow$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ETHYL FREE RADICAL $\cdot$ 1-HUTENE, 2,3,3-TRIMETHYL- REACTION ORDER: 2. 72 KBR/PAR	322-364	7.8(+9)	0	2800	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot (\text{CH}_3)_2\text{C}=\text{CHCH}=\text{C}(\text{CH}_3)_2$ $\rightarrow$ $(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\cdot)\text{CH}=\text{C}(\text{CH}_3)_2$ $\cdot (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}=\text{C}(\text{CH}_3)_2$ ETHYL FREE RADICAL $\cdot$ 2,4-HEXADIENE, 2,5-DIMETHYL- REACTION ORDER: 2. 72 KBR/PAR	328-420	6.2(+10)	0	3300	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot \text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2$ $\rightarrow$ $\text{CH}_3(\text{CH}_2)_5\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ETHYL FREE RADICAL $\cdot$ 1-OCTENE REACTION ORDER: 2. 72 KBR/PAR	339-425	1.2(+11)	0	3825	
$\text{CH}_3\text{CH}_2 \cdot$ $\cdot (\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $\rightarrow$ $(\text{CH}_3)_3\text{CCH}_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot (\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ ETHYL FREE RADICAL $\cdot$ 1-PENTENE, 2,4,4-TRIMETHYL- REACTION ORDER: 2. 72 KBR/PAR	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
ETHANE 70 BEN/e'N	REACTION ORDER: 1. -----	298-858	5.6(+16)	0	45045	
CH <sub>3</sub> CH <sub>3</sub> + O → CH <sub>3</sub> CH <sub>2</sub> + OH ETHANE + OXYGEN ATOM 73 HER/HUI	REACTION ORDER: 2. -----		2.5(+13)	0	3200	0.7 1.3
CH <sub>3</sub> CH <sub>3</sub> + H → CH <sub>3</sub> CH <sub>2</sub> + H <sub>2</sub> ETHANE + HYDROGEN ATOM 72 IGN	REACTION ORDER: 2. -----	285-1440	1.0(+14)	0	4815470	0.8 1.2
CH <sub>3</sub> CH <sub>3</sub> + OH → CH <sub>3</sub> CH <sub>2</sub> + H <sub>2</sub> O ETHANE + HYDROXYL FREE RADICAL 72 IGM	REACTION ORDER: 2. -----		1.3(+14)	0	1998	
CH <sub>3</sub> CH <sub>3</sub> + H <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> + H <sub>2</sub> O ETHANE + HYDROPEROXYL FREE RADICAL 74 ILC	REACTION ORDER: 2. -----	300-1000	1.0(+12)	0	7000	0.1 10.
NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS k <sub>ref</sub> FOR H <sub>2</sub> + CO → HC + CO <sub>2</sub>						
CH <sub>3</sub> CH <sub>3</sub> + CH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> + CH <sub>4</sub> ETHANE + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----		5.6(+11)	0	58404250	0.7 1.3
CH <sub>3</sub> CH <sub>3</sub> + CD <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> + CD <sub>3</sub> H ETHANE + METHYL-d <sub>3</sub> FREE RADICAL 72 IGM	REACTION ORDER: 2. -----	390-800	1.0(+12)	0	60854165	0.7 1.4
CH <sub>3</sub> CD <sub>3</sub> + CD <sub>3</sub> → CH <sub>3</sub> CD <sub>2</sub> + CD <sub>4</sub> ETHANE-1,1,1-d <sub>3</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----	500-750	4.3(+11)	0	68454250	0.7 1.3
CD <sub>3</sub> CH <sub>3</sub> + CD <sub>3</sub> → CD <sub>3</sub> CH <sub>2</sub> + CD <sub>3</sub> H ETHANE-1,1,1-d <sub>3</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----		3.0(+11)	0	59004250	0.7 1.3
CD <sub>3</sub> CD <sub>3</sub> + CH <sub>3</sub> → CD <sub>3</sub> CD <sub>2</sub> + CH <sub>3</sub> D ETHANE-d <sub>6</sub> + METHYL FREE RADICAL 76 KER/PAR	REACTION ORDER: 2. -----	500-900	5.6(+11)	0	66004250	0.7 1.3
CD <sub>3</sub> CD <sub>3</sub> + CD <sub>3</sub> → CD <sub>3</sub> CD <sub>2</sub> + CD <sub>4</sub> ETHANE-d <sub>3</sub> + METHYL-d <sub>3</sub> FREE RADICAL 72 IGM	REACTION ORDER: 2. -----		4.6(+11)	0	6405	
CH <sub>2</sub> =C=O + O → products ETHENONE + OXYGEN ATOM 73 HER/HUI	REACTION ORDER: 2. -----	298	5.3(+11)	-	-	0.7 1.3
HOOCCOOH → HCOOH + CO <sub>2</sub> ETHANEDIC ACID 70 BEN/e'N	REACTION ORDER: 1. -----	390-420	7.9(+11)	0	15100	

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	k factors F
273-413	1.5(+10)	0	6790±115	0.7	1.4
$\text{CH}_3\text{C}(\theta)$ , - $\text{CH}_3$ + $\text{C}\theta$ ETHYL, 1-CXG-, FREE RADICAL 72 KEN REACTION ORDER: 1.					
298-500	2.0(+10)	0	7550	0.5	2.0
$\text{CH}_3\text{C}(\theta)$ , - $\text{CH}_3$ + $\text{C}\theta$ ETHYL, 1-CXG-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.					
300-525	1.4(+13)	0	1140	0.4	1.6
$\text{CH}_3\text{C}\theta$ + $\theta$ - products ACETALDEHYDE + OXYGEN ATOM 73 HHR/HUI REACTION ORDER: 2.					
300-500	8.5(+10)	0	3000±250	0.5	1.5
$\text{CH}_3\text{C}\theta$ + $\text{CH}_3$ - $\text{CH}_3\text{C}(\theta)$ + $\text{CH}_4$ ACETALDEHYDE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
298	1.0(+11)	0	3975±500	0.5	1.5
$\text{CH}_3\text{C}\theta$ + $\text{CH}_3$ - $\text{CH}_3\text{C}(\theta)$ + $\text{CH}_3\text{D}$ ACETALDEHYDE-1-d + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
350-500	7.0(+8)	-	-	0.6	1.5
$\text{cy-CH}_2\text{CH}_2\theta$ + $\theta$ - products OXIRANE + OXYGEN ATOM 73 HHR/HUI REACTION ORDER: 2.					
350-550	2.5(+11)	0	5435±750	0.5	2.0
$\text{cy-CH}_2\text{CH}_2\theta$ + $\text{CH}_3$ - $\text{cy-CH}_2\text{CH}(\theta)\theta$ + $\text{CH}_4$ OXIRANE + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
350-550	2.0(+11)	0	4900±500	0.5	1.5
$\text{HC}\theta\theta\text{CH}_3$ + $\text{CH}_3$ - $\text{C}\theta\theta\text{CH}_3$ + $\text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
350-550	1.6(+11)	0	5635±500	0.5	1.5
$\text{HC}\theta\theta\text{CH}_3$ + $\text{CH}_3$ - $\text{HC}\theta\theta\text{CH}_2$ + $\text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
350-550	3.0(+11)	0	4980±500	0.5	1.5
$\text{HC}\theta\theta\text{CH}_3$ + $\text{CH}_3$ - $\text{C}\theta\theta\text{CH}_3$ + $\text{HC}\theta\theta\text{CH}_3$ + $\text{CH}_4$ FORMIC ACID METHYL ESTER + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
350-550	2.5(+11)	0	5900±500	0.5	1.5
$\text{DC}\theta\theta\text{CH}_3$ + $\text{CH}_3$ - $\text{C}\theta\theta\text{CH}_3$ + $\text{CH}_3\text{D}$ FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2.					
773-973	1.6(+11)	0	5635±500	0.5	1.5
$\text{DC}\theta\theta\text{CH}_3$ + $\text{CH}_3$ - $\text{DC}\theta\theta\text{CH}_2$ + $\text{CH}_4$ FORMIC-d ACID METHYL ESTER + METHYL FREE RADICAL 76 KHR/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.					
773-973	8.9(+12)	0	33970	0.5	1.5
$\text{CH}_3\text{C}\theta\theta$ - $\text{CH}_2\text{-C-}\theta$ + $\text{H}_2\theta$ ACETIC ACID 70 HEN/G'N REACTION ORDER: 1. NOTE: SUSPECT VALUE.					

## CHEMICAL REACTIONS

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



## CHEMICAL REACTIONS

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

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
350-500	2.9(+11)	0	4200±500	0.5 2.0
423	4.0(+5)	-	-	-
350-650	1.6(+11)	0	3500±500	0.5 2.0
350-650	6.5(+10)	0	3200±500	0.5 2.0
350-500	2.9(+11)	0	4400±500	0.5 1.5
350-500	1.0(+11)	0	4300±500	0.5 1.5
552-600	3.2(+16)	0	26400	-
300-500	1.1(+11)	0	3975±250	-
300-450	5.0(+10)	0	3040±355	-
300-500	6.6(+10)	0	4125±500	-
350-500	3.8(+11)	0	4200±500	-
350-500	2.0(+11)	0	4430±500	-

CD<sub>3</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub> → CH<sub>4</sub> + CH<sub>3</sub>D + CD<sub>3</sub>CH(•)NH<sub>2</sub> + •CD<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>  
 ETHAN-2,2,2-d<sub>3</sub>-AMINE + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

CD<sub>3</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub> → CD<sub>3</sub>CH<sub>2</sub>NH• + CH<sub>4</sub>  
 ETHAN-2,2,2-d<sub>3</sub>-AMINE + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.  
 NOTE: TENTATIVE k VALUE.

(CH<sub>3</sub>)<sub>2</sub>NH + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>N• + •CH<sub>2</sub>NH(CH<sub>3</sub>) + CH<sub>4</sub>  
 METHANAMINE, N-METHYL- + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>2</sub>NH + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>N• + CH<sub>4</sub>  
 METHANAMINE, N-METHYL- + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>2</sub>ND + CH<sub>3</sub> → CH<sub>2</sub>NDCH<sub>3</sub> + CH<sub>4</sub>  
 METHANAMINE-d, N-METHYL-, + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>2</sub>ND + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>N• + CH<sub>3</sub>D  
 METHANAMINE-d, N-METHYL-, + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

CH<sub>3</sub>N=NCH<sub>3</sub> → CH<sub>3</sub>• + CH<sub>3</sub>N=N•  
 DIAZENE, DIMETHYL-  
 70 BEN/6'N REACTION ORDER: 1.

CH<sub>3</sub>N=NCH<sub>3</sub> + CH<sub>3</sub> → CH<sub>2</sub>N=NCH<sub>3</sub> + CH<sub>4</sub>  
 DIAZENE, DIMETHYL- + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

CH<sub>3</sub>N=NCH<sub>3</sub> + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>NN(•)CH<sub>3</sub>  
 DIAZENE, DIMETHYL- + METHYL FREE RADICAL  
 72 KCN REACTION ORDER: 2.  
 CD<sub>3</sub>N=NCD<sub>3</sub> + CD<sub>3</sub> → •CD<sub>2</sub>N=NCD<sub>3</sub> + CD<sub>4</sub>  
 DIAZENE, DI(METHYL-d<sub>3</sub>)-, + METHYL-d<sub>3</sub> FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

NH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub> → •NHCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub>  
 + NH<sub>2</sub>CH(•)CH<sub>2</sub>NH<sub>2</sub> + CH<sub>4</sub>  
 ETHANEDIAMINE + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

NH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub> → •NHCH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>4</sub>  
 ETHANEDIAMINE + METHYL FREE RADICAL  
 76 KHR/PAR REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.  
 ND<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>ND<sub>2</sub> + CH<sub>3</sub> → •NDCH<sub>2</sub>CH<sub>2</sub>ND<sub>2</sub> + CH<sub>3</sub>D

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
ETHAN(DIAMINE-d <sub>2</sub> ) * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- ND <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> ND <sub>2</sub> * CH <sub>3</sub> ° → ND <sub>2</sub> CH(•)CH <sub>2</sub> ND <sub>2</sub> * CH <sub>4</sub> ETHANEDIAMINE-d <sub>2</sub> ) * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	3.2(*11)	0	5100*500	
(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → (CH <sub>3</sub> ) <sub>2</sub> NNH• * CH <sub>4</sub> HYDRAZINE, 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → (CH <sub>3</sub> ) <sub>2</sub> NH• * •CH <sub>2</sub> N(CH <sub>3</sub> )NH <sub>2</sub> * CH <sub>4</sub> HYDRAZINE, 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	2.0(*11)	0	4025*500	
(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → (CH <sub>3</sub> ) <sub>2</sub> NND• * CH <sub>3</sub> D HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → CH <sub>2</sub> N(CH <sub>3</sub> )ND <sub>2</sub> * CH <sub>4</sub> HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	1.7(*11)	0	2870*500	
(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → (CH <sub>3</sub> ) <sub>2</sub> NND• * CH <sub>3</sub> D HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → CH <sub>2</sub> N(CH <sub>3</sub> )ND <sub>2</sub> * CH <sub>4</sub> HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	2.4(*11)	0	2970*500	
(CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → (CH <sub>3</sub> ) <sub>2</sub> NND• * CH <sub>3</sub> D HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> NNH <sub>2</sub> * CH <sub>3</sub> ° → CH <sub>2</sub> N(CH <sub>3</sub> )ND <sub>2</sub> * CH <sub>4</sub> HYDRAZINE-d <sub>2</sub> , 1,1-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	2.1(*11)	0	3400*500	
CH <sub>3</sub> NHCH <sub>3</sub> * CH <sub>3</sub> ° → CH <sub>3</sub> N(•)NHCH <sub>3</sub> * •CH <sub>2</sub> NHCH <sub>3</sub> * CH <sub>4</sub> HYDRAZINE, 1,2-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CH <sub>3</sub> NHCH <sub>3</sub> * CH <sub>3</sub> ° → CH <sub>3</sub> N(•)NHCH <sub>3</sub> * •CH <sub>2</sub> NHCH <sub>3</sub> * CH <sub>4</sub> HYDRAZINE, 1,2-DIMETHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	3.2(*11)	0	4125*750	
CH <sub>3</sub> NDNDCH <sub>3</sub> * CH <sub>3</sub> ° → CH <sub>3</sub> N(•)NDCH <sub>3</sub> * CH <sub>3</sub> D HYDRAZINE-d <sub>2</sub> , 1,2-DIMETHYL * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CH <sub>3</sub> NDNDCH <sub>3</sub> * CH <sub>3</sub> ° → CH <sub>3</sub> N(•)NDCH <sub>3</sub> * CH <sub>3</sub> D HYDRAZINE-d <sub>2</sub> , 1,2-DIMETHYL * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-500	2.5(*11)	0	2400*250	
CH <sub>3</sub> CH=N•H → CH <sub>3</sub> CH=N• * •H ACETALDEHYDE, EXIME 70 BEN/6'N REACTION ORDER: 1. ----- HC•NHCH <sub>3</sub> * CH <sub>3</sub> ° → •C•NHCH <sub>3</sub> * HC•N(•)CH <sub>3</sub> * HC•NHCH <sub>2</sub> ° * CH <sub>4</sub> FORMAMIDE, N-METHYL-, * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	603-713	6.8(*12)	0	23655	
CH <sub>3</sub> CONH <sub>2</sub> * CH <sub>3</sub> ° → CH <sub>3</sub> CONH• * •CH <sub>2</sub> CONH <sub>2</sub> * CH <sub>4</sub> ACETAMIDE * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CH <sub>3</sub> CONH <sub>2</sub> * CH <sub>3</sub> ° → CH <sub>3</sub> CONH• * •CH <sub>2</sub> CONH <sub>2</sub> * CH <sub>4</sub> ACETAMIDE * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	400-600	7.9(*10)	0	3800*500	
CH <sub>3</sub> CONH <sub>2</sub> * CH <sub>3</sub> ° → •CH <sub>2</sub> CONH <sub>2</sub> * CH <sub>4</sub> ACETAMIDE * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- CH <sub>3</sub> CONH <sub>2</sub> * CH <sub>3</sub> ° → •CH <sub>2</sub> CONH <sub>2</sub> * CH <sub>4</sub> ACETAMIDE * METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----	350-600	2.1(*11)	0	5235*500	
CD <sub>3</sub> CONH <sub>2</sub> * CD <sub>3</sub> ° → •CD <sub>2</sub> CONH <sub>2</sub> * CD <sub>4</sub> REACTION ORDER: 2. -----	350-600	1.0(*11)	0	5200*500	

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f F
ACETAMIDE-2,2,2-d <sub>3</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KHE/PAR REACTION ORDER: 2. -----	350-600	1.4(+11)	0	5800±500	
CD <sub>3</sub> CNH <sub>2</sub> + CD <sub>3</sub> → CD <sub>3</sub> CNH <sub>2</sub> + CD <sub>3</sub> H ACETAMIDE-2,2,2-d <sub>3</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KHE/PAR REACTION ORDER: 2. -----	350-600	1.1(+11)	0	5235±500	
CH <sub>3</sub> CH <sub>2</sub> NO <sub>2</sub> → CH <sub>2</sub> =CH <sub>2</sub> + HONO ETHANE, NITRO- 70 HBN/G*N REACTION ORDER: 1. -----	583-715	2.5(+12)	0	22645	
CH <sub>3</sub> CH <sub>2</sub> NO <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> O <sub>2</sub> + NO NITROUS ACID ETHYL ESTER 70 HBN/G*N REACTION ORDER: 1. -----	484-505	1.2(+16)	0	20400	
CH <sub>3</sub> CH <sub>2</sub> NO <sub>2</sub> → CH <sub>3</sub> CH <sub>2</sub> O <sub>2</sub> + NO <sub>2</sub> NITRIC ACID ETHYL ESTER 70 HBN/G*N REACTION ORDER: 1. -----	434-474	3.2(+16)	0	19830	
CH <sub>2</sub> NOCH <sub>2</sub> CH <sub>2</sub> NO <sub>2</sub> → Products 1,2-ETHANEDIOL, DINITRATE 70 HBN/G*N REACTION ORDER: 1. -----	358-378	7.9(+15)	0	19630	
CH <sub>3</sub> N(O)N(O)CH <sub>3</sub> → CH <sub>3</sub> NO + CH <sub>3</sub> NO DIAZENE, DIMETHYL-1,2-DIOXIDE- 70 HBN/G*N REACTION ORDER: 1. -----	374-404	2.5(+13)	0	11600	
CH <sub>3</sub> C=CH + O → Products 1-PROPENE + OXYGEN ATOM 73 HBR/HUI REACTION ORDER: 2. -----	298	4.0(+11)	-	-	0.5 2.0
CH <sub>3</sub> C=CH + H → CH <sub>3</sub> CH=CH <sub>2</sub> + CH <sub>3</sub> C(•)-CH <sub>2</sub> 1-PROPENE + HYDROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. -----	298	2.5(+11)	-	-	
NOTE: k TAKEN AS LOWER LIMIT.					
CH <sub>3</sub> C=CH + S → cy-CH <sub>3</sub> C=CHS 1-PROPENE + SULFUR ATOM 72 KHE/PAR REACTION ORDER: 2. -----	298	1.1(+12)	-	-	
CH <sub>3</sub> C=CH + N → Products 1-PROPENE + NITROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. -----	320-550	6.9(+10)	0	745	
CH <sub>3</sub> C=CH + N → Products 1-PROPENE + NITROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. -----	435	-	-	-	
NOTE: k <sub>ref</sub> : CHCH + N					
CH <sub>3</sub> C=CH + CH <sub>3</sub> → (CH <sub>3</sub> ) <sub>2</sub> C=CH <sub>2</sub> + CH <sub>3</sub> C(•)-CH <sub>3</sub> 1-PROPENE + METHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. -----	379-465	5.0(+11)	0	4400	
NOTE: TENTATIVE k VALUE. CH <sub>3</sub> ADDITION OCCURS					

## CHEMICAL REACTIONS

T/K	A	B	E/R (ln OK)	k factors f
360-439	1.9(+9)	0	2870	
PREDOMINANTLY AT TERMINAL C ATOM. ----- $\text{CH}_3\text{C}=\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{C}(\cdot)\text{CH}_3$ 1-PROPENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR NOTE: SUSPECT k VALUE.				
360-439	5.0(+8)	0	2770	
----- $\text{CH}_3\text{C}=\text{CH} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)\cdot\text{CH}_2$ + $(\text{CH}_3)_3\text{CC}=\text{C}(\cdot)\text{CH}_3$ 1-PROPENE + ETHYL-, 1,1-DIMETHYL-, FREE RADICAL 72 KER/PAR NOTE: SUSPECT k VALUE.				
373-483	2.0(+11)	0	4100	
----- $\text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
379-465	3.2(+11)	0	4630	
----- $\text{CH}_3\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\cdot)(\text{CH}_3)$ 1,2-PROPADIENE + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.				
366-473	3.6(+10)	0	3660	
----- $\text{CH}_2=\text{C}=\text{CH}_2 + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{C}(\cdot)=\text{CH}_2$ 1,2-PROPADIENE + ETHYL, 1-METHYL-, FREE RADICAL 72 KER/PAR NOTE: TENTATIVE k VALUE.				
953-1143	2.0(+15)	0	4900	
----- $\text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2 \cdot + \text{H}$ 1-PROPENE 70 BEN/6'N REACTION ORDER: 1.				
200-500	2.5(+12)	0	38	0.8 1.2
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{C} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{C}$ 1-PROPENE + OXYGEN ATOM 73 BEN/HUI REACTION ORDER: 2.				
298	11.2(+12)	0	1460	
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 \cdot$ 1-PROPENE + HYDROGEN ATOM 72 KER/PAR NOTE: TENTATIVE k VALUE.				
298	7.2(+12)	0	600	
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_3$ 1-PROPENE + HYDROGEN ATOM 72 KER/PAR REACTION ORDER: 2.				
300	6.6(+12)	-	-	
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH} \rightarrow \text{CH}_3\text{CH}(\cdot)\text{CH}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2 \cdot$ 1-PROPENE + HYDROXYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. NOTE: ADDITION TO TERMINAL CARBON OF DOUBLE BOND IS PROBABLY 95%.				
----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM				

CHEMICAL REACTIONS	T/K	A	B	E/R (in oK)	k factors f
72 KER/PAR REACTION ORDER: 2. ----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{S} \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 6.9 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{S}$	298	5.8(+12)	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{S}^*(1\text{D}) \rightarrow \text{cy}-(\text{CH}_3)\text{CHCH}_2\text{S}$ 1-PROPENE + SULFUR ATOM(1D) 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 1.7 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{S}^*(1\text{D})$	300	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-PROPENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. ----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{N} \rightarrow \text{products}$ 1-PROPENE + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 2.8 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{N}$	320-550	1.2(+11)	0	655	
$\text{CH}_3\text{CH}=\text{CH}_2 + {}^1\text{CH}_2 \rightarrow \text{products}$ 1-PROPENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 1.27 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + {}^1\text{CH}_2$	435	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + {}^3\text{CH}_2 \rightarrow \text{products}$ 1-PROPENE + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 1.0 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + {}^3\text{CH}_2$	297	-	-	-	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \rightarrow [\text{C}_3\text{H}_5\cdot] + \text{CH}_4$ 1-PROPENE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- $\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \rightarrow [\text{C}_3\text{H}_5\cdot] + \text{CH}_4$ 1-PROPENE + METHYL FREE RADICAL 72 KEN REACTION ORDER: 2.	350-600	1.4(+11)	0	4430+500	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\cdot$ 1-PROPENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2.	350-580	3.2(+10)	0	3775+300	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}_2\cdot$ 1-PROPENE + METHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 0.72 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{CH}_3$	353-453	1.7(+11)	0	3770	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CCl}_4 \rightarrow \text{CH}_3\text{CH}=\text{C}=\text{CH}_2 + \text{CCl}_3$ 1-PROPENE + CARBON TETRACHLORIDE 72 KER/PAR REACTION ORDER: 2. $k/k_{\text{ref}}$ : 5.7 NOTE: $k_{\text{ref}}$ : $\text{CH}_2=\text{CH}_2 + \text{CCl}_4$	453	-	-	-	-

## CHEMICAL REACTIONS

T/K	A	B	E/R (in OK)	k factors f
381-412	6.3(+10)	0	3725	
300-750	5.8(+14)	0	16880*350	
297-564	4.0(+13)	0	16660	
296-723	6.3(+13)	0	9100	
375-503	1.9(+10)	0	3070	
298	-	-	3630	
298	-	-	4370	
298	-	-	4515	
298	-	-	3410	
65C-814	1.9(+11)	0	16045*1150	
673-777	2.00(+14)	0	20800	

NOTE: k<sub>rel</sub>: CH<sub>2</sub>-CH<sub>2</sub> • CCE

CH<sub>3</sub>CH=CH<sub>2</sub> • CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)CH(CH<sub>3</sub>)CH<sub>2</sub>•  
 • CH<sub>3</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)CH<sub>2</sub>CH(•)CH<sub>3</sub>  
 1-PROPENE • PROPYL, 1-METHYL-, FREE RADICAL  
 REACTION ORDER: 2.  
 72 KER/PAR

NOTE: TENTATIVE k VALUE.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• → CH<sub>3</sub>• + CH<sub>2</sub>-CH<sub>2</sub>  
 1-PROPYL FREE RADICAL  
 72 KGN

REACTION ORDER: 1.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• → CH<sub>3</sub>• + CH<sub>2</sub>-CH<sub>2</sub>  
 1-PROPYL FREE RADICAL  
 70 BEN/6'N

REACTION ORDER: 1.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• → CH<sub>3</sub>CH=CH<sub>2</sub> + H  
 1-PROPYL FREE RADICAL  
 70 BEN/6'N

REACTION ORDER: 1.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• + CH<sub>2</sub>-CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>•  
 1-PROPYL FREE RADICAL • ETHENE  
 72 KGN

REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• + CH<sub>3</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>  
 1-PROPYL FREE RADICAL • 1-BUTENE  
 72 KER/PAR

REACTION ORDER: 2.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• + cis-CH<sub>3</sub>CH=CHCH<sub>3</sub> → CH<sub>3</sub>CH(CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>)CH(•)CH<sub>3</sub>  
 1-PROPYL FREE RADICAL • cis-2-BUTENE  
 72 KER/PAR

REACTION ORDER: 2.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• + trans-CH<sub>3</sub>CH=CHCH<sub>3</sub> →  
 CH<sub>3</sub>CH(CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>)CH(•)CH<sub>3</sub>  
 1-PROPYL FREE RADICAL • trans-2-BUTENE  
 72 KER/PAR

REACTION ORDER: 2.

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>• + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH=CH<sub>2</sub> →  
 CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>  
 1-PROPYL FREE RADICAL • 1-PENTENE  
 72 KER/PAR

REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>2</sub>CH• → CH<sub>3</sub>• + CH<sub>2</sub>-CH<sub>2</sub>  
 ETHYL, 1-METHYL-, FREE RADICAL  
 72 KGN

REACTION ORDER: 1.

(CH<sub>3</sub>)<sub>2</sub>CD• → CH<sub>3</sub>CD=CH<sub>2</sub> + H.  
 ETHYL-1-d, 1-METHYL-, FREE RADICAL  
 70 BEN/6'N

REACTION ORDER: 1.

(CH<sub>3</sub>)<sub>2</sub>CH• + CH<sub>2</sub>=CH → (CH<sub>3</sub>)<sub>2</sub>CHCH=CH•  
 ETHYL, 1-METHYL, FREE RADICAL • ETHYLENE

## CHEMICAL REACTIONS

T/K	A	B	E/R (in OK)	k factors f
363-577	5.0(+10)	0	3475	
72 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- $(CH_3)_2CH \cdot + CH_2=CH_2 \rightarrow (CH_3)_2CHCH_2CH_2 \cdot$ ETHYL, 1-METHYL-, FREE RADICAL + ETHENE REACTION ORDER: 2. ----- 72 KER/PAR $(CH_3)_2CH \cdot + CH_3C \equiv CH \rightarrow (CH_3)_2CHCH_2C(\cdot)CH_3$ ETHYL, 1-METHYL-, FREE RADICAL + 1-BUTYNE REACTION ORDER: 2. NOTE: SUSPECT k VALUE. ----- 72 KER/PAR $(CH_3)_2CH \cdot + CH_2=C=CH_2 \rightarrow (CH_3)_2CHCH_2C(\cdot)=CH_2$ ETHYL, 1-METHYL-, FREE RADICAL + 1,2-PROPADIENE REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- 72 KER/PAR $(CH_3)_2CH \cdot + CH_3CH_2CH=CH_2 \rightarrow (CH_3)_2CHCH_2CH(\cdot)CH_2CH_3$ ETHYL, 1-METHYL-, FREE RADICAL + 1-BUTENE REACTION ORDER: 2. NOTE: CRITICAL ENERGY OF REACTION. ----- 72 KER/PAR $(CH_3)_2CH \cdot + cis-CH_3CH=CH_2 \rightarrow CH_3CH[CH(CH_3)_2]CH(\cdot)CH_3$ ETHYL, 1-METHYL-, FREE RADICAL + cis-2-BUTENE REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. ----- 72 KER/PAR $(CH_3)_2CH \cdot + trans-CH_3CH=CH_2 \rightarrow CH_3CH[CH(CH_3)_2]CH(\cdot)CH_3$ ETHYL, 1-METHYL-, FREE RADICAL + trans-2-BUTENE REACTION ORDER: 2. NOTE: CRITICAL ENERGY OF REACTION. ----- 72 KER/PAR $CH_3CH_2CH_3 + e \rightarrow$ products PROPANE + OXYGEN ATOM 73 KER/HUI REACTION ORDER: 2. ----- $CH_3CH_2CH_3 + H \rightarrow (CH_3)_2CH \cdot + CH_3CH_2CH_2 \cdot + H_2$ PROPANE + HYDROGEN ATOM 72 KGN REACTION ORDER: 2. ----- $CH_3CH_2CH_3 + H_2 \rightarrow (CH_3)_2CH \cdot + H_2^{\delta 2}$ PROPANE + HYDROGENXYL FREE RADICAL 74 LL6 REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS $k_{ref}$ FOR $H_2 + H_2^{\delta 2} \rightarrow H_2^{\delta 2} + H_2$ ----- $CH_3CH_2CH_3 + CH_3 \cdot \rightarrow (CH_3)_2CH \cdot + CH_4$ PROPANE + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. ----- $CH_3CD_2CH_3 + CD_3 \cdot \rightarrow (CH_3)_2CD \cdot + CD_4$ PROPANE-2,2-d <sub>2</sub> + METHYL-d <sub>3</sub> FREE RADICAL 76 KER/PAR REACTION ORDER: 2. -----				
340-457	6.9(+10)	0	3475	
360-439	1.90(+9)	0	2870	
366-473	3.6(+10)	0	3600	
298	-	-	3480	
298	-	-	3950	
298	-	-	4065	
298	5.0(+9)	-	-	0.7 2.0
332-933	1.0(+13)	0	3130*180	
300-1000	2.0(+11)	0	5300	
550-750	2.0(+11)	0	4820*250	
550-750	2.5(+11)	0	5735*250	



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

## 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.

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

(CH<sub>3</sub>)<sub>2</sub>CHOH + O → products

2-PROPANOL + OXYGEN ATOM

73 KER/PAR

(CH<sub>3</sub>)<sub>2</sub>COH + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>C(O)OH + CH<sub>3</sub>D

2-PROPAN-2-d-OL + METHYL FREE RADICAL

76 KER/PAR REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>2</sub>CHOH + CD<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>C(O)OH + ·CH<sub>2</sub>CH(CH<sub>3</sub>)OH + CD<sub>3</sub>H2-PROPANOL-d + METHYL-d<sub>3</sub> FREE RADICAL

76 KER/PAR REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>2</sub>CHOH → (CH<sub>3</sub>)<sub>2</sub>CHO + OH

HYDROPEROXIDE, 1-METHYLETHYL

70 BEN/G'N REACTION ORDER: 1.

CY-CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>S + CH<sub>3</sub> → CY-CH<sub>2</sub>CH(O)CH<sub>2</sub>S + CH<sub>4</sub>

THIETANE + METHYL FREE RADICAL

76 KER/PAR REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

(CH<sub>3</sub>)<sub>2</sub>CHSH + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>CHS + (CH<sub>3</sub>)<sub>2</sub>C(O)SH·CH<sub>2</sub>CH(CH<sub>3</sub>)SH + CH<sub>4</sub>

2-PROPANETHIOL + METHYL FREE RADICAL

76 KER/PAR REACTION ORDER: 2.

NOTE: TENTATIVE k VALUE.

CH<sub>2</sub>=CHCN + CH<sub>3</sub>CH<sub>2</sub>· → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(O)CN + ·CH<sub>2</sub>CH(CH<sub>2</sub>CH<sub>3</sub>)CN

2-PROPENITRILE + ETHYL FREE RADICAL

72 KER/PAR REACTION ORDER: 2.

CH<sub>3</sub>CH<sub>2</sub>CN → CH<sub>3</sub>· + ·CH<sub>2</sub>CN

PROPANENITRILE

70 BEN/G'N REACTION ORDER: 1.

CH<sub>3</sub>CH<sub>2</sub>CN + CD<sub>3</sub>· → CH<sub>3</sub>CH(O)CN + ·CH<sub>2</sub>CH<sub>2</sub>CN + CD<sub>3</sub>HPROPANENITRILE + METHYL-d<sub>3</sub> FREE RADICAL

76 KER/PAR REACTION ORDER: 2.

(CH<sub>3</sub>)<sub>3</sub>N + CH<sub>3</sub>· → ·CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> + CH<sub>4</sub>

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

76 KER/PAR REACTION ORDER: 2.

O<sub>2</sub>NOCCH<sub>2</sub>CH(OH)<sub>2</sub>CH<sub>2</sub>OH<sub>2</sub> → products

1,2,3-TRIFLUORETHYL, TRINITRATE

70 BEN/G'N REACTION ORDER: 1.

## CHEMICAL REACTIONS

k factors f	E/R (in oK)	B	A	T/K	
	18800	0	1.6(+15)	353-373	$\sigma_2\text{NOCH}_2\text{CH}(\sigma\text{NO}_2)\text{CH}_3$ - products 1,2-PROPANEDICL, DINITRATE REACTION ORDER: 1. 70 BEN/ $\sigma'$ N
	19175	0	1.6(+15)	358-383	$\sigma_2\text{NOCH}_2\text{CH}_2\text{CH}_2\text{ONO}_2$ - products 1,3-PROPANEDICL, DINITRATE REACTION ORDER: 1. 70 BEN/ $\sigma'$ N
	3600*500	0	6.3(+10)	400-600	$\text{HCON}(\text{CH}_3)_2 + \text{CH}_3 - \text{CON}(\text{CH}_3)_2 + \text{HCO}-(\text{CH}_3)\text{NCH}_2 + \text{CH}_4$ FORMAMIDE, N,N-DIMETHYL-, + METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE.
	24005	0	2.50(+13)	687-733	$\text{CH}_3\text{CH}_2\text{CH}_2\text{NO}_2 - \text{CH}_3\text{CH}=\text{CH}_2 + \text{HONO}$ PROPANE, 1-NITRO- REACTION ORDER: 1. 70 BEN/ $\sigma'$ N
	20130	0	2.0(+11)	800-1000	$\text{CH}_3\text{CH}(\text{NO}_2)\text{CH}_3 - \text{CH}_3\text{CH}=\text{CH}_2 + \text{HONO}$ PROPANE, 2-NITRO- REACTION ORDER: 1. 70 BEN/ $\sigma'$ N
	20230	0	1.6(+16)	443-483	$\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}_2 - \text{CH}_3\text{CH}_2\text{CH}_2\sigma + \text{NO}$ NITROUS ACID PEROXY ESTER REACTION ORDER: 1. 70 BEN/ $\sigma'$ N
	18600	0	3.2(+16)	443-483	$(\text{CH}_3)_2\text{CHONO} - (\text{CH}_3)_2\text{CH}\sigma + \text{NO}$ NITROUS ACID, 1-METHYL ETHYL ESTER REACTION ORDER: 1. 70 BEN/ $\sigma'$ N
	-	-	5.0(+11)	300	$\text{CH}=\text{CC}=\text{CH} + \sigma - \text{products}$ 1,3-BUTADIENE + OXYGEN ATOM REACTION ORDER: 2. 73 KER/HUI
	1125	0	3.5(+11)	320-550 435	$\text{CH}_3\text{CH}_2\text{C}=\text{CH} + \text{N} - \text{products}$ 1-BUTYNE + NITROGEN ATOM REACTION ORDER: 2. 72 KER/PAR NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH + N k/k <sub>ref</sub> : 13.0
	5135*500	0	1.9(+12)	456-620	$\text{CH}_3\text{CH}_2\text{C}=\text{CH} + \text{CH}_3 - \text{CH}_3\text{CH}(\sigma)\text{C}=\text{CH} + \sigma\text{CH}_2\text{CH}_2\text{C}=\text{CH}$ + $\text{CH}_3\text{CH}_2\text{C}=\text{C}\sigma + \text{CH}_4$ 1-BUTYNE + METHYL FREE RADICAL REACTION ORDER: 2. 76 KER/PAR NOTE: TENTATIVE k VALUE.
	-	-	1.9(+13)	298	$\text{CH}_3\text{C}=\text{CCH}_3 + \text{S} - \text{cy}-(\text{CH}_3)\text{C}=\text{C}(\text{CH}_3)\text{S}$ 2-BUTYNE + SULFUR ATOM REACTION ORDER: 2. 72 KER/PAR
	526	0	1.9(+11)	320-550 435	$\text{CH}_3\text{C}=\text{CCH}_3 + \text{N} - \text{products}$ 2-BUTYNE + NITROGEN ATOM REACTION ORDER: 2. 72 KER/PAR k/k <sub>ref</sub> : 12.0

0.7 1.4

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
486-619	1.1(+12)	0	4900±500	
NOTE: $k_{ref}$ : $CH_3CH \cdot N$ $CH_3COCCH_3 \cdot CH_3 \rightarrow CH_3C=CH_2 \cdot + CH_4$ 2-BUTYNE $\cdot$ METHYL FREE RADICAL 76 KHE/PAR REACTION ORDER: 2. NOTE: TENTATIVE $k$ VALUE.				
304	-	-	-	
$CH_3COCCH_3 \cdot C \rightarrow$ products 2-HUTYME $\cdot$ CARBON OXIDE( $C_2O$ ) 72 KHE/PAR REACTION ORDER: 2. $k/k_{ref}$ : 8.5				
298-400	3.4(+12)	0	- 380	0.7 1.3
NOTE: $k_{ref}$ : $CH_2=CH_2 \cdot CCl$ $CH_2=CHCH=CH_2 \cdot C \rightarrow$ products 1,3-BUTADIENE $\cdot$ OXYGEN ATOM 73 KHE/YUI REACTION ORDER: 2.				
298	4.10(+13)	0	655	
$CH_2=CHCH=CH_2 \cdot H \rightarrow CH_2=CHCH(\cdot)CH_3 + CH_2=CHCH_2CH_2\cdot$ 1,3-BUTADIENE $\cdot$ HYDROGEN ATOM 72 KHE/PAR REACTION ORDER: 2. NOTE: AVERAGED $k$ .				
300	-	-	-	
NOTE: $k_{ref}$ : $CH_3CH=CH_2 \cdot H$ $CH_2=CHCH=CH_2 \cdot S \rightarrow cy-(CH_2=CH)CHCH_2S$ 1,3-BUTADIENE $\cdot$ SULFUR ATOM 72 KHE/PAR REACTION ORDER: 2.				
298	6.0(+13)	-	-	
NOTE: $k_{ref}$ : $CH_3CH=CH_2 \cdot H$ $CH_2=CHCH=CH_2 \cdot N \rightarrow$ products 1,3-BUTADIENE $\cdot$ NITROGEN ATOM 72 KHE/PAR REACTION ORDER: 2.				
340	3.5(+10)	-	-	
$CH_2=CHCH=CH_2 \cdot ^1CH_2 \rightarrow$ products 1,3-BUTADIENE $\cdot$ METHYLENE FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. $k/k_{ref}$ : 3.2				
297	-	-	-	
NOTE: $k_{ref}$ : $CH_2=CH_2 \cdot ^1CH_2$ ASSUMING $10^4$ $^3CH_2$ $CH_2=CHCH=CH_2 \cdot CH_3 \rightarrow CH_3CH_2CH(\cdot)CH=CH_2$ 1,3-BUTADIENE $\cdot$ METHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2.				
353-453	8.1(+10)	0	2065	
$CH_2=CHCH=CH_2 \cdot CH_3 \rightarrow CH_3CH_2CH(\cdot)CH=CH_2$ $\cdot CH_2CH(CH_3)CH=CH_2$ 1,3-BUTADIENE $\cdot$ METHYL FREE RADICAL 72 KHE/PAR REACTION ORDER: 2. $k/k_{ref}$ : 12.0				
435	-	-	-	
NOTE: $k_{ref}$ : $CH_2=CH_2 \cdot CH_3$ $CH_2=CHCH=CH_2 \cdot CCl \rightarrow CH_2=C=CHCH=CH_2 \cdot CCl$ 1,3-BUTADIENE $\cdot$ CARBON DIBROMIDE( $C_2Br_2$ ) 72 KHE/PAR REACTION ORDER: 2. $k/k_{ref}$ : 210.				
298	-	-	-	
NOTE: $k_{ref}$ : $CH_2=CH_2 \cdot CCl$ $CH_3CH_2CH=CH_2 \cdot O \rightarrow cy-(CH_3CH_2)CHCH_2O$ 1-BUTENE $\cdot$ OXYGEN ATOM				

CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f F
73 IER/HUI CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • H → CH <sub>3</sub> CH <sub>2</sub> CH(•)CH <sub>3</sub> • CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> • 1-BUTENE • HYDROGEN ATOM 72 IER/PAR	REACTION ORDER: 2. ----- REACTION ORDER: 2. k/k <sub>ref</sub> : 1.03	298 298 300	2.3(•12) 8.7(•11) -	- - -	- - -	0.8 1.2
NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH-CH <sub>2</sub> • H ----- CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • H → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> • 1-BUTENE • HYDROGEN ATOM 72 IER/PAR	REACTION ORDER: 2. ----- REACTION ORDER: 2. ----- NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTANE.	298	5.0(•10)	-	-	
CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • H → CH <sub>3</sub> CH <sub>2</sub> CH(•)CH <sub>3</sub> 1-BUTENE • HYDROGEN ATOM 72 IER/PAR	REACTION ORDER: 2. ----- NOTE: CALCULATED ON THE BASIS OF 5.7% NON-TERMINAL ADDITION OF H TO 1-BUTENE.	298	8.1(•11)	-	-	
CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • S → cy-(CH <sub>3</sub> CH <sub>2</sub> ) <sub>2</sub> CHCH <sub>2</sub> S 1-BUTENE • SULFUR ATOM 72 IER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : 10.0	298 298	9.3(•12) -	- -	- -	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> -CH <sub>2</sub> • S ----- CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • N → Products 1-BUTENE • NITROGEN ATOM 72 IER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : 3.4	320-550 435	1.6(•11) -	0 -	660 -	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> -CH <sub>2</sub> • N ----- CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • <sup>1</sup> CH <sub>2</sub> → Products 1-BUTENE • METHYLENE FREE RADICAL 72 IER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : 1.63	297	-	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> -CH <sub>2</sub> • <sup>1</sup> CH <sub>2</sub> ----- CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • <sup>3</sup> CH <sub>2</sub> → Products 1-BUTENE • METHYLENE FREE RADICAL 72 IER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : 1.6	297	-	-	-	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> -CH <sub>2</sub> • <sup>3</sup> CH <sub>2</sub> ----- CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • CH <sub>3</sub> → CH <sub>3</sub> CH(•)CH-CH <sub>2</sub> • CH <sub>4</sub> 1-BUTENE • METHYL FREE RADICAL 76 IER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : 12.0	350-650	2.5(•11)	0	4200±500	0.6 1.4
CH <sub>3</sub> CH <sub>2</sub> CH-CH <sub>2</sub> • CH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> CH(•)CH <sub>2</sub> CH <sub>3</sub> • CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH <sub>2</sub> • 1-BUTENE • METHYL FREE RADICAL 72 IER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : 3600	353-453 453	1.0(•11) -	0 -	3600 -	
NOTE: k <sub>ref</sub> : CH <sub>2</sub> -CH <sub>2</sub> • CH <sub>3</sub>						

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
298	-	-	-	-
298	-	-	3675	-
298	-	-	3630	-
298	-	-	3480	-
900-1051	1.00(±16)	0	36900	-
298-333	1.6(±9)	-	-	-
686-742	6.00(±13)	0	31600	-
250-500	5.9(±12)	0	- 165	0.8 1.2
208	4.6(±11)	-	-	-
300	-	-	-	-
298	1.4(±13)	-	-	-
298	-	-	-	-
320-550	2.3(±11)	0	995	-
435	-	-	-	-

$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CCl}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{Cl})_2 + \text{C}\dot{\text{C}}\text{l}$   
 1-BUTENE + CARBON DIBROMIDE (C<sub>2</sub>Br<sub>2</sub>)  
 72 KBR/PAR REACTION ORDER: 2.  $k/k_{\text{ref}}$ : 7.0  
 NOTE:  $k_{\text{ref}}$ :  $\text{CH}_2=\text{CH}_2 + \text{CCl}_2$

$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\dot{\text{C}}\text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$   
 1-BUTENE + ETHYL FREE RADICAL  
 72 KBR/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\dot{\text{C}}\text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$   
 1-BUTENE + PROPYL FREE RADICAL  
 72 KBR/PAR REACTION ORDER: 2.

$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}\dot{\text{C}}\text{H} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$   
 1-BUTENE + ISOPROPYL, 1-METHYL-, FREE RADICAL  
 72 KBR/PAR REACTION ORDER: 2.

$\text{CH}_2=\text{CHCH}_2\text{CH}_3 + \dot{\text{C}}\text{H}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\dot{\text{C}}\text{H}_3$   
 1-BUTENE  
 70 HEN/6'N REACTION ORDER: 1.  
 NOTE:  $k$  ESTIMATED.

$\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_3 + \text{CH}_3\dot{\text{S}} \rightarrow \text{CH}_3\text{CH}(\text{SCH}_3)\text{CH}(\text{CH}_3)\text{CH}_3$   
 2-BUTENE + METHYLTHIO FREE RADICAL  
 72 KBR/PAR REACTION ORDER: 2.  
 NOTE: cis-trans EQUILIBRIUM - WEIGHTED  $k$ .

$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3$   
 cis-2-BUTENE  
 70 HEN/6'N REACTION ORDER: 1.

$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{O} \rightarrow \text{Products}$   
 cis-2-BUTENE + OXYGEN ATOM  
 73 KBR/HUI REACTION ORDER: 2.

$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_3$   
 cis-2-BUTENE + HYDROGEN ATOM  
 72 KBR/PAR REACTION ORDER: 2.  
 NOTE: NO KINETIC DATA ON REVERSE RADICAL DECOMPOSITION.  
 $k/k_{\text{ref}}$ : 0.47

$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{S} \rightarrow \text{Products}$   
 cis-2-BUTENE + SULFUR ATOM  
 72 KBR/PAR REACTION ORDER: 2.  
 $k/k_{\text{ref}}$ : 16.0

$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{N} \rightarrow \text{Products}$   
 cis-2-BUTENE + NITROGEN ATOM  
 72 KBR/PAR REACTION ORDER: 2.  
 $k/k_{\text{ref}}$ : 2.4

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
297	-	-	-	-
297	-	-	-	-
350-650	1.8(+11)	0	4100±500	-
353-453	4.5(+10)	0	3675	-
297	-	-	-	-
298	-	-	4265	-
298	-	-	4370	-
298	-	-	3950	-
298	1.4(+13)	-	-	0.7 1.3
298	5.6(+11)	-	-	-
300	-	-	-	-

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.  $k/k_{ref}$ : 1.37NOTE:  $k_{ref}$ :  $CH_2=CH_2 + ^1CH_2$  $cis-CH_3CH=CHCH_3 + ^3CH_2 \rightarrow$  products $cis-2-BUTENE + METHYLENE FREE RADICAL$ 

72 KER/PAR

REACTION ORDER: 2.  $k/k_{ref}$ : 0.94NOTE:  $k_{ref}$ :  $CH_2=CH_2 + ^3CH_2$  $cis-CH_3CH=CHCH_3 + CH_3 \rightarrow CH_3CH=CHCH_2 + CH_4$  $cis-2-BUTENE + METHYL FREE RADICAL$ 

76 KER/PAR

REACTION ORDER: 2.

 $cis-CH_3CH=CHCH_3 + CH_3 \rightarrow (CH_3)_2CHCH(\cdot)CH_3$  $cis-2-BUTENE + METHYL FREE RADICAL$ 

72 KER/PAR

REACTION ORDER: 2.  $k/k_{ref}$ : 0.2NOTE:  $k_{ref}$ :  $CH_2=CH_2 + CH_3$  $cis-CH_3CH=CHCH_3 + CCO \rightarrow cis-CH_3CH=C=CHCH_3 + CO$  $cis-2-BUTENE + CARBON OXIDE(C_2O)$ 

72 KER/PAR

REACTION ORDER: 2.  $k/k_{ref}$ : 9.1NOTE:  $k_{ref}$ :  $CH_2=CH_2 + CCO$  $cis-CH_3CH=CHCH_3 + CH_3CH_2 \rightarrow CH_3CH(CH_2CH_3)CH(\cdot)CH_3$  $cis-2-BUTENE + ETHYL FREE RADICAL$ 

72 KER/PAR

REACTION ORDER: 2.

NOTE: CRITICAL ENERGY OF REACTION.

 $cis-CH_3CH=CHCH_3 + CH_3CH_2CH_2 \rightarrow CH_3CH(CH_2CH_2CH_3)CH(\cdot)CH_3$  $cis-2-BUTENE + PROPYL FREE RADICAL$ 

72 KER/PAR

REACTION ORDER: 2.

 $cis-CH_3CH=CHCH_3 + (CH_3)_2CH \rightarrow CH_3CH(CH_3)_2CH(\cdot)CH_3$  $cis-2-BUTENE + ETHYL, 1-METHYL-, FREE RADICAL$ 

72 KER/PAR

REACTION ORDER: 2.

 $trans-CH_3CH=CHCH_3 + O \rightarrow$  products $trans-2-BUTENE + OXYGEN ATOM$ 

73 KER/HUI

REACTION ORDER: 2.

 $trans-CH_3CH=CHCH_3 + H \rightarrow CH_3CH_2CH(\cdot)CH_3$  $trans-2-BUTENE + HYDROGEN ATOM$ 

72 KER/PAR

REACTION ORDER: 2.

NOTE: AVERAGE  $k$ .NOTE:  $k_{ref}$ :  $CH_3CH=CH_2 + H$  $trans-CH_3CH=CHCH_3 + S \rightarrow cy-(CH_3CH)C(CH_3)S$

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



CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors 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 BER/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. NOTE: SUGGESTED $k$ VALUE. -----	300	1.0(+ 8)	-	-	0.1 10.
$(CH_3)_2C=CH_2 + S \rightarrow cy-[(CH_3)_2]CCH_2S$ 1-PROPENE, 2-METHYL-, + SULFUR ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 50.0$ NOTE: $k_{ref}: CH_2=CH_2 + S$ -----	298 298	4.0(+13)	- -	- -	
$(CH_3)_2C=CH_2 + S^*(^1D) \rightarrow$ products 1-PROPENE, 2-METHYL-, + NITROGEN ATOM 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 3.5$ NOTE: $k_{ref}: CH_2=CH_2 + S^*(^1D)$ -----	300	-	-	-	
$(CH_3)_2C=CH_2 + N \rightarrow$ 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. $k/k_{ref}: 4.1$ NOTE: $k_{ref}: CH_2=CH_2 + N$ -----	435	-	-	-	
$(CH_3)_2C=CH_2 + ^1CH_2 \rightarrow$ products 1-PROPENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $k/k_{ref}: 1.96$ NOTE: $k_{ref}: CH_2=CH_2 + ^1CH_2$ -----	297	-	-	-	

CHEMICAL REACTIONS	T/K	A	B	E/R. (in °K)	k factors f
<p>-----</p> <p><math>(CH_3)_2C=CH_2 + ^3CH_2 \rightarrow</math> products 1-PROPENE, 2-METHYL-, + METHYLENE FREE RADICAL 72 KHE/FAR REACTION ORDER: 2. <math>k/k_{ref}</math>: 2.86</p> <p>NOTE: <math>k_{ref}</math>: <math>CH_2=CH_2 + ^3CH_2</math></p>	297	-	-	-	
<p>-----</p> <p><math>(CH_3)_2C=CH_2 + CH_3 \rightarrow</math> <math>CH_2C(CH_3)=CH_2 + CH_4</math> 1-PROPENE, 2-METHYL-, + METHYL FREE RADICAL 76 KHE/FAR REACTION ORDER: 2.</p>	350-600	3.0(+11)	0	4500±500	0.6 1.4
<p>-----</p> <p><math>(CH_3)_2C=CH_2 + CH_3 \rightarrow (CH_3)_3CCH_2 + (CH_3)_2C(·)CH_2CH_3</math> 1-PROPENE, 2-METHYL-, + METHYL FREE RADICAL 72 KHE/FAR REACTION ORDER: 2. <math>k/k_{ref}</math>: 1.1</p>	353-453	1.4(+11)	0	3475	-
<p>-----</p> <p>NOTE: <math>k_{ref}</math>: <math>CH_2=CH_2 + CH_3</math></p> <p><math>(CH_3)_2C=CH_2 + CCl \rightarrow (CH_3)_2C=CH_2 + CCl</math> 1-PROPENE, 2-METHYL-, + CARBON CHLORIDE(C<sub>2</sub>Cl) 72 KHE/FAR REACTION ORDER: 2. <math>k/k_{ref}</math>: 50.0</p>	297	-	-	-	-
<p>-----</p> <p>NOTE: <math>k_{ref}</math>: <math>CH_2=CH_2 + CCl</math></p> <p><math>CH_3CH_2CH_2CH_2 \rightarrow CH_3CH_2 \cdot + CH_2=CH_2</math> BUTYL FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.</p>	334-689	4.0(+13)	0	14600	
<p>-----</p> <p><math>CH_3CH_2CH_2CH_2 \cdot + CH_2=CH_2 \rightarrow CH_3(CH_2)_4CH_2 \cdot</math> BUTYL FREE RADICAL + ETHENE 72 KHE/FAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE <math>k</math> VALUE.</p>	352-405	2.3(+10)	0	3370	
<p>-----</p> <p><math>CH_3CH_2CH(·)CH_3 \rightarrow CH_3CH=CH_2 + CH_3</math> PROPYL, 1-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.</p> <p><math>CH_3CH_2CH(·)CH_3 + CH_3 \rightarrow CH_3CH_2CH(CH_3)CH(CH_3)CH_2 \cdot</math> + <math>CH_3CH_2CH(CH_3)CH_2CH(·)CH_3</math> PROPYL, 1-METHYL-, FREE RADICAL + 1-PREPENE 72 KHE/FAR REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE <math>k</math> VALUE.</p>	523-622	1.4(+14)	0	17060	
<p>-----</p> <p><math>(CH_3)_2CHCH_2 \cdot \rightarrow CH_3 \cdot + CH_3CH=CH_2</math> PROPYL, 2-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.</p>	381-412	6.3(+10)	0	3725	
<p>-----</p> <p><math>(CH_3)_2CHCH_2 \cdot \rightarrow (CH_3)_3C=CH_2 + H</math> PROPYL, 2-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.</p>	299-691	1.6(+14)	0	16455	
<p>-----</p> <p><math>(CH_3)_2CHCH_2 \cdot \rightarrow (CH_3)_3C=CH_2 + H</math> PROPYL, 2-METHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.</p>	299-691	5.0(+13)	0	16420	
<p>-----</p> <p><math>(CH_3)_3C \cdot \rightarrow (CH_3)_2C=CH_2 + H</math> ETHYL, 1,1-DIMETHYL-, FREE RADICAL 70 HEN/G'N REACTION ORDER: 1.</p>	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	
$(\text{CH}_3)_3\text{C} \cdot + \text{CH}=\text{CH} \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH} \cdot$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL ♦ ETHYNE REACTION ORDER: 2. 72 KEE/PAR NOTE: TENTATIVE k VALUE.				
300-650	2.8(♦10)	0	3575	
$(\text{CH}_3)_3\text{C} \cdot + \text{CH}_2=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}_2 \cdot$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL ♦ ETHENE REACTION ORDER: 2. 72 KEE/PAR				
360-439	5.0(♦8)	0	2770	
$(\text{CH}_3)_3\text{C} \cdot + \text{CH}_3\text{C}=\text{CH} \rightarrow (\text{CH}_3)_3\text{C}(\text{CH}_3)-\text{CH} \cdot + (\text{CH}_3)_3\text{CCH}=\text{C}(\cdot)\text{CH}_3$ ETHYL, 1,1-DIMETHYL-, FREE RADICAL ♦ 1-PROPENE REACTION ORDER: 2. 72 KEE/PAR NOTE: SUSPECT k VALUE.				
653-803	4.0(♦17)	0	43230	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}_2 \cdot$ BUTANE 70 HEN/σ'N REACTION ORDER: 1. NOTE: k ESTIMATED.				
653-803	1.9(♦17)	0	41170	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 \cdot + \text{CH}_3\text{CH}_2 \cdot$ BUTANE 70 HEN/σ'N REACTION ORDER: 1.				
298-650	3.0(♦13)	0	2920	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \cdot + \text{OH}$ BUTANE ♦ OXYGEN ATOM 73 HEE/HUI REACTION ORDER: 2.				
298-650	4.6(♦13)	0	2410	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{O} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{OH}$ BUTANE ♦ OXYGEN ATOM 73 HEE/HUI REACTION ORDER: 2.				
320-930	4.1(♦12)	0	2637♦320	0.5 2.0
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \cdot + \text{H}_2$ BUTANE ♦ HYDROGEN ATOM 72 KGN REACTION ORDER: 2.				
300-1000	5.0(♦11)	0	5285	0.1 10.
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{H}_2\text{O}$ BUTANE ♦ HYDROPEROXYL FREE RADICAL 74 LLG REACTION ORDER: 2. NOTE: UPPER LIMIT RECOMMENDED. RATIO DATA VERSUS $k_{\text{ref}}$ for $\text{H}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}_2$				
350-500	1.6(♦11)	0	4540♦150	0.7 1.4
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$ $+ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \cdot + \text{CH}_4$ BUTANE ♦ METHYL FREE RADICAL 72 KGN REACTION ORDER: 2.				
350-750	4.0(♦11)	0	4830♦250	0.7 1.3
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3 \cdot \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4$ BUTANE ♦ METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2.				
600-750	4.5(♦11)	0	5735♦250	0.7 1.3
$\text{CH}_3\text{CD}_2\text{CH}_2\text{CH}_3 + \text{CD}_3 \cdot \rightarrow \text{CH}_3\text{CD}_2\text{CD}(\cdot)\text{CH}_3 + \text{CD}_4$ BUTANE-2,2,3,3-d <sub>4</sub> ♦ METHYL-d <sub>3</sub> FREE RADICAL 76 KEE/PAR REACTION ORDER: 2.				

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
<p>-----</p> <p><math>\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}</math>  HUTANE-2,2,3,3-d<sub>4</sub> + METHYL-d<sub>3</sub> FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>-----</p> <p><math>(\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</math>  PROPANE, 2-METHYL-, + HYDROGEN ATOM  REACTION ORDER: 2.  72 KGN</p> <p>-----</p> <p><math>(\text{CH}_3)_3\text{CH} + \text{H}_2 \rightarrow (\text{CH}_3)_3\text{C} \cdot + \text{H}_2^{\delta 2}</math>  PROPANE, 2-METHYL-, + HYDROPEROXYL FREE RADICAL.  REACTION ORDER: 2.  74 ILC</p> <p>NOTE: UPPER LIMIT RECOMMENDED. RATIC DATA VERSUS <math>k_{\text{ref}}</math> for  <math>\text{H}_2 + \text{H}_2 \rightarrow \text{H}_2^{\delta 2} + \text{H}_2</math></p> <p>-----</p> <p><math>(\text{CH}_3)_3\text{CH} + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{C} \cdot + \text{CH}_4</math>  PROPANE, 2-METHYL-, + METHYL FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>-----</p> <p><math>(\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</math>  PROPANE, 2-METHYL-, + METHYL FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>-----</p> <p><math>(\text{CH}_3)_3\text{CD} + \text{CD}_3 \rightarrow (\text{CH}_3)_3\text{C} \cdot + \text{CD}_4</math>  PROPANE-2-d, 2-METHYL-, + METHYL-d<sub>3</sub> FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>-----</p> <p><math>(\text{CH}_3)_3\text{CD} + \text{CD}_3 \rightarrow (\text{CH}_3)_2\text{CDCH}_2 \cdot + \text{CD}_3\text{H}</math>  PROPANE-2-d, 2-METHYL-, + METHYL-d<sub>3</sub> FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>-----</p> <p><math>\text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}=\text{C}(\text{CH}_3) \cdot + \text{CH}_4</math>  2-BUTENAL + METHYL FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>NOTE: TENTATIVE k VALUE.</p> <p>-----</p> <p><math>\text{CH}_2=\text{CHCH}_2\text{C}(\text{CH}_3)_2 + \text{C}_6\text{H}_6</math>  3-BUTENIC ACID  70 HHR/G'N</p> <p>-----</p> <p><math>\text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2 \cdot \rightarrow \text{CH}_3\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_2)\text{CH}_2 \cdot</math>  + <math>\text{CH}_3\text{C}(\text{CH}_3)=\text{CH} + \text{CH}_3\text{CH}_2</math>  ACETIC ACID ETHERYL ESTER + ETHYL FREE RADICAL  REACTION ORDER: 2.  72 KHR/PAR</p> <p>-----</p> <p><math>\text{CH}_3\text{C}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{CH}_3)_2 \cdot + \text{CH}_4</math>  2,3-BUTANEDIONE + METHYL FREE RADICAL  REACTION ORDER: 2.  76 KHR/PAR</p> <p>-----</p> <p><math>\text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{C}(\text{CH}_3) \cdot + \text{CH}_3\text{C}(\text{CH}_3) \cdot</math>  2,3-BUTANEDIONE  70 HHR/G'N</p>	<p>600-750</p> <p>300-800</p> <p>300-1000</p> <p>550-750</p> <p>300-500</p> <p>550-750</p> <p>550-750</p> <p>350-500</p> <p>587-651</p> <p>303-417</p> <p>300-800</p> <p>626-698</p>	<p>4.8(+11)</p> <p>1.9(+13)</p> <p>1.0(+11)</p> <p>9.6(+10)</p> <p>8.3(+10)</p> <p>1.2(+11)</p> <p>6.0(+11)</p> <p>1.0(+11)</p> <p>2.2(+11)</p> <p>7.8(+10)</p> <p>2.2(+11)</p> <p>1.6(+16)</p>	<p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p> <p>0</p>	<p>5735*250</p> <p>2680*85</p> <p>3500</p> <p>3975*250</p> <p>4000*500</p> <p>4800*250</p> <p>5735*250</p> <p>3400*500</p> <p>20435</p> <p>3475</p> <p>4300*500</p> <p>33970</p>	<p>0.7 1.3</p> <p>0.8 1.2</p> <p>0.1 10.</p> <p>0.7 1.3</p> <p>0.5 2.0</p> <p>0.7 1.3</p> <p>0.7 1.3</p> <p>0.4 2.5</p> <p>0.5 1.5</p>

CHEMICAL REACTIONS	T/K	A	B	E/R. (in °K)	k factors f
(CH <sub>3</sub> CO) <sub>2</sub> O → CH <sub>3</sub> COOH + CH <sub>2</sub> =C=O ACETIC ACID ANHYDRIDE 70 HEN/°N REACTION ORDER: 1. -----	553-646	1.0(+12)	0	17365	
(CH <sub>3</sub> CO) <sub>2</sub> O + CH <sub>3</sub> → CH <sub>3</sub> COCCOCH <sub>2</sub> + CH <sub>4</sub> ACETIC ACID ANHYDRIDE + METHYL FREE RADICAL REACTION ORDER: 2. -----	300-500	1.8(+11)	0	4830*500	0.6 1.4
CH <sub>3</sub> C(O)COCC(O)CH <sub>3</sub> → CH <sub>3</sub> C(O)O + CH <sub>3</sub> C(O)O PEROXIDE, DIACETYL 70 HEN/°N REACTION ORDER: 1. -----	363-463	1.8(+14)	0	14845	
CH <sub>3</sub> CH <sub>2</sub> COCH <sub>3</sub> + CH <sub>3</sub> → CH <sub>3</sub> CH(O)COCH <sub>3</sub> + •CH <sub>2</sub> CH <sub>2</sub> COCH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> COCH <sub>2</sub> • + CH <sub>4</sub> 2-BUTANONE + METHYL FREE RADICAL REACTION ORDER: 2. -----	300-500	8.2(+10)	0	3700*500	0.5 1.5
HCOCCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → HCOCCH <sub>2</sub> + CH <sub>3</sub> CH=CH <sub>2</sub> FORMIC ACID PROPYL ESTER 70 HEN/°N REACTION ORDER: 1. -----	613-673	1.3(+12)	0	24006	
HCOCCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> • → •COCCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>4</sub> FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL REACTION ORDER: 2. -----	347-455	1.3(+10)	0	3675	
HCOCCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> • → •COCCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> + HCOCCH(O)CH <sub>2</sub> CH <sub>3</sub> + HCOCCH <sub>2</sub> CH(O)CH <sub>3</sub> + CH <sub>3</sub> • + HCOCCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> • + CH <sub>4</sub> FORMIC ACID PROPYL ESTER + METHYL FREE RADICAL REACTION ORDER: 2. -----	350-500	2.5(+11)	0	5000*500	0.5 2.0
NOTE: TENTATIVE k VALUE.					
HCOCCH(CH <sub>3</sub> ) <sub>2</sub> → HCOCCH + CH <sub>3</sub> CH=CH <sub>2</sub> FORMIC ACID 1-METHYLETHYL ESTER 70 HEN/°N REACTION ORDER: 1. -----	721-811	4.0(+12)	0	22145	
HCOCCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> • → •COCCH(CH <sub>3</sub> ) <sub>2</sub> + HCOCCH(O)(CH <sub>3</sub> ) <sub>2</sub> + HCOCCH(CH <sub>3</sub> )CH <sub>2</sub> • + CH <sub>4</sub> FORMIC ACID 1-METHYLETHYL ESTER + METHYL FREE RADICAL REACTION ORDER: 2. -----	350-500	2.5(+11)	0	4980*500	0.5 2.0
NOTE: TENTATIVE k VALUE.					
CH <sub>3</sub> COCCOCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> COOH + CH <sub>2</sub> =CH <sub>2</sub> ACETIC ACID ETHYL ESTER 70 HEN/°N REACTION ORDER: 1. -----	725-883	3.9(+12)	0	24155	
CH <sub>3</sub> COCCOCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> COH + CO <sub>2</sub> + CH <sub>2</sub> =CH <sub>2</sub> CARBONIC ACID ETHYL METHYL ESTER 70 HEN/°N REACTION ORDER: 1. -----	573-648	4.0(+12)	0	21640	
CH <sub>3</sub> CH(O)COCH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CHO + CH <sub>3</sub> CH <sub>2</sub> • ETHYL, 1-ETHOXY-, FREE RADICAL 70 HEN/°N REACTION ORDER: 1. -----	418-453	8.1(+10)	0	11825	
NOTE: log <sub>a</sub> PROBABLY LOW.					

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

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
<p>cis-2-BUTENENITRILE + ETHYL FREE RADICAL REACTION ORDER: 2.</p> <p>-----</p> <p>trans-CH<sub>3</sub>CH=CHCN + CH<sub>3</sub>CH<sub>2</sub>• → CH<sub>3</sub>CH(CF<sub>2</sub>CH<sub>3</sub>)CH(•)CN + CH<sub>3</sub>CH(•)CH(CH<sub>2</sub>CH<sub>3</sub>)CN</p> <p>trans-2-BUTENENITRILE + ETHYL FREE RADICAL REACTION ORDER: 2.</p> <p>-----</p> <p>CH<sub>2</sub>=C(CH<sub>3</sub>)CN + CH<sub>3</sub>CH<sub>2</sub>• → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>C(•)(CH<sub>3</sub>)CN + •CH<sub>2</sub>C(CH<sub>3</sub>)(CH<sub>2</sub>CH<sub>3</sub>)CN</p> <p>2-PROPENENITRILE, 2-METHYL-, + ETHYL FREE RADICAL REACTION ORDER: 2.</p> <p>-----</p> <p>CH<sub>3</sub>CH=NN=CHCH<sub>3</sub> + CH<sub>3</sub>• → CH<sub>3</sub>C(•)-NN=CHCH<sub>3</sub> + •CH<sub>2</sub>CH=NN=CHCH<sub>3</sub> + CH<sub>4</sub></p> <p>ACETALDEHYDE ETHYLIDENEHYDRAZONE + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>-----</p> <p>CH<sub>3</sub>CH<sub>2</sub>N=NCH<sub>2</sub>CH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>N=N• + CH<sub>3</sub>CH<sub>2</sub>•</p> <p>DIAZENE, DIETHYL- REACTION ORDER 1.</p> <p>-----</p> <p>CH<sub>3</sub>N=NCH(CH<sub>3</sub>)<sub>2</sub> → CH<sub>3</sub>N=N• + (CH<sub>3</sub>)<sub>2</sub>CH•</p> <p>DIAZENE, METHYL(1-METHYLETHYL)- REACTION ORDER 1.</p> <p>-----</p> <p>CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH• + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)NH<sub>2</sub> + •CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub></p> <p>1-BUTANAMINE + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	323-454	1.5(+10)	0	2500	0.5 2.0
<p>(CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>NH + CH<sub>3</sub>• → (CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>N• + CH<sub>3</sub>CH(•)NHCH<sub>2</sub>CH<sub>3</sub> + •CH<sub>2</sub>CH<sub>2</sub>NHCH<sub>2</sub>CH<sub>3</sub> + CH<sub>4</sub></p> <p>ETHANAMINE, N-ETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	323-754	3.1(+10)	0	2600	0.5 2.0
<p>CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub>• + •CH<sub>2</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub></p> <p>ETHANAMINE, N,N-DIMETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	312-400	2.5(+11)	0	2300	0.5 2.0
<p>CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> + CH<sub>3</sub>• → (CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>N• + CH<sub>3</sub>CH(•)NHCH<sub>2</sub>CH<sub>3</sub> + •CH<sub>2</sub>CH<sub>2</sub>NHCH<sub>2</sub>CH<sub>3</sub> + CH<sub>4</sub></p> <p>ETHANAMINE, N-ETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	350-600	2.5(+11)	0	3975±500	0.5 2.0
<p>CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub>• + (CH<sub>3</sub>)<sub>2</sub>CH•</p> <p>DIAZENE, METHYL(1-METHYLETHYL)- REACTION ORDER 1.</p> <p>-----</p> <p>CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH• + CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)NH<sub>2</sub> + •CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>NH<sub>2</sub></p> <p>1-BUTANAMINE + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	543-605	2.0(+16)	0	25165	0.5 2.0
<p>(CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>NH + CH<sub>3</sub>• → (CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>N• + CH<sub>3</sub>CH(•)NHCH<sub>2</sub>CH<sub>3</sub> + •CH<sub>2</sub>CH<sub>2</sub>NHCH<sub>2</sub>CH<sub>3</sub> + CH<sub>4</sub></p> <p>ETHANAMINE, N-ETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	426	3.2(+7)	-	-	0.5 2.0
<p>CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> + CH<sub>3</sub>• → CH<sub>3</sub>CH(•)N(CH<sub>3</sub>)<sub>2</sub> + •CH<sub>2</sub>CH<sub>2</sub>N(CH<sub>3</sub>)<sub>2</sub> + CH<sub>3</sub>CH<sub>2</sub>N(CH<sub>3</sub>)CH<sub>2</sub>• + CH<sub>4</sub></p> <p>ETHANAMINE, N,N-DIMETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.</p> <p>NOTE: TENTATIVE k VALUE.</p>	350-500	2.2(+11)	0	3550±500	0.5 2.0
<p>(CH<sub>3</sub>)<sub>2</sub>NN=NN(CH<sub>3</sub>)<sub>2</sub> → (CH<sub>3</sub>)<sub>2</sub>NN=N• + (CH<sub>3</sub>)<sub>2</sub>N•</p> <p>2-TETRAZENE, 1,1,4,4-TETRAMETHYL- REACTION ORDER: 1.</p> <p>-----</p> <p>CH<sub>3</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → CH<sub>3</sub>CH• + CH<sub>2</sub>=CH<sub>2</sub></p> <p>ETHENE, ETHOXY- REACTION ORDER: 1.</p> <p>-----</p> <p>CH<sub>2</sub>=CHCH<sub>2</sub>CH<sub>2</sub>• → CH<sub>3</sub>CH• + CH<sub>3</sub>CH=CH<sub>2</sub> + HCHO</p>	420	2.6(+7)	-	-	0.5 2.0
<p>CH<sub>3</sub>CH<sub>2</sub>CH=CH<sub>2</sub> → CH<sub>3</sub>CH• + CH<sub>2</sub>=CH<sub>2</sub></p> <p>ETHENE, ETHOXY- REACTION ORDER: 1.</p> <p>-----</p> <p>CH<sub>2</sub>=CHCH<sub>2</sub>CH<sub>2</sub>• → CH<sub>3</sub>CH• + CH<sub>3</sub>CH=CH<sub>2</sub> + HCHO</p>	466-539	2.5(+14)	0	18170	0.5 2.0
<p>CH<sub>2</sub>=CHCH<sub>2</sub>CH<sub>2</sub>• → CH<sub>3</sub>CH• + CH<sub>3</sub>CH=CH<sub>2</sub> + HCHO</p>	640-659	4.0(+11)	0	22345	0.5 2.0





CHEMICAL REACTIONS		T/K	A	B	E/R (in °K)	k factors f
72 KER/PAR	REACTION ORDER: 2. ----- cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + O → Products cis-2-PENTENE + OXYGEN ATOM	298	-	-	3410	
73 HBR/HUI	REACTION ORDER: 2. ----- cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + H → CH <sub>3</sub> CH <sub>2</sub> CH(•)CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(•)CH <sub>3</sub> cis-2-PENTENE + HYDROGEN ATOM	298	1.1(+13)	-	-	0.7 1.03
72 KER/PAR	REACTION ORDER: 2. ----- NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H k/k <sub>ref</sub> : 0.39 cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> • → CH <sub>3</sub> CH <sub>2</sub> CH(•)CH(CH <sub>3</sub> ) <sub>2</sub> cis-2-PENTENE + METHYL FREE RADICAL	298 300	3.8(+11)	-	-	
72 KER/PAR	REACTION ORDER: 2. ----- cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> • → CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(•)CH <sub>3</sub> cis-2-PENTENE + METHYL FREE RADICAL	298	-	-	4060	
72 KER/PAR	REACTION ORDER: 2. ----- cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> • → CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH(•)CH <sub>3</sub> cis-2-PENTENE + METHYL FREE RADICAL	298	-	-	4125	
72 KER/PAR	REACTION ORDER: 2. ----- cis-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> • → CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>2</sub> CH <sub>3</sub> )CH(•)CH <sub>3</sub> cis-2-PENTENE + ETHYL FREE RADICAL	298	-	-	4300	
72 KER/PAR	REACTION ORDER: 2. ----- trans-CH <sub>3</sub> CH <sub>2</sub> CH=CHCH <sub>3</sub> + H → CH <sub>3</sub> CH <sub>2</sub> CH(•)CH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH(•)CH <sub>3</sub> trans-2-PENTENE + HYDROGEN ATOM	300	-	-	-	
72 KER/PAR	REACTION ORDER: 2. k/k <sub>ref</sub> : 0.44 ----- NOTE: k <sub>ref</sub> : CH <sub>3</sub> CH=CH <sub>2</sub> + H	298	4.1(+11)	-	-	
72 KER/PAR	REACTION ORDER: 2. ----- CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> + H → CH <sub>3</sub> CH <sub>2</sub> C(•)(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> CH <sub>2</sub> CH(CH <sub>3</sub> )CH <sub>2</sub> • 1-BUTENE, 2-METHYL-, + HYDROGEN ATOM	298	9.1(+11)	-	-	
72 KER/PAR	REACTION ORDER: 2. ----- CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> + D → CH <sub>3</sub> CH <sub>2</sub> C(•)(CH <sub>3</sub> )CH <sub>2</sub> D + CH <sub>3</sub> CH <sub>2</sub> CD(CH <sub>3</sub> )CH <sub>2</sub> • 1-BUTENE, 2-METHYL-, + DEUTERIUM ATOM	298	2.0(+12)	-	-	
72 KER/PAR	REACTION ORDER: 2. ----- CH <sub>3</sub> CH <sub>2</sub> C(CH <sub>3</sub> )=CH <sub>2</sub> + S → cy-(CH <sub>3</sub> ) <sub>2</sub> C(CH <sub>3</sub> )CH <sub>2</sub> S 1-BUTENE, 2-METHYL-, + SULFUR ATOM	298	7.4(+13)	-	-	
72 KER/PAR	REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> CHCH=CH <sub>2</sub> + H → (CH <sub>3</sub> ) <sub>2</sub> CHCH(•)CH <sub>3</sub> + (CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> CH <sub>2</sub> • 1-BUTENE, 3-METHYL-, + HYDROGEN ATOM	298	7.4(+11)	-	-	
72 KER/PAR	REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> CHCH=CH <sub>2</sub> + D → (CH <sub>3</sub> ) <sub>2</sub> CHCH(•)CH <sub>2</sub> D + (CH <sub>3</sub> ) <sub>2</sub> CHCHDCH <sub>2</sub> • 1-BUTENE, 3-METHYL-, + DEUTERIUM ATOM	298	7.6(+11)	-	-	

CHEMICAL REACTIONS	T/K	A	B	E/R (ln OK)	k factors f F
<p>-----  <math>(CH_3)_2CCH=CH_2 + CH_3 \rightarrow (CH_3)_2CCH(\cdot)CH_2CH_3</math>            1-BUTENE, 3-METHYL-, + METHYL FREE RADICAL            72 KHR/PAR            REACTION ORDER: 2.            -----</p> <p> <math>(CH_3)_2CCH=CH_2 + CH_3 \rightarrow (CH_3)_2C(\cdot)CH=CH_2 + CH_4</math>            1-BUTENE, 3-METHYL-, + METHYL FREE RADICAL            72 KHR/PAR            REACTION ORDER: 2.            -----</p> <p> <math>(CH_3)_2CCH=CH_2 + CH_3CH_2 \rightarrow (CH_3)_2CCH(\cdot)CH_2CH_2CH_3</math>            1-BUTENE, 3-METHYL-, + ETHYL FREE RADICAL            72 KHR/PAR            REACTION ORDER: 2.            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + O \rightarrow</math> products            2-BUTENE, 2-METHYL-, + OXYGEN ATOM            73 KHR/HUI            REACTION ORDER: 2.            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + H \rightarrow (CH_3)_2CCH(\cdot)CH_3 + (CH_3)_2C(\cdot)CH_2CH_3</math>            2-BUTENE, 2-METHYL-, + HYDROGEN ATOM            73 KHR/HUI            REACTION ORDER: 2.            k/k<sub>ref</sub>: 1.03            -----</p> <p>           NOTE: k<sub>ref</sub>: <math>CH_3CH=CH_2 + H</math>            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + S \rightarrow cy-[(CH_3)_2CCH(CH_3)]S</math>            2-BUTENE, 2-METHYL-, + SULFUR ATOM            72 KHR/PAR            REACTION ORDER: 2.            k/k<sub>ref</sub>: 56.0            -----</p> <p>           NOTE: k<sub>ref</sub>: <math>CH_2=CH_2 + S</math>            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + N \rightarrow</math> products            2-BUTENE, 2-METHYL-, + NITROGEN ATOM            72 KHR/PAR            REACTION ORDER: 2.            k/k<sub>ref</sub>: 3.5            -----</p> <p>           NOTE: k<sub>ref</sub>: <math>CH_2=CH_2 + N</math>            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + ^1CH_2 \rightarrow</math> products            2-BUTENE, 2-METHYL-, + METHYLENE FREE RADICAL            72 KHR/PAR            REACTION ORDER: 2.            k/k<sub>ref</sub>: 2.12            -----</p> <p>           NOTE: k<sub>ref</sub>: <math>CH_2=CH_2 + ^1CH_2</math>            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + ^3CH_2 \rightarrow</math> products            2-BUTENE, 2-METHYL-, + METHYL FREE RADICAL            72 KHR/PAR            REACTION ORDER: 2.            k/k<sub>ref</sub>: 1.83            -----</p> <p>           NOTE: k<sub>ref</sub>: <math>CH_2=CH_2 + ^3CH_2</math>            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + CH_3 \rightarrow (CH_3)_2C=CHCH_2 + CH_4</math>            2-BUTENE, 2-METHYL-, + METHYL FREE RADICAL            76 KHR/PAR            REACTION ORDER: 2.            NOTE: TENTATIVE k VALUE.            -----</p> <p> <math>(CH_3)_2C=CHCH_3 + CH_3 \rightarrow (CH_3)_3CCH(\cdot)CH_3</math>            -----</p>	<p>298</p> <p>450-600</p> <p>298</p> <p>298-400</p> <p>298 300</p> <p>298 298</p> <p>320-550 435</p> <p>297</p> <p>400-500</p>	<p>-</p> <p>4.4(+11)</p> <p>-</p> <p>3.9(+12)</p> <p>9.1(+11)</p> <p>6.5(+13)</p> <p>9.3(+10)</p> <p>-</p> <p>4.9(+11)</p>	<p>-</p> <p>0</p> <p>-</p> <p>0</p> <p>-</p> <p>-</p> <p>0</p> <p>0</p>	<p>3500</p> <p>4225±750</p> <p>3620</p> <p>- 680</p> <p>-</p> <p>-</p> <p>433</p> <p>-</p> <p>-</p> <p>4300±500</p>	<p>0.5 1.5</p> <p>0.5 1.5</p> <p>0.8 1.2</p> <p>0.5 1.5</p>

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
<p>• (CH<sub>3</sub>)<sub>2</sub>C(•)CH(CH<sub>3</sub>)<sub>2</sub> 2-BUTENE, 2-METHYL-, • METHYL FREE RADICAL 72 KER/PAR NOTE: TENTATIVE k VALUE.</p>	403-455	1.4(•10)	0	3070	0.7
<p>NOTE: k<sub>ref</sub>: CH<sub>2</sub>-CH<sub>2</sub> • CH<sub>3</sub> k/k<sub>ref</sub>: 0.4</p>	453	-	-	-	-
<p>(CH<sub>3</sub>)<sub>2</sub>C-CHCH<sub>3</sub> • CCG - (CH<sub>3</sub>)<sub>2</sub>C-C-CHCH<sub>3</sub> • C6 2-BUTENE, 2-METHYL-, • CARBON GILIE(C<sub>2</sub>O) 72 KER/PAR NOTE: k<sub>ref</sub>: CH<sub>2</sub>-CH<sub>2</sub> • CCG REACTION ORDER: 2. k/k<sub>ref</sub>: 100.</p>	298	-	-	-	-
<p>(CH<sub>3</sub>)<sub>3</sub>CCCH<sub>2</sub> • - (CH<sub>3</sub>)<sub>2</sub>C-CH<sub>2</sub> • CH<sub>3</sub> PROPYL, 2,2-DIMETHYL-, FREE RADICAL 70 BEN/G'N REACTION ORDER: 1.</p>	762	1.0(•14)	0	18875	0.7
<p>(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>2</sub> • • CH<sub>2</sub>-CH<sub>2</sub> - (CH<sub>3</sub>)<sub>2</sub>CH(CH<sub>2</sub>)<sub>3</sub>CH<sub>2</sub> • BUTYL, 3-METHYL-, FREE RADICAL • ETHENE 72 KER/PAR NOTE: TENTATIVE k VALUE. REACTION ORDER: 2.</p>	340-413	1.2(•10)	0	3235	0.7
<p>CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> • 6 - CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub> • 6H PENTANE • OXYGEN ATOM 73 BER/HUI REACTION ORDER: 2.</p>	298-650	2.9(•13)	0	2920	0.7
<p>CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> • 6 - CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub> • CH<sub>3</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>3</sub> • CH PENTANE • OXYGEN ATOM 73 BER/HUI REACTION ORDER: 2.</p>	298-650	8.0(•13)	0	2320	0.7
<p>CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> • CH<sub>3</sub> • - CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub> • CH<sub>4</sub> PENTANE • METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE. REACTION ORDER: 2.</p>	350-600	4.8(•11)	0	5600±250	0.7
<p>CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> • CH<sub>3</sub> • - CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>2</sub>CH<sub>3</sub> • CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH(•)CH<sub>3</sub> • CH<sub>4</sub> PENTANE • METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE. REACTION ORDER: 2.</p>	350-600	6.0(•11)	0	4830±250	0.7
<p>(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> • 6 - [C<sub>5</sub>H<sub>11</sub>•] • 6H BUTANE, 2-METHYL-, • OXYGEN ATOM 73 BER/HUI REACTION ORDER: 2.</p>	307	8.0(•10)	-	-	0.7
<p>(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> • CH<sub>3</sub> • - (CH<sub>3</sub>)<sub>2</sub>C(•)CH<sub>2</sub>CH<sub>3</sub> • CH<sub>4</sub> BUTANE, 2-METHYL-, • METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE. REACTION ORDER: 2.</p>	350-750	9.6(•10)	0	3975±250	0.7
<p>(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> • CH<sub>3</sub> • - (CH<sub>3</sub>)<sub>2</sub>CHCH(•)CH<sub>3</sub> • CH<sub>4</sub> BUTANE, 2-METHYL-, • METHYL FREE RADICAL 76 KER/PAR NOTE: TENTATIVE k VALUE. REACTION ORDER: 2.</p>	350-750	2.0(•11)	0	4830±250	0.7

CHEMICAL REACTIONS	T/K	A	B	E/R (in OK)	k factors f
NOTE: TENTATIVE k VALUE. $(CH_3)_2CHCH_2CH_3 + CH_3 \rightarrow (CH_3)_2CHCH_2CH_2$ $\cdot CH_2CH(CH_3)CH_2CH_3 + CH_4$ BUTANE, 2-METHYL-, + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE. $(CH_3)_4C + (CH_3)_3C \cdot + CH_3$ PROPANE, 2,2-DIMETHYL- 70 BEN/C'N REACTION ORDER: 1. $(CH_3)_4C + C \rightarrow (CH_3)_3CCH_2 \cdot + 6H$ 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-ETHENYLIC- 70 BEN/C'N REACTION ORDER: 1. $cis-CH_3CH=CHC_6H_5 \rightarrow trans-CH_3CH=CHC_6H_5$ $cis-2-BUTENOIC ACID METHYL ESTER$ 70 BEN/C'N REACTION ORDER: 1. $trans-CH_3CH=CHC_6H_5 \rightarrow cis-CH_3CH=CHC_6H_5$ $trans-2-BUTENOIC ACID METHYL ESTER$ 70 BEN/C'N REACTION ORDER: 1. $CH_3C_6H_4CH_2CH=CH_2 + CH_3CH_2 \cdot \rightarrow CH_3C_6H_4CH_2CH_2CH_3$ $+ CH_3C_6H_4CH_2CH_2CH_2CH_3$ ACETIC ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL 72 KER/PAR REACTION ORDER: 2. $(CH_3COO)_2CH_2 \rightarrow (CH_3CO)_2C + HCHO$ METHANEDICHL, DIACETATE 70 BEN/C'N REACTION ORDER: 1. $(CH_3)_2CHCH=CH_2 \rightarrow CH_3CH=CH_2 + CH_3CH_2$ PROPANE, 2-(ETHENYLIC)- 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. $CH_3CH_2CH_2CH_2CH_3 + CH_3 \rightarrow CH_3CH_2CH_2CH_2C(\cdot) + CH_4$ PENTANAL + METHYL FREE RADICAL 76 KER/PAR REACTION ORDER: 2. NOTE: TENTATIVE k VALUE.	350-750	7.1(+11)	0	5800±250	0.7 1.3
REACTION ORDER: 1.	803-1200	5.0(+16)	0	40465	
REACTION ORDER: 2.	298-650	5.9(+13)	0	2920	0.7 1.4
REACTION ORDER: 2.	400-600	8.3(+11)	0	5940±350	0.6 1.4
REACTION ORDER: 1.	440-473	5.0(+11)	0	15400	
REACTION ORDER: 1.	673-833	1.6(+11)	0	29090	
REACTION ORDER: 1.	673-833	4.0(+12)	0	29190	
REACTION ORDER: 2.	308-448	2.5(+11)	0	3900	
REACTION ORDER: 1.	493-578	5.0(+10)	0	18300	
REACTION ORDER: 1.	720-794	3.8(+12)	0	21920	
REACTION ORDER: 1.	625-663	8.5(+11)	0	20600	
REACTION ORDER: 2.	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
<p>CH<sub>3</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)C + CH<sub>3</sub> → CH<sub>3</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)C(•), + CH<sub>4</sub>            BUTANAL, 2-METHYL-, + METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
350-500	1.0(+11)	0	3070±500	0.4	1.6
<p>(CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>CH<sub>3</sub> + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>CHCH<sub>2</sub>C(•), + CH<sub>4</sub>            BUTANAL, 3-METHYL-, + METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
350-500	1.0(+11)	0	3170±500	0.5	2.0
<p>(CH<sub>3</sub>)<sub>3</sub>CCCH<sub>3</sub> + CH<sub>3</sub> → (CH<sub>3</sub>)<sub>3</sub>C(•), + CH<sub>4</sub>            PROPANAL, 2,2-DIMETHYL-, + METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
300-450	1.9(+11)	0	3675±500	0.5	1.5
<p>(CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>CC + CH<sub>3</sub> → CH<sub>3</sub>CH(•)CCH<sub>2</sub>CH<sub>3</sub>            + •CH<sub>2</sub>CH<sub>2</sub>CCCH<sub>2</sub>CH<sub>3</sub> + CH<sub>4</sub>            3-PENTANONE + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.</p>					
500-600	2.0(+11)	0	5535±500	0.5	2.0
<p>(CH<sub>3</sub>CD<sub>2</sub>)<sub>2</sub>CC + CH<sub>3</sub> → CH<sub>3</sub>CD<sub>2</sub>CCD(•)CH<sub>3</sub> + CH<sub>4</sub>            3-PENTANONE-2,2,4,4-d<sub>4</sub> + METHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.</p>					
500-600	1.3(+11)	0	4200±500	0.5	2.0
<p>(CH<sub>3</sub>CH<sub>2</sub>)<sub>2</sub>CC + CH<sub>3</sub> → •CH<sub>2</sub>CH<sub>2</sub>CCCH<sub>2</sub>CH<sub>3</sub> + CH<sub>3</sub>CH<sub>3</sub>            3-PENTANONE + ETHYL FREE RADICAL            76 KER/PAR            REACTION ORDER: 2.</p>					
300-520	2.8(+11)	0	3986±100	0.4	2.2
<p>HC(•)(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub> + CH<sub>3</sub> → •C(•)(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub> + HC(•)CH(•)(CH<sub>2</sub>)<sub>2</sub>CH<sub>3</sub>            + HC(•)CH<sub>2</sub>CH(•)(CH<sub>2</sub>)CH<sub>3</sub> + HC(•)CH<sub>2</sub>CH<sub>2</sub>CH(•)(CH<sub>3</sub>)            + HC(•)(CH<sub>2</sub>)<sub>3</sub>CH<sub>2</sub>• + CH<sub>4</sub>            FORMIC ACID BUTYL ESTER + METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.</p>					
503-573	7.9(+12)	0	19730		
<p>HC(•)C(CH<sub>3</sub>)<sub>3</sub> → (CH<sub>3</sub>)<sub>2</sub>C-CH<sub>2</sub> + HC(•)CH<sub>3</sub>            FORMIC ACID 1,1-DIMETHYL ETHYL ESTER            70 BEN/G'N            REACTION ORDER: 1.</p>					
725-810	2.5(+12)	0	24006		
<p>CH<sub>3</sub>CC(•)CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> → CH<sub>3</sub>CH-CH<sub>2</sub> + CH<sub>3</sub>CC(•)H            ACETIC ACID PROPYL ESTER            70 BEN/G'N            REACTION ORDER: 1.            NOTE: RELIABILITY NO BETTER THAN AN ORDER OF MAGNITUDE.</p>					
586-801	1.0(+13)	0	22645		
<p>CH<sub>3</sub>CC(•)CH(CH<sub>3</sub>)<sub>2</sub> → CH<sub>3</sub>CH-CH<sub>2</sub> + CH<sub>3</sub>CC(•)H            ACETIC ACID 1-METHYLETHYL ESTER            70 BEN/G'N            REACTION ORDER: 1.</p>					

## 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	-	-	-	
320-550 435	3.4(+11)	0	1102	
320-550 435	-	-	-	

$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_2 + \text{CH}_2-\text{CH}_2$   
 PROPANIC ACID ETHYL ESTER  
 70 KBR/G'N  
 REACTION ORDER: 1.

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

$\text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2-\text{C}(\text{O})\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\cdot$   
 ACETIC ACID (2-METHYL ETHYL) ESTER  
 70 KBR/G'N  
 REACTION ORDER: 1.

$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\cdot + \text{CH}_2-\text{CH}_2$   
 PROPANIC ACID ETHYL ESTER  
 70 KBR/G'N  
 REACTION ORDER: 1.

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

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

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

NOTE: TENTATIVE k VALUE.

$(\text{CH}_3)_2\text{N}(\text{O})\text{N}(\text{CH}_3)_2 + \text{CH}_3 \rightarrow \cdot\text{CH}_2(\text{CH}_3)\text{N}(\text{O})\text{N}(\text{CH}_3)_2 + \text{CH}_4$   
 UREA, TETRAMETHYL-, + METHYL FREE RADICAL  
 76 KBR/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 KBR/G'N  
 REACTION ORDER: 1.

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

k/k<sub>ref</sub>: 14.0

NOTE: k<sub>ref</sub>: CHCH + N.

$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_3 + \text{N} \rightarrow \text{products}$   
 3-HEXYNE + NITROGEN ATOM  
 72 KBR/PAR  
 REACTION ORDER: 2.

k/k<sub>ref</sub>: 14.0

NOTE: k<sub>ref</sub>: CH<sub>3</sub>CH + N

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
474-518	6.3(+10)	0	16355	
<p> <math>\text{cis-CH}_2\text{-CHCH-CHCH}_2\text{CH}_3</math>  <math>\text{cis-1,3-HEXADIENE}</math>            REACTION ORDER: 1.            -----            70 BEN/6'N         </p>				
530	1.3(+11)	0	17865	
<p> <math>\text{CD}_2\text{-CHCH}_2\text{CH}_2\text{CH-CD}_2</math>  <math>\text{1,5-HEXADIENE-1,1,6,6-D}_4</math>            REACTION ORDER: 1.            -----            70 BEN/6'N         </p>				
473-510	5.2(+11)	0	18199	
<p> <math>(\text{CH}_3)_2\text{C=CHCH-CH}_2</math>  <math>\text{1,3-PENTADIENE, 4-METHYL-}</math>            REACTION ORDER: 1.            -----            70 BEN/6'N         </p>				
318-414	1.6(+11)	0	2265	
<p> <math>\text{CH}_2\text{-C}(\text{CH}_3)_2\text{C}(\text{CH}_3)\text{-CH}_2</math>  <math>\text{1,3-PENTADIENE, 2,3-DIMETHYL-}</math>  <math>\text{1,3-BUTADIENE, 2,3-DIMETHYL-}</math>            REACTION ORDER: 2.            -----            72 KER/PAR         </p>				
473	1.7(+11)	0	16485	
<p> <math>\text{cis-CH}_2\text{-C}(\text{CH}_3)\text{CH=CHCH}_3</math>  <math>\text{cis-1,3-PENTADIENE, 2-METHYL-}</math>            REACTION ORDER: 1.            -----            70 BEN/6'N         </p>				
298	3.1(+12)	-	-	0.7 1.3
<p> <math>\text{CH}_3(\text{CH}_2)_3\text{CH-CH}_2</math>  <math>\text{1-HEXENE}</math>            REACTION ORDER: 2.            -----            73 HER/HUI         </p>				
338-435	3.9(+10)	0	3400	
<p> <math>\text{CH}_2(\text{CH}_2)_3\text{CH-CH}_2</math>  <math>\text{1-HEXENE}</math>            REACTION ORDER: 2.            -----            72 KER/PAR         </p>				
298	-	-	4060	
<p> <math>\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH-CHCH}_3</math>  <math>\text{cis-2-HEXENE}</math>            REACTION ORDER: 2.            -----            72 KER/PAR         </p>				
298	-	-	4150	
<p> <math>\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH-CHCH}_3</math>  <math>\text{cis-2-HEXENE}</math>            REACTION ORDER: 2.            -----            72 KER/PAR         </p>				
298	-	-	3450	
<p> <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2</math>  <math>\text{1-PENTENE, 2-METHYL-}</math>            REACTION ORDER: 2.            -----            72 KER/PAR         </p>				
298	-	-	4390	
<p> <math>\text{cis-}(\text{CH}_3)_2\text{CHCH=CHCH}_3</math>  <math>\text{cis-2-PENTENE, 4-METHYL-}</math>            REACTION ORDER: 2.            -----            72 KER/PAR         </p>				
298-400	3.4(+12)	0	-790	0.8 1.2
<p> <math>(\text{CH}_3)_2\text{C-C}(\text{CH}_3)_2</math>  <math>\text{2-BUTENE, 2,3-DIMETHYL-}</math>            REACTION ORDER: 2.            -----            73 HER/HUI         </p>				
<p> <math>(\text{CH}_3)_2\text{C-C}(\text{CH}_3)_2</math>  <math>\text{2-BUTENE, 2,3-DIMETHYL-}</math>            REACTION ORDER: 2.            -----            73 HER/HUI         </p>				

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
72 KER/PAR NOTE: $k_{ref}$ : $CH_3\dot{C}H=CH_2 + H$ ----- $(CH_3)_2C=C(CH_3)_2 + S \rightarrow cy-[(CH_3)_2]C\dot{C}(CH_3)_2$ 2-BUTENE, 2,3-DIMETHYL-, + SULFUR ATOM REACTION ORDER: 2.0 72 KER/PAR	298 300	7.8(+11) -	-	-	
$(CH_3)_2C=C(CH_3)_2 + N \rightarrow$ products 2-BUTENE, 2,3-DIMETHYL-, + NITROGEN ATOM REACTION ORDER: 2.0 72 KER/PAR NOTE: $k_{ref}$ : $CH_2=CH_2 + N$ ----- $(CH_3)_2C=C(CH_3)_2 + ^1CH_2 \rightarrow$ products 2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL REACTION ORDER: 2.0 72 KER/PAR NOTE: $k_{ref}$ : $CH_2=CH_2 + ^1CH_2$ ----- $(CH_3)_2C=C(CH_3)_2 + ^3CH_2 \rightarrow$ products 2-BUTENE, 2,3-DIMETHYL-, + METHYLENE FREE RADICAL REACTION ORDER: 2.0 72 KER/PAR NOTE: $k_{ref}$ : $CH_2=CH_2 + ^3CH_2$ ----- $(CH_3)_2C=C(CH_3)_2 + CH_3 \rightarrow (CH_3)_2C(CH_3)C\dot{C}H_2 + CH_4$ 2-BUTENE, 2,3-DIMETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.0 76 KER/PAR	298 320-550 435	8.5(+13) 1.7(+11) -	0	690	
$(CH_3)_2C=C(CH_3)_2 + CH_3 \rightarrow (CH_3)_3CC\dot{C}(CH_3)_2$ 2-BUTENE, 2,3-DIMETHYL-, + METHYL FREE RADICAL REACTION ORDER: 2.0 72 KER/PAR NOTE: TENTATIVE $k$ VALUE. ----- NOTE: $k_{ref}$ : $CH_2=CH_2 + CH_3$ ----- $(CH_3)_2C=C(CH_3)_2 + C\dot{C}l \rightarrow (CH_3)_2C-C\dot{C}(CH_3)_2 + C\dot{C}l$ 2-BUTENE, 2,3-DIMETHYL-, + CARBON DIIDE( $C_2\dot{C}$ ) REACTION ORDER: 2.0 72 KER/PAR NOTE: $k_{ref}$ : $CH_2=CH_2 + C\dot{C}l$ ----- $CH_3\dot{C}H(CH_3)CH_2CH_2CH_3 \rightarrow CH_3\dot{C}H=CH_2 + CH_3CH_2CH_2\dot{C}H_2$ PENTYL, 1-METHYL-, FREE RADICAL REACTION ORDER: 1.0 70 BEN/G'N $CH_3(CH_2)_4CH_3 + \dot{C} \rightarrow CH_3(CH_2)_4CH_2\dot{C} + \dot{C}H$ HEXANE + OXYGEN ATOM REACTION ORDER: 2.0 73 HBR/HUI $CH_3(CH_2)_4CH_3 + \dot{C} \rightarrow CH_3CH_2\dot{C}(CH_3)CH_2CH_2CH_3$ + $CH_3CH_2CH_2\dot{C}(CH_3)CH_2CH_3 + \dot{C}H$ HEXANE + OXYGEN ATOM REACTION ORDER: 2.0 73 HBR/HUI	257 257 403-614 403-453 453 298 822 298-650 298-650	-	0	4400±500 3400	0.6 1.4 0.6 1.4 0.7 1.3 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
<p>-----  <math>\text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_2 \cdot + \text{CH}_4</math>            HEXANE <math>\rightarrow</math> METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.            REACTION ORDER: 2.</p>				
350-800	7.9(+11)	0	4830±250	0.7 1.3
<p>-----  <math>\text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_3 \cdot + \text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3</math>  <math>\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\cdot)\text{CH}_3 + \text{CH}_4</math>            HEXANE <math>\rightarrow</math> METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.            REACTION ORDER: 2.</p>				
1000-1200	3.2(+16)	0	39250	
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}\cdot + (\text{CH}_3)_2\text{C}\cdot</math>            BUTANE, 2,3-DIMETHYL-            70 HEN/Ø'N            REACTION ORDER: 1.</p>				
1000-1200	1.0(+17)	0	41800	
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_3\cdot</math>            BUTANE, 2,3-DIMETHYL-            70 HEN/Ø'N            REACTION ORDER: 1.</p>				
298-650	5.9(+13)	0	2920	0.7 1.3
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 + \text{Ø} \rightarrow \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{ØH}</math>            BUTANE, 2,3-DIMETHYL-, <math>\rightarrow</math> OXYGEN ATOM            73 HER/HUI            REACTION ORDER: 2.</p>				
298-650	3.1(+13)	0	1650	0.7 1.3
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 + \text{Ø} \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{ØH}</math>            BUTANE, 2,3-DIMETHYL-, <math>\rightarrow</math> OXYGEN ATOM            73 HER/HUI            REACTION ORDER: 2.</p>				
350-750	9.5(+11)	0	5800±250	0.7 1.3
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4</math>            BUTANE, 2,3-DIMETHYL-, <math>\rightarrow</math> METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.            REACTION ORDER: 2.</p>				
350-750	1.9(+11)	0	3975±250	0.7 1.3
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_4</math>            BUTANE, 2,3-DIMETHYL-, <math>\rightarrow</math> METHYL FREE RADICAL            76 KER/PAR            NOTE: TENTATIVE k VALUE.            REACTION ORDER: 2.</p>				
300-500	5.0(+10)	0	3445	
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 + \text{CH}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2</math>  <math>\rightarrow \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4</math>            BUTANE, 2,3-DIMETHYL-, <math>\rightarrow</math> METHYL FREE RADICAL            72 KØN            REACTION ORDER: 2.</p>				
439-566	4.7(+11)	0	4525	
<p>-----  <math>(\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2 + \text{CD}_3\cdot \rightarrow (\text{CH}_3)_2\text{C}(\cdot)\text{CH}(\text{CH}_3)_2</math>  <math>\rightarrow \cdot\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CD}_3\text{H}</math>            BUTANE, 2,3-DIMETHYL-, <math>\rightarrow</math> METHYL-d3 FREE RADICAL            72 KØN            REACTION ORDER: 2.</p>				
416-467	5.4(+11)	0	14745	
<p>-----  <math>\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{C}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_2</math>            1-PROPENE, 3-(1-METHYLETHENYLØXY)-            70 HEN/Ø'N            REACTION ORDER: 1.</p>				
<p>-----  <math>\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{C}\cdot</math></p>				

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
1-PROPENE, 2-METHYL-3-(ETHENYLOXY)- 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_2=\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$ 1-PROPENE, 3-METHYL-3-(ETHENYLOXY)- 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_2=\text{CH}(\text{CH}_3)_2\text{C}(\text{O}^\ominus\text{H}) \rightarrow \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 + \text{C}_6\text{H}_6$ 3-BUTENOIC ACID, 2,2-DIMETHYL- 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_3\text{CH}_2\text{C}(\text{O}^\ominus\text{H})\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{O}^\ominus$ $\text{CH}_3\text{CH}_2\text{C}(\text{O}^\ominus\text{H})\text{CH}_2\text{CH}(\text{O}^\ominus\text{C}_6\text{H}_5)\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{C}(\text{O}^\ominus\text{H})\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{O}^\ominus$ PROPANOIC ACID 2-PROPENYL ESTER + ETHYL FREE RADICAL REACTION ORDER: 2. ----- $(\text{CH}_3\text{C}(\text{O}^\ominus))_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{C}(\text{O}^\ominus)\text{C}(\text{O}^\ominus)\text{CH}_3 + \text{CH}_3\text{C}(\text{O}^\ominus)\text{H}$ 1,1-ETHANEDIOL, DIACETATE 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_3\text{CH}_2\text{C}(\text{O}^\ominus)\text{C}(\text{O}^\ominus)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O}^\ominus)\text{O}^\ominus + \text{CH}_3\text{CH}_2\text{C}(\text{O}^\ominus)\text{O}^\ominus$ PEROXIDE, BIS(1-CYCLOPENTYL)- 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_2=\text{CHCH}_2\text{C}(\text{O}^\ominus)(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{C}(\text{O}^\ominus)$ 4-PENTEN-2-OL, 2-METHYL- 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_3$ BUTANE, 1-(ETHENYLOXY)- 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{O}^\ominus \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O}^\ominus + (\text{CH}_3)_3\text{C}^\ominus$ $+ \text{CH}_2\text{CH}(\text{CH}_2)_3\text{CH}_3 + (\text{CH}_2)_3\text{CH}_3$ BUTANE, 1-ETHENYLOXY-, + ETHYL FREE RADICAL 70 BEN/6'N REACTION ORDER: 2. ----- $\text{CH}_3\text{C}(\text{O}^\ominus)(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{C}(\text{O}^\ominus)\text{H}$ ACETIC ACID BUTYL ESTER 72 KBR/FAR REACTION ORDER: 1. ----- $\text{CH}_3\text{C}(\text{O}^\ominus)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O}^\ominus)\text{H} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$ $+ \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$ ACETIC ACID 1-METHYLPROPYL ESTER 70 BEN/6'N REACTION ORDER: 1. ----- NOTE: 57% 1-BUTENE: trans/cis-2-BUTENE = 0.64. ----- $\text{CH}_3\text{C}(\text{O}^\ominus)\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{C}(\text{O}^\ominus)\text{H}$ ACETIC ACID 2-METHYLPROPYL ESTER 70 BEN/6'N REACTION ORDER: 1. ----- $\text{CH}_3\text{C}(\text{O}^\ominus)(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{C}(\text{O}^\ominus)\text{H}$ ACETIC ACID 1,1-DIMETHYLETHYL ESTER	423-461  423-461  511-548  352-453  493-541  373-464  607-643  590-650  303-435  725-810  576-710  725-810	1.4(+11)  2.1(+11)  1.4(+11)  2.5(+11)  1.9(+10)  2.5(+14)  1.4(+12)  1.4(+11)  2.5(+10)  1.6(+12)  2.0(+13)  7.9(+11)	0  0  0  0  0  0  0  0  0  0  0	14645  14025  18400  3675  16560  15100  20500  21330  3070  23150  23450  23600	

## 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. ----- (CH <sub>3</sub> ) <sub>2</sub> C(OH)CH <sub>2</sub> COCH <sub>3</sub> → (CH <sub>3</sub> ) <sub>2</sub> CO + (CH <sub>3</sub> ) <sub>2</sub> CO 2-PENTANONE, 4-HYDROXY-4-METHYL- 70 HEN/O'N REACTION ORDER: 1. ----- CH <sub>3</sub> COCH(CH <sub>3</sub> )CH <sub>2</sub> COCH <sub>3</sub> → CH <sub>3</sub> COOH + CH <sub>2</sub> =CHCH <sub>2</sub> COCH <sub>3</sub> + cis- and trans-CH <sub>3</sub> CH=CHCOCH <sub>3</sub> 2-PROPANOL, 1-METHOXY-, ACETATE 70 HEN/O'N REACTION ORDER: 1. ----- NOTE: 58% PROPENE, 3-METHOXY- ----- CH <sub>3</sub> COCH <sub>2</sub> CH <sub>2</sub> COCH <sub>2</sub> CH <sub>3</sub> → CH <sub>2</sub> =CHCOCH <sub>2</sub> CH <sub>3</sub> + CH <sub>3</sub> COOH ETHANOL, 2-ETHOXY-, ACETATE 70 HEN/O'N REACTION ORDER: 1. ----- (CH <sub>3</sub> ) <sub>2</sub> CHCOCH(CH <sub>3</sub> ) <sub>2</sub> → CH <sub>3</sub> CH=CH <sub>2</sub> + (CH <sub>3</sub> ) <sub>2</sub> CHOH PROPANE, 2,2'-OXYBIS- 70 HEN/O'N REACTION ORDER: 1. ----- NOTE: SUSPECT RATE CONSTANT. ----- (CH <sub>3</sub> ) <sub>2</sub> CHCOCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> → (CH <sub>3</sub> ) <sub>2</sub> C(•)COCH(CH <sub>3</sub> ) <sub>2</sub> + •CH <sub>2</sub> CH(CH <sub>3</sub> )COCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>4</sub> PROPANE, 2,2'-OXYBIS- + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. ----- CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> COCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> → CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> • + CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CO• PEROXIDE, DIPEPYL 70 HEN/O'N REACTION ORDER: 1. ----- (CH <sub>3</sub> ) <sub>2</sub> CHCOCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> • → (CH <sub>3</sub> ) <sub>2</sub> C(•)COCH(CH <sub>3</sub> ) <sub>2</sub> + •CH <sub>2</sub> CH(CH <sub>3</sub> )COCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>4</sub> PEROXIDE, BIS(1-METHYLETHYL)-, + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. ----- CH <sub>3</sub> CH=NC(CH <sub>3</sub> ) <sub>3</sub> + CH <sub>3</sub> • → CH <sub>3</sub> C(•)=NC(CH <sub>3</sub> ) <sub>3</sub> + •CH <sub>2</sub> CH=NC(CH <sub>3</sub> ) <sub>3</sub> + CH <sub>3</sub> CH=NC(CH <sub>3</sub> ) <sub>2</sub> CH <sub>2</sub> • + CH <sub>4</sub> 2-PROPANIMINE, N-ETHYLIDENE-2-METHYL-, + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. ----- (CH <sub>3</sub> ) <sub>2</sub> CHN=NCH(CH <sub>3</sub> ) <sub>2</sub> → (CH <sub>3</sub> ) <sub>2</sub> CHN=N• + (CH <sub>3</sub> ) <sub>2</sub> CH• DIAZENE, BIS(1-METHYLETHYL)- 70 HEN/O'N REACTION ORDER: 1. ----- (CH <sub>3</sub> ) <sub>2</sub> CHNCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>3</sub> • → (CH <sub>3</sub> ) <sub>2</sub> CHN(•)CH(CH <sub>3</sub> ) <sub>2</sub> + (CH <sub>3</sub> ) <sub>2</sub> C(•)NCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>2</sub> CH(CH <sub>3</sub> )NCH(CH <sub>3</sub> ) <sub>2</sub> + CH <sub>4</sub> 2-PROPANAMINE, N-(1-METHYLETHYL)-, + METHYL FREE RADICAL 76 KEE/PAR REACTION ORDER: 2. ----- NOTE: TENTATIVE K VALUE. ----- (CH <sub>3</sub> CH <sub>2</sub> ) <sub>3</sub> N + CH <sub>3</sub> • → CH <sub>3</sub> CH(•)N(CH <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub> + •CH <sub>2</sub> CH <sub>2</sub> N(CH <sub>2</sub> CH <sub>3</sub> ) <sub>2</sub> + CH <sub>4</sub>			

CHEMICAL REACTIONS	T/K	A	B	E/R (in °K)	k factors f
ETHANAMINE, N,N-DIETHYL-, • METHYL FREE RADICAL 76 KEE/PAR NOTE: TENTATIVE k VALUE.	350-600	5.0(•11)	0	4000±500	0 2.0
$\text{CH}_2=\text{C}=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CH}=\text{CH}_2$ 1,2,6-HEPTADIENE 70 HEN/6'N REACTION ORDER: 1.	445-491	9.3(•9)	0	14330	
$\text{CH}_3(\text{CH}_2)_4\text{CCH} \cdot \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{C}(\cdot) - \text{CHCH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{C}(\text{CH}_2\text{CH}_3) - \text{CH} \cdot$ 1-HEPTYNE • ETHYL FREE RADICAL 72 KEE/PAR REACTION ORDER: 2.	451-523	1.3(•11)	0	16355	
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$ 1,5-HEPTADIENE 70 HEN/6'N REACTION ORDER: 1.	451-523	1.3(•11)	0	17590	
$\text{CH}_2-\text{CHCH}(\text{CH}_3)\text{CH}_2-\text{CH}=\text{CH}_2$ 1,5-HEXADIENE, 3-METHYL- 70 HEN/6'N REACTION ORDER: 1.	304	-	-	-	
$(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \cdot \text{CCl} \rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CCl}$ 2,3-PHTADIENE, 2,4-DIMETHYL-, • CARBON OXIDE(C <sub>2</sub> O) 70 HEN/6'N REACTION ORDER: 2. k/k <sub>ref</sub> : 113.	355-439	6.2(•10)	0	3500	
NOTE: k <sub>ref</sub> : $\text{CH}_2=\text{CH}_2 \cdot \text{CCl}$ . $\text{CH}_3(\text{CH}_2)_4\text{CH}=\text{CH}_2 \cdot \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ 1-HEPTYNE • ETHYL FREE RADICAL 72 KEE/PAR REACTION ORDER: 2.	298	1.6(•12)	-	-	
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 \cdot \text{H} \rightarrow (\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2 \cdot$ $\cdot (\text{CH}_3)_3\text{CC}(\cdot)(\text{CH}_3)_2$ 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 $(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)=\text{CH}_2 \cdot \text{CH}_3\text{CH}_2 \cdot$ $\text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\cdot)(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ $\cdot \text{CH}_3\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)(\text{CH}_2\text{CH}_3)\text{CH}_2 \cdot$ 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
$\text{CH}_3(\text{CH}_2)_5\text{CH}_3 \cdot \text{Cl} \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2 \cdot + \text{HCl}$ HEPTANE • OXYGEN ATOM 73 HEN/HUI REACTION ORDER: 2.	298-650	1.2(•14)	0	2190	0.7 1.3
$\text{CH}_3(\text{CH}_2)_5\text{CH}_3 \cdot \text{Cl} \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3$ $\cdot \text{CH}_3(\text{CH}_2)_2\text{CH}(\cdot)(\text{CH}_2)\text{CH}_3 \cdot \text{Cl}$ HEPTANE • OXYGEN ATOM 73 HEN/HUI REACTION ORDER: 2.	298-650	1.2(•14)	0	2190	0.7 1.3

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f	k factors F
307	6.5(+10)	-	-	0.7	1.4
307	1.0(+11)	-	-	0.7	1.4
350-750	9.5(+10)	0	3975±250	0.7	1.3
350-750	6.0(+11)	0	4830±250	0.7	1.3
350-750	7.1(+11)	0	5800±250	0.7	1.3
1065-1197	1.1(+16)	0	36335		
447-488	7.1(+10)	0	16560		
526-564	5.5(+11)	0	20300		
564-628	2.0(+13)	0	22345		
525-570	7.9(+11)	0	18800		
493-578	5.0(+10)	0	18300		
725-810	1.6(+12)	0	23350		

$(CH_3)_3C(CH_2)_2CH_3 + \theta$  - Products  
 PENTANE, 2,2-DIMETHYL-, + OXYGEN ATOM  
 REACTION ORDER: 2.  
 73 BEN/HUI

$(CH_3)_2CHCH_2CH(CH_3)_2 + e$  - Products  
 PENTANE, 2,4-DIMETHYL-, + OXYGEN ATOM  
 REACTION ORDER: 2.  
 73 BEN/HUI

$(CH_3CH_2)_3CH + CH_3 \rightarrow (CH_3CH_2)_3C + CH_4$   
 PENTANE, 3-ETHYL-, + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: TENTATIVE & VALUE.

$(CH_3CH_2)_3CH + CH_3 \rightarrow (CH_3CH_2)_2CHCH_2 + CH_4$   
 PENTANE, 3-ETHYL-, + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: TENTATIVE & VALUE.

$(CH_3CH_2)_3CH + CH_3 \rightarrow (CH_3CH_2)_2CHCH_2CH_2 + CH_4$   
 PENTANE, 3-ETHYL-, + METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: TENTATIVE & VALUE.

$(CH_3)_3CCH(CH_3)_2 \rightarrow (CH_3)_3C + (CH_3)_2CH$   
 BUTANE, 2,2,3-TRIMETHYL-  
 70 BEN/6'N  
 REACTION ORDER: 1.

$CH_2=C(CH_3)C(CH_3)_2COOH \rightarrow (CH_3)_2C=C(CH_3)_2 + CO_2$   
 3-BUTENOIC ACID 2,2,3-TRIMETHYL-  
 70 BEN/6'N  
 REACTION ORDER: 1.

$trans-CH_3CH=CH(CH_3)_2COOH \rightarrow CH_3CH_2CH=C(CH_3)_2 + CO_2$   
 trans-3-PENTENOIC ACID, 2,2-DIMETHYL-  
 70 BEN/6'N  
 REACTION ORDER: 1.

$CH_3COCH(CH_3)CH_2CH=CH_2 \rightarrow CH_3COCH + CH_2=CHCH_2CH=CH_2$   
 + 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.

$CH_3COCH(CH_3)CH_2COCH_3 \rightarrow CH_3CH=CHCOCH_3 + CH_3COCH$   
 2-2-PENTANONE, 4-ACETYL-  
 70 BEN/6'N  
 REACTION ORDER: 1.

$(CH_3CH_2CO)_2CH_2 \rightarrow (CH_3CH_2CO)_2\theta + HCHO$   
 METHANEDIOL, DIPROPANATE  
 70 BEN/6'N  
 REACTION ORDER: 1.

$CH_3COCH(CH_2)_4CH_3 \rightarrow CH_3CH_2CH_2CH=CH_2 + CH_3COCH$   
 ACETIC ACID PENTYL ESTER  
 70 BEN/6'N  
 REACTION ORDER: 1.

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
650-710	5.0(+12)	0	21995	
<p>-----  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{cis-}</math>, and <math>\text{trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2</math>            ACETIC ACID 1-METHYL ETHYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            NOTE: 55% 1-FENTENE.            -----</p>				
650-710	1.2(+13)	0	22500	
<p>-----  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{cis-}</math>, and <math>\text{trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3</math>            ACETIC ACID 1-ETHYLPROPYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            -----</p>				
725-810	7.9(+11)	0	23500	
<p>-----  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3</math>            ACETIC ACID 2-METHYL BUTYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            -----</p>				
501-562	2.5(+13)	0	20300	
<p>-----  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2</math>            ACETIC ACID 1,1-DIMETHYL PROPYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            NOTE: 75% 1-BUTENE, 2-METHYL-.            -----</p>				
725-810	1.6(+12)	0	23350	
<p>-----  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3</math>            ACETIC ACID 3-METHYL BUTYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            -----</p>				
635-694	4.0(+12)	0	24200	
<p>-----  <math>(\text{CH}_3)_3\text{C}(\text{CH}_2)_2\text{CH}_3 \rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3) + \text{CH}_2=\text{CH}_2</math>            PROPANIC ACID, 2,2-DIMETHYL-, ETHYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            -----</p>				
513-569	6.3(+12)	0	19730	
<p>-----  <math>\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2\text{CH}_3</math>            PROPANIC ACID, 1,1-DIMETHYL ETHYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            -----</p>				
650-710	6.3(+12)	0	22245	
<p>-----  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\text{N}(\text{CH}_3)_2 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2</math>  <math>\downarrow</math>  <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3</math>            ACETIC ACID 1-METHYL-2-DIMETHYLAMINOETHYL ESTER            70 BEN/6°N            REACTION ORDER: 1.            -----</p>				
328-420	6.2(+10)	0	3300	
<p>-----  <math>(\text{CH}_3)_2\text{C}=\text{CHCH}=\text{C}(\text{CH}_3)_2 + 3\text{CH}_3\text{CH}_2</math>  <math>(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\text{CH}_3)\text{C}(\text{CH}_3)_2</math>  <math>\downarrow</math>  <math>(\text{CH}_3)_2\text{C}(\text{CH}_2\text{CH}_3)\text{CH}(\text{CH}_3)\text{C}(\text{CH}_3)_2</math>            2,4-HEADIENE, 2,5-DIMETHYL-, ETHYL FREE RADICAL            72 KEE/PAR            REACTION ORDER: 2.            -----</p>				
339-425	1.2(+11)	0	3625	
<p>-----  <math>\text{CH}_3(\text{CH}_2)_5\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2</math>  <math>\downarrow</math>  <math>\text{CH}_3(\text{CH}_2)_5\text{CH}(\text{CH}_2\text{CH}_3)\text{CH}_2</math>            1-OCTENE + ETHYL FREE RADICAL            72 KEE/PAR            REACTION ORDER: 2.            -----</p>				
<p>-----  <math>(\text{CH}_3)_3\text{CC}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3\text{CH}_2</math>  <math>(\text{CH}_3)_3\text{CC}(\text{CH}_3)\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3</math>  <math>\downarrow</math>  <math>(\text{CH}_3)_3\text{CC}(\text{CH}_3)\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3</math>            REACTION ORDER: 2.            -----</p>				

## CHEMICAL REACTIONS

T/K	A	B	E/R (in °K)	k factors f
309-364	1.9(+10)	0	2870	
<p>1-PENTENE, 2,4,4-TRIMETHYL-, + ETHYL FREE RADICAL            REACTION ORDER: 2.            -----            72 KER/PAR</p>				
298-650	2.9(+13)	0	2920	0.7 1.3
<p><math>\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}</math>            OCTANE + OXYGEN ATOM            REACTION ORDER: 2.            -----            73 KER/HUI</p>				
298-650	9.3(+13)	0	2030	0.7 1.3
<p><math>\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</math>            + <math>\text{CH}_3(\text{CH}_2)_4\text{CH}(\cdot)\text{CH}_2\text{CH}_3</math> + <math>\text{CH}_3(\text{CH}_2)_3\text{CH}(\cdot)(\text{CH}_2)_2\text{CH}_3</math> + <math>\theta\text{H}</math>            OCTANE + OXYGEN ATOM            REACTION ORDER: 2.            -----            73 KER/HUI</p>				
350-800	4.8(+11)	0	5800±250	0.7 1.3
<p><math>\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</math>            OCTANE + METHYL FREE RADICAL            REACTION ORDER: 2.            -----            76 KER/PAR</p>				
350-800	1.2(+12)	0	4830±250	0.7 1.3
<p>NOTE: TENTATIVE k VALUE.            -----            76 KER/PAR</p>				
307	5.5(+10)	-	-	0.6 1.5
<p><math>(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + \theta \rightarrow</math> products            PENTANE, 2,2,4-TRIMETHYL-, + OXYGEN ATOM            REACTION ORDER: 2.            -----            73 KER/HUI</p>				
350-750	2.0(+11)	0	4830±250	0.7 1.3
<p><math>(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_3\text{CCH}(\cdot)\text{CH}(\text{CH}_3)_2 + \text{CH}_4</math>            PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL            REACTION ORDER: 2.            -----            76 KER/PAR</p>				
350-750	9.5(+10)	0	3975±250	0.7 1.3
<p>NOTE: TENTATIVE k VALUE.            -----            76 KER/PAR</p>				
350-750	1.2(+12)	0	5800±250	0.7 1.3
<p><math>(\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2 \cdot</math>            + <math>\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2 + \text{CH}_4</math>            PENTANE, 2,2,4-TRIMETHYL-, + METHYL FREE RADICAL            REACTION ORDER: 2.            -----            76 KER/PAR</p>				
307	3.0(+10)	-	-	0.6 1.5
<p>NOTE: TENTATIVE k VALUE.            -----            73 KER/HUI</p>				
350-750	1.2(+12)	0	5800±250	0.7 1.3
<p><math>(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \theta \rightarrow</math> products            PENTANE, 2,3,4-TRIMETHYL-, + OXYGEN ATOM            REACTION ORDER: 2.            -----            73 KER/HUI</p>				
350-750	1.2(+12)	0	5800±250	0.7 1.3
<p><math>(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_3 \cdot \rightarrow</math>            + <math>\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CH}_4</math>            PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL            REACTION ORDER: 2.            -----            76 KER/PAR</p>				
<p>NOTE: TENTATIVE k VALUE.            -----            76 KER/PAR</p>				

## CHEMICAL REACTIONS

T/K	A	B	E/R (in OK)	k factors f
350-750	2.9(+11)	0	3975±250	0.7 1.3
<p><math>(CH_3)_2CHCH(CH_3)CH(CH_3)_2 + CH_3 \rightarrow (CH_3)_2C(\cdot)CH(CH_3)_2 + CH_4</math>  <math>(CH_3)_2CHC(\cdot)(CH_3)CH(CH_3)_2 + (CH_3)_2C(\cdot)CH(CH_3)_2 + CH_4</math>            PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL            76 KEE/PAR            NOTE: TENTATIVE k VALUE.</p>				
414-605	4.7(+11)	0	4575	
<p><math>(CH_3)_2CHCH(CH_3)CH(CH_3)_2 + CH_3 \rightarrow [C_6H_{17}\cdot] + CH_4</math>            PENTANE, 2,3,4-TRIMETHYL-, + METHYL FREE RADICAL            72 ION            REACTION ORDER: 2.</p>				
985-1119	5.0(+16)	0	33800	
<p><math>(CH_3)_3CC(CH_3)_3 \rightarrow (CH_3)_3C\cdot + (CH_3)_3C\cdot</math>            BUTANE, 2,2,3,3-TETRAMETHYL-            70 BEN/G'N            REACTION ORDER: 1.</p>				
307	8.0(+9)	-	-	0.6 1.5
<p><math>(CH_3)_3CC(CH_3)_3 + \theta \rightarrow</math> Products            BUTANE, 2,2,3,3-TETRAMETHYL-            73 BER/HUI            REACTION ORDER: 2.</p>				
350-800	1.4(+12)	0	5800±250	0.7 1.3
<p><math>(CH_3)_3CC(CH_3)_3 + CH_3 \rightarrow \cdot CH_2C(CH_3)_2CC(CH_3)_2 + CH_4</math>            BUTANE, 2,2,3,3-TETRAMETHYL-, + METHYL FREE RADICAL            76 KEE/PAR            REACTION ORDER: 2.            NOTE: TENTATIVE k VALUE.</p>				
492-533	1.3(+11)	0	16600	
<p><math>(CH_3COO)_2CHCH=CHCH_3 \rightarrow (CH_3CO)_2\theta + cis-CH_3CH=CHCHO</math>            2-BUTENE-1,1-DIOL, DIACETATE            70 BEN/G'N            REACTION ORDER: 1.            NOTE: PROBABLY RELIABLE k.</p>				
484-538	3.0(+10)	0	16560	
<p><math>(CH_3COO)_2CHCH_2CH_2CH_3 \rightarrow (CH_3CO)_2\theta + CH_3CH_2CH_2CHO</math>            1,1-BUTANEDIOL, DIACETATE            70 BEN/G'N            REACTION ORDER: 1.            NOTE: PROBABLY RELIABLE k.</p>				
484-538	2.5(+10)	0	16560	
<p><math>(CH_3CH_2COO)_2CHCH_3 \rightarrow (CH_3CH_2CO)_2\theta + CH_3CHO</math>            1,1-ETHANEDIOL, DIPROPIONATE            70 BEN/G'N            REACTION ORDER: 1.</p>				
370-452	2.0(+14)	0	14900	
<p><math>CH_3CH_2C(\theta)C(\theta)CH_2CH_3 \rightarrow CH_3CH_2C(\theta)C(\theta)\theta</math>  <math>+ CH_3CH_2C(\theta)C(\theta)\theta</math>            PEROXIDE, BIS(1-ETHYL-)            70 BEN/G'N            REACTION ORDER: 1.</p>				
560-610	1.4(+13)	0	19400	
<p><math>CH_3COOC(CH_2CH_3)_2CH_3 \rightarrow cis-</math>, end <math>trans-CH_3CH=C(CH_3)CH_2CH_3</math>  <math>+ CH_2=C(CH_2CH_3)_2 + CH_3COH</math>            ACETIC ACID 1-ETHYL-1-METHYLPROPYL ESTER            70 BEN/G'N            REACTION ORDER: 1.            NOTE: 65% 1-BUTENE, 2-ETHYL-</p>				
725-810	7.9(+11)	0	23050	
<p><math>CH_3COOC(CH_2CH_3)_2 \rightarrow (CH_3CH_2)_2C=CH_2 + CH_3COH</math>            ACETIC ACID 2-ETHYLBUYL ESTER            70 BEN/G'N            REACTION ORDER: 1.</p>				
<p><math>CH_3COOC(CH_3)CH(CH_3)CH_2CH_3 \rightarrow CH_2=CHCH(CH_3)CH_2CH_3</math></p>				



## CHEMICAL REACTIONS

\* cis-, and trans- $\text{C}_3\text{H}_7\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$  +  $\text{CH}_3\text{COOH}$   
 ACETIC ACID 1,2-DIMETHYLBUTYL ESTER  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76% 1-PENTENE, 3-METHYL-

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 $\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}_2\text{CH}_2\text{CH}_3$  -  $\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$   
 +  $(\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_3$  +  $\text{CH}_3\text{COOH}$   
 ACETIC ACID 1,1-DIMETHYLBUTYL ESTER  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 72% 1-PENTENE, 2-METHYL-

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$\text{CH}_3\text{COOC}(\text{CH}_3)_2\text{CH}(\text{CH}_3)_2$  -  $(\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$

+  $\text{CH}_2\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$  +  $\text{CH}_3\text{COOH}$   
 ACETIC ACID 1,1,2-TRIMETHYLPROPYL ESTER  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 90% 1-BUTENE, 2,3-DIMETHYL-

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$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3$  -  $(\text{CH}_3)_3\text{CO}$  +  $(\text{CH}_3)_3\text{CO}$

PEROXIDE, BIS(1,1-DIMETHYLETHYL)  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3$  +  $\text{CH}_3\cdot$  -  $\text{CH}_2\text{C}(\text{CH}_3)_2\text{OC}(\text{CH}_3)_3$  +  $\text{CH}_4$   
 PEROXIDE, BIS(1,1-DIMETHYLETHYL)-, \* METHYL FREE RADICAL  
 76 KER/PAR  
 REACTION ORDER: 2.  
 NOTE: 76 KER/PAR

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 $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_2\text{CH}_3$  -  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{N}$   
 +  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\cdot$   
 DIAZENE, DIBUTYL-  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{NCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$  -  $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{N}$   
 +  $\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$   
 DIAZENE, BIS(1-METHYLPROPYL)-  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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$(\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{NCH}_2\text{CH}(\text{CH}_3)_2$  -  $(\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{N}$   
 +  $(\text{CH}_3)_2\text{CHCH}_2\cdot$   
 DIAZENE, BIS(2-METHYLPROPYL)-  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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$(\text{CH}_3)_3\text{CN}=\text{N}(\text{CH}_3)_3$  -  $(\text{CH}_3)_3\text{CN}=\text{N}$  +  $(\text{CH}_3)_3\text{C}\cdot$   
 DIAZENE, BIS(1,1-DIMETHYLETHYL)-  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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$(\text{CH}_3\text{CH}_2)_2\text{NN}=\text{N}(\text{CH}_2\text{CH}_3)_2$  -  $(\text{CH}_3\text{CH}_2)_2\text{NN}=\text{N}$  +  $(\text{CH}_3\text{CH}_2)_2\text{N}\cdot$   
 2-TETRAZENE, 1,1,4,4-TETRAETHYL-  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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$(\text{CH}_3)_2\text{CHCH}_2\text{N}(\text{CH}_3)\text{CH}_2\text{CH}(\text{CH}_3)_2$  -  $(\text{CH}_3)_2\text{CHCH}_2\text{N}\cdot$   
 +  $(\text{CH}_3)_2\text{CHCH}_2\text{N}\cdot$   
 PROPANE, 1-NITROSC-2-METHYL-, DIMERIC  
 70 BEN/0'N  
 REACTION ORDER: 1.  
 NOTE: 76 KER/PAR

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T/K	A	B	E/R (in °K)	k factors f
650-710	4.0(+12)	0	21740	
560-610	1.5(+13)	0	19525	
560-610	1.3(+13)	0	19075	
403-443	4.0(+15)	0	18800	
350-500	1.8(+12)	0	5900±150	0.3 3
472-673	3.2(+16)	0	25165	
535-618	4.0(+16)	0	23500	
473-673	1.7(+16)	0	24660	
473-673	1.4(+17)	0	21900	
471-508	2.5(+14)	0	17365	
374-402	2.5(+14)	0	12900	

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

APPENDIX: CONVERSION TABLES  
EQUIVALENT SECOND ORDER RATE CONSTANTS

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

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

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

See note to Table for Second Order Rate Constants

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16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)  A table of recommended rate constants for gas phase chemical reactions occurring in combustion is presented. Specifically, it gives in tabular form the values of the parameters for the modified Arrhenius equation $k = AT^p \exp(-E/RT)$ . The table covers reactions occurring in the combustion, oxidation and decomposition of aliphatic saturated or unsaturated C <sub>1</sub> to C <sub>10</sub> hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides and their free radicals, as well as the reactions of O, O <sub>2</sub> , H, H <sub>2</sub> , OH, H <sub>2</sub> O, H <sub>2</sub> O <sub>2</sub> , N, N <sub>2</sub> , NO, N <sub>2</sub> O, NO <sub>2</sub> , N <sub>2</sub> O <sub>4</sub> , N <sub>2</sub> O <sub>5</sub> , S, S <sub>2</sub> , SH, SO, SO <sub>2</sub> , SOH, NS <sub>2</sub> with each other. The table includes approximately 170 first order reactions 760 second order reactions and 50 third order reactions. There are 1805 entries covering about 1100 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.			
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