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Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1979)

Francis Wesley

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Center for Thermodynamic and Molecular Science
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National Bureau of Standards
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Washington, D.C. 20234

July 1980

Marketing Report

Prepared for

Morgantown Energy Technology Center
Department of Energy
Morgantown, West Virginia 26505

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PHASE CHEMICAL REACTIONS OF
SULFUR COMPOUNDS (1971-1979)**

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Interim Report

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and

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Washington, D.C. 20234



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TABLES OF RATE CONSTANTS FOR GAS PHASE CHEMICAL
REACTIONS OF SULFUR COMPOUNDS (1971-1979)*

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A table of rate constants for gas phase chemical reactions of sulfur compounds 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 the reactions of sulfur containing molecules and free radicals - S, S₂, SO, SO₂, SO₃, S₂O, SH, H₂S, CS, CS₂, COS, CH₃S·, CH₃SH, cy-CH₂CH₂S, CH₃SCH₂· and a number of thiols, thioethers and thioesters - with other compounds. The table includes 16 unimolecular, 187 bimolecular, and 11 termolecular reactions totalling 214 distinct chemical reactions. There are 348 distinct entries, distributed as follows: 26 for first order reactions, 294 for second order reactions and 28 for third order reactions. The kinetic data were compiled from 109 experimental papers and 6 critical reviews published between 1970 and 1979.

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

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

INTRODUCTION

This publication consists of a table of rate constants for reactions of inorganic and organic sulfur compounds in the gas phase, as well as of their reactions with other bodies. The table is a compilation of rate constants given in 109 experimental papers and 6 critical reviews published between 1970 and 1979. Its purpose is to provide the kineticist and combustion modeler with a comprehensive and easy-to-use source on kinetic data for chemical processes involving sulfur compounds. The table gives 348 distinct reaction rate constants from the above mentioned sources. A list of references including the 115 papers, arranged alphabetically by author for each separate year, is appended at the end of the table.

For ease of reference the sulfur-containing reactant in a bimolecular or termolecular reaction is always placed first, so that a grouping of the reactions according to the standard order of sulfur compounds is obtained. However, 14 bimolecular reactions and one termolecular reaction involve two sulfur-containing reactants. For that reason, these 15 reactions are listed twice, the second time with the order of the sulfur-containing reactants reversed. (E.g.: $\text{COS} + \text{S} \rightarrow \text{CO} + \text{S}_2$ is also listed as: $\text{S} + \text{COS} \rightarrow \text{S}_2 + \text{CO}$.) As a result, the total number of tabulated entries is 363, although the real number of distinct entries is only 347. The arrangement of the tables and the standard order of chemical compounds are described in detail below, in the "Guidelines for the User".

The presentation of kinetic data is standardized and simplified as much as possible. Rate constants are expressed in terms of 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 E/R 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. Conversion tables for other units are appended at the end of this publication.

This publication is not the result of the effort of a single person, but of the whole staff of the Chemical Kinetics Division. My thanks to all of them. In particular, I wish to thank Dr. David Garvin, Deputy Director of the Center for Thermodynamics and Molecular Science, 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, and Dr. John T. Herron of the Chemical Kinetics Division, for their encouragement; Dr. Bert R. Staples, Chief of the Electrolyte Data Center, for allowing us to program the tables through a computer; 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; and Mrs. Janice L. Jones and Mrs. Delores E. Dorman for typing a difficult typescript 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. Units of rate constants used in this table 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 formulas used to transform any form of uncertainty limits into the standard form were given and discussed at length in the introduction of a previous publication* and will not be repeated here.

Arrangement of the table

This publication is in two parts:

Part I. The table arranged in nine columns gives the chemical reaction, the order of reaction n , the "third body" collision partner M , the rate constants' ratio k/k_{ref} , the temperature range in kelvins, 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 109 experimental papers and 6 critical reviews from which the present table was compiled. Following the bibliography, two conversion tables for equivalent second and third order rate constant units are appended.

The arrangement of the table in part I is as follows:

Column 1 the chemical reaction indicating both the reactants and the products. In the same column, under each chemical reaction, the

* Westley, Francis, "Tables of Recommended Rate Constants for Chemical Reactions Occurring in Combustion", NBSIR 79-1941 (1979) (1st ed.); NSRDS-NBS 67 (1980) (2nd ed.).

names of the reactants are given. The chemical nomenclature adopted is the one used in the Chemical Substance Indexes of Chemical Abstracts. Alternative names are not given. The chemical names of the products are not given. The line with chemical names is indented with respect to the line above it. Under the chemical names, the short reference to the reviewer's book or article is given. It includes the last two digits of the year of the publication followed by the first three letters of the 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.:

78 MAR/HER indicates the experimental rate constant for the reaction between dimethyl sulfide and ozone, published by Martinez and Herron in 1978.

The last line of column 1, placed under the line including the short reference, 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 a value for the ratio k/k_{ref} is given in column 3, or other information pertinent to the reaction indicated above. For a couple of reactions taken from Baulch, et al. (76 BAU/DRY) the relationship $k_1 = Kk_{-1}$ included in the note indicates that the 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, does not allow the forward rate constant of a reaction to be followed immediately by its reverse rate constant. The reader will have to locate the rate constant of a reverse in its proper place in the table.

Column 2, with the heading n , indicates the order of the reaction displayed in column 1. The value of n is 1, 2, or 3, which defines the proper standard units for the reactions, as follows:

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

The reaction order is indicated for every reaction included in the table and the digit indicating its value is aligned with the short reference.

Column 3, with the heading M , defines the inert reaction partner ("third body") when the chemical reaction displayed in column 1 includes the letter M . Most of the third bodies displayed in column 3 include no more than three characters (e.g.: Ar, He, H_2O , N_2 , N_2O , SO_2 , SO_3 , CO_2). For the reaction $\text{SO}_2 + \text{OH} + \text{M} \rightarrow \text{HOSO}_2 + \text{M}$ the third body, a mixture of N_2 and O_2 , is indicated in the note, in column 1. No indication is given if M is undefined in the paper. When displayed, the third body is aligned with the short reference and the reaction order.

Column 4, with the heading k/k_{ref} , gives the ratio of the rate constant of the reaction indicated in column 1 and the rate constant of a reference reaction. In most cases this ratio is a dimensionless number. However, when the order of the reaction indicated in column 1 is different from the order of the reference reaction, the ratio of the rate constants is no longer dimensionless and the expression for the ratio of rate constants is not given in column 3 (for lack of space), but in the note, at the end of column 1. The reference reaction is always indicated in the notes. The dimensionless rate ratios given in column 3 are aligned with the short reference given in column 1 and with the reaction order given in column 2.

Column 5, with the heading T/K, gives the temperature range of validity for the corresponding rate parameters. For some reactions only one temperature is given, meaning that the reaction was studied only at one temperature. If no temperature is indicated, it means that the kinetic parameters of the corresponding reaction are valid throughout. The data estimated by Benson and Golden in their report "Estimating the Kinetics of Combustion" (75 BEN/GOL) are in this category. The temperatures are aligned with the short references given in column 1, as well as with the reaction order given in column 2.

Column 6, with the heading A, gives the value of A for the equation $k = AT^B \exp(-E/RT)$. A is expressed as a number less than 10 followed by the exponent in parenthesis. 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. 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. 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. In such a case a rate ratio is given in column 4.

Column 7, with the heading B, gives the value of B for the equation $k = AT^B \exp(-E/RT)$. The value of B usually lies between 0 and 4, negative or positive. No more than one digit is given after the decimal dot. A dash in this column means that no B value was reported by the evaluator. The data for B are aligned with the short reference and reaction order information.

Column 8, with the heading E/R, indicates the value of E/R for the equation $k = AT^B \exp(-E/RT)$. Since E is the activation energy in cal mol⁻¹ and R the gas constant with a value of 1.987 cal mol⁻¹ K⁻¹, it follows that the units of E/R are kelvins. The values given in column 5 for E/R may vary from 0 to over 100000 kelvins. The E/R values may be positive or negative. Some of the E/R values included in the table are followed by an uncertainty with plus or minus signs. As pointed out in the introduction, these uncertainties may be ignored, as they are included in the lower and upper k factors indicated in the right column of the table. A dash in this column means that no E/R value was reported by the evaluator. The values for the E/R factor are aligned with the short reference and reaction order information.

Column 9, 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 in (1): $fk_0 < k < Fk_0$. 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. The k factors are aligned with the short reference and reaction order information.

Ordering of chemical reactions.

The general rule for ordering the chemical reactions listed in column 1 of the table is the standard order of arrangement as described in NBS Technical Note 270-3^{*}. A detailed discussion of this rule was presented in the introduction to the publication noted in the preceding footnote (NBSIR 79-1941/1979, or NSRDS-NBS 67/1980) - and will

^{*} 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).

not be repeated here. It suffices to say that this rule is applied to the first reactants of the reactions listed in this table, as well as to the reactants following the first, and that the first reactant of a reaction takes precedence over the following ones. The compounds listed in the Table of Contents, which give only the first reactants of the chemical reactions included in this work, are in the standard order (S, S₂, SO, SO₂, SO₃, S₂O, SH, H₂S, CS, CS₂, COS, CH₃S·, cy-CH₂CH₂S, etc.) and are each part of the S-O-H-C system. (The first reactant always includes an S atom, and may include any of the O, H, or C atoms). The second, or the third reactants may include any of the O, H, S, N, or C atoms, and this sequence - arranged according to the standard order - defines the O-H-S-N-C system.

A number of second and third order reactions includes a second and - respectively - third body M. For this type reactions, M will always be placed after all other reactants. (e.g.: SO₃ + M → SO₂ + O + M, or SO + O + M → SO₂ + M).

Most of the chemical reactions included in the table are balanced. There are a number of reactions with unspecified products. In such a case, the word "products" appears after the arrow (e.g.: SO₂ + HO₂ → products).

Display of Chemical Reactions and Formulae

In order to define the reaction products, the reactants are written using semi-structural formulas. All saturated normal hydrocarbons are written so as to show separately each methyl and methylene group in the chain: CH₄, CH₃CH₃, CH₃CH₂CH₃. Unsaturated hydrocarbons are written so as to show the position of double or triple bonds. The unpaired electron

of an alkyl radical is always indicated, with the exception of Methyl free radical, e.g.:

Methyl free radical	CH_3 (no dot)
Ethyl, 1-methyl-, free radical (Isopropyl)	$(\text{CH}_3)_2\text{CH}\cdot$
Methyl, hydroxy-, free radical	$\cdot\text{CH}_2\text{OH}$
Methylthio free radical	$\text{CH}_3\text{S}\cdot$

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) $\text{CH}_3\text{CH}_2\text{CH}(\cdot)\text{CH}_3$

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: $(\text{CH}_3)_2\text{C}(\text{O}\cdot)\text{CH}_2\text{CH}_3$.

The rules for writing peroxy, 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, C, and simple radicals like OH, HO_2 , SH, NH, CH, CH_2 , CH_3 , CS, CN are written without dot.

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f F
S + SO → SO + S Sulfur atom + Sulfur monoxide ZS BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
S + SH → S ₂ + H								
Sulfur atom + Mercapto free radical ZS BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
S + SH → SH + S Sulfur atom + Mercapto free radical ZS BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	4000	
S + N ₂ → NS + N Sulfur atom + Nitrogen molecule ZS BENZOL NOTE: Semi-empirical evaluation.	2				4.0(+12)	0.5	55200	
S*(¹ D) + N ₂ → products Sulfur atom + Nitrogen molecule ZS LI/DAL	2		0.062	300	-	-	-	
E: k _{ref} , S*(¹ D) + CH ₂ =CH ₂ → products								
S + NO → SO + N Sulfur atom + Nitrogen oxide(NO) ZS BENZOL NOTE: Semi-empirical evaluation.	2				4.0(+11)	0.5	17260	
S + NO → NS + O Sulfur atom + Nitrogen oxide(NO) ZS BENZOL NOTE: Semi-empirical evaluation.	2				1.0(+12)	0.5	17365	
S*(¹ D) + NO → products Sulfur atom + Nitrogen oxide(NO) ZS LI/DAL NOTE: k _{ref} , S*(¹ D) + CH ₂ =CH ₂ → products	2		0.68		-	-	-	
S + NO + H + SNO + H Sulfur atom + Nitrogen oxide(NO) ZS VANZONI NOTE: Limiting high-pressure k.	2	CO2		298	9.3(+12)	-	-	0.8 1.2
NOTE: k ₀ (low pressure).	3	CO2		298	1.9(+17)	-	-	

CHEMICAL REACTIONS

	n	M	k/k _{ref}	T/K	A	B	E/R [*] (in K)	k factors f F
S + CS + H → CS ₂ + M Sulfur atom + Carbon monosulfide free radical Z6 10X/DKX NOTE: k ₁ = Kk ₁ . Recommended k	3			1600-2700	0.7(+13)	0	-4370	0.5 1.5
S + CS ₂ → S ₂ + CS Sulfur atom + Carbon disulfide Z6 10X/DKX NOTE: Recommended k	2			290	3.9(+11)	-	-	0.5 1.5
S + COS → S ₂ + CO Sulfur atom + Carbon oxide sulfide Z6 10X/DKX NOTE: Evaluation. Z4 KLEZDAV Z6 10X/DKX NOTE: Recommended k	2			290	1.1(+10)	-	-	
S*(¹ D) + COS + S ₂ + CO Sulfur atom + Carbon oxide sulfide Z6 11ZDAE NOTE: k _{ref} = S*(¹ D) + CH ₂ =CH ₂ → products	2		1.5	233-245 230-2600 300	9.2(+11) 1.7(+12)	0	1025±60 2050±230	0.9 1.1 0.3 3.0
S + CN → CS + N Sulfur atom + Cyanogen free radical Z5 10N/CO NOTE: Semi-empirical evaluation.	2			300	6.3(+11)	0.5	0	0.7 1.3
S + C ₂ → S + C Sulfur atom + Carbon dimer Z5 10N/CO NOTE: Semi-empirical evaluation.	2			290-450	6.3(+11)	0.5	0	
S + Cl-Cl → cy-Cl=ClS Sulfur atom + Fluorine Z1 51E/2E4 NOTE: k/k _{ref} = 6.2exp(-1007/T). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method. Z2 11R/2ER NOTE: Recommended k	2			290	1.7(+11)	-	-	
S + Cl-Cl → products Sulfur atom + Fluorine Z8 96R/2AE NOTE: Recommended k	2			290-400	3.4(+13)	0	1510±200	0.4 1.6
S + Cl-Cl → products Sulfur atom + Fluorine Z8 96R/2AE NOTE: Recommended k	2			290	2.3(+11)	-	-	0.0 1.2

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F
<p>S + CH₂=CH₂ + cy-CH₂CH₂S Sulfur atom + Ethene Z1 CONZVAN</p> <p>NOTE: Flash photolysis method.</p> <p>NOTE: k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p> <p>Z2 DAV/ALF2 Z3 KERZEBAB</p> <p>NOTE: Recommended k.</p>	2		1.0	290 290-450	9.0(+11) -	-	-	0.9 1.1
<p>S + CD₂=CH₂ + cy-CD₂CH₂S Sulfur atom + Ethene-1,1-d₂ Z4 SIRZD'G</p> <p>NOTE: k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p> <p>S + cis-CHD=CHD + cy-CHDCHDS Sulfur atom + cis-Ethene-1,2-d₂ Z1 SIRZD'G</p> <p>NOTE: k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p> <p>S + CD₂=CD₂ + cy-CD₂CD₂S Sulfur atom + Ethene-d₄ Z1 SIRZD'G</p> <p>NOTE: k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p>	2		1.07	298-450	-	-	-	
<p>S*(¹D) + CH₃CH₃ + products Sulfur atom + Ethane Z3 LILZDAL</p> <p>NOTE: k_{ref}: S*(¹D) + CH₂=CH₂ + products</p> <p>S + cy-CH₂CH₂S + S₂ + CH₂=CH₂ Sulfur atom + Ethane Z1 SIRZD'G</p> <p>NOTE: k/k_{ref}: 0.3exp(+906/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p> <p>Z3 KLEZDAVI</p>	2		0.17	300	-	-	-	
<p>S + cy-CH₂CH₂S + S₂ + CH₂=CH₂ Sulfur atom + Ethane Z1 SIRZD'G</p> <p>NOTE: k/k_{ref}: 0.3exp(+906/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p> <p>Z3 KLEZDAVI</p>	2			290-450	-	-	-	
<p>S + cy-CH₂CH₂S + S₂ + CH₂=CH₂ Sulfur atom + Ethane Z1 SIRZD'G</p> <p>NOTE: k/k_{ref}: 0.3exp(+906/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p> <p>Z3 KLEZDAVI</p>	2			290-355	2.7(+13)	0	0	0.9 1.1

CHEMICAL REACTIONS	n	M	k _r /k _{ref}	T/K	A	B	E/R (in K)	k factors f F
<p>S + CH₃C≡CH + cy-(CH₃)C=CHS Sulfur atom + 1-Propyne Z1 SIRZOC</p> <p>NOTE: k/k_{ref}: 6.2exp(-453/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method. Z2 KERZPAR</p> <p>NOTE: Recommended k.</p>	2			298-450	-	-	-	
<p>S + CH₃C≡CH + products Sulfur atom + Propyne Z0 VANZSAE</p>	2			298-449	2.0(+13)	0	453±100	0.4 1.6
<p>S + CH₃CH=CH₂ + cy-(CH₃)CICH₂S Sulfur atom + Propene Z1 DONZVAN</p> <p>NOTE: Flash photolysis method. Z1 SINZOC</p> <p>NOTE: k/k_{ref}: 1.0exp(+574/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method. Z2 KERZPAR</p> <p>NOTE: Recommended k. Z2 KERZPAR</p> <p>NOTE: k/k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method. Z3 KLEZDVSZ</p>	2		6.9	298	6.0(+12)	-	-	0.8 1.2
<p>S*(¹D) + CH₃CH=CH₂ + cy-(CH₃)CICH₂S Sulfur atom + Propene Z2 KERZPAR</p> <p>NOTE: k/k_{ref}: S*(¹D) + CH₂=CH₂ + cy-CH₂CH₂S Recommended ratio.</p>	2		1.7	300	-	-	-	
<p>S + cy-(CH₃)CICH₂S + S₂ + CH₃CH=CH₂ Sulfur atom + Ithiane, methyl- Z1 SIRZOC</p> <p>NOTE: k/k_{ref}: 0.4exp(+1057/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂S Conventional photolysis method.</p>	2			298-450	-	-	-	
<p>S + CH₃CH₂C≡CH + products Sulfur atom + 1-Butyne Z0 VANZSAE</p>	2			298	3.3(+12)	-	-	0.9 1.1

CHEMICAL REACTIONS

	n	M	k/k _{ref}	T/K	A	B	E/H (in K)	k factors f
$S + (CH_3)_2C=CH_2 \rightarrow cy-(CH_3)_2C=C(CH_3)_2$ Solfor atom + 2-Butylene ZA SIRZOC NOTE: k/k _{ref} = 2.7exp(+654/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method. Z2 KERZPAR NOTE: Recommended k.	2			290-450	-	-	-	
$S + CH_3C=CCH_3 \rightarrow$ products Solfor atom + 2-Butylene ZB VANZSAF	2			298	1.9(+13)	-	-	0.9 1.1
$S + CH_2=CH-CH_2 \rightarrow cy-(CH_2=CH)CHCH_2S$ Solfor atom + 1,3-Butadiene ZA SIRZOC NOTE: k/k _{ref} = 2.4exp(+1027/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method. Z2 KERZPAR NOTE: Recommended k.	2			290-450	-	-	-	
$S + CH_3CH_2CH=CH_2 \rightarrow cy-(CH_3CH_2)CHCH_2S$ Solfor atom + 1-Butene ZA CUBZOD NOTE: Flash photolysis method. ZA SIRZOC NOTE: k/k _{ref} = 0.75exp(+866/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method. Z2 KERZPAR NOTE: Recommended k.	2		10.0	290	9.0(+12)	-	-	0.9 1.1
$S + cis-CH_3CH=CHCH_3 \rightarrow cy-(CH_3)CHCH(CH_3)_2S$ Solfor atom + cis-2-Butene ZA SIRZOC NOTE: k/k _{ref} = 0.53exp(+1050/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method. Z2 KERZPAR NOTE: Recommended k.	2			290 450	-	-	-	
$S + CH_2=CH_2 \rightarrow cy-CH_2CH_2S$ Recommended ratio. ZA KLEZDAV2	2			216-475	4.5(+12)	0	180±45	0.1 4.0
$S + CH_2=CH_2 \rightarrow cy-CH_2CH_2S$ Recommended ratio.	2		16.0	290	-	-	-	

CHEMICAL REACTIONS

Chemical Reaction	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f
<p>S + cis-CH₃CH=CHCH₃ → products Sulfur atom + cis-2-Pentene Z1 VAN/VAE</p>	2			219-500	2.0(+12)	0	-116±15	0.9 1.1
<p>S + trans-CH₃CH=CHCH₃ → cy-(CH₃)CHCH(CH₃)B Sulfur atom + trans-2-Pentene Z1 VAN/VAN</p>	2			298	1.2(+13)	-	-	0.8 1.2
<p>NOTE: Flash photolysis method. Z1 SIR/VAE</p>	2			298-450	-	-	-	
<p>NOTE: k/k_{ref} = 0.65exp(+1010/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂B Conventional photolysis method. Z2 KER/PAB</p>	2			298	1.4(+13)	-	-	
<p>NOTE: Recommended k. k_{ref}: B + CH₂=CH₂ + cy-CH₂CH₂B Recommended ratio.</p>	2		20.0	298	-	-	-	
<p>S + (CH₃)₂C=CH₂ + cy-(CH₃)₂CCH₂B Sulfur atom + 1-Propene, 2-methyl- Z1 VAN/VAN</p>	2			298	3.6(+13)	-	-	0.9 1.1
<p>NOTE: Flash photolysis method. Z1 SIR/VAE</p>	2			290-450	-	-	-	
<p>NOTE: k/k_{ref} = 0.97exp(+1190/T) k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂B Conventional photolysis method. Z2 KER/PAB</p>	2			298	4.0(+13)	-	-	
<p>NOTE: Recommended k. k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂B Recommended ratio.</p>	2		50.0	298	-	-	-	
<p>S*(¹D) + (CH₃)₂C=CH₂ + cy-(CH₃)₂CCH₂B Sulfur atom + 1-Propene, 2-methyl- Z2 KER/PAB</p>	2			300	-	-	-	
<p>NOTE: k_{ref}: S*(¹D) + CH₂=CH₂ + cy-CH₂CH₂B Recommended ratio.</p>	2		3.5					
<p>S + CH₃CH₂C=CCCH₃ + products Sulfur atom + 2-Pentynone Z1 VAN/VAE</p>	2			298	1.8(+13)	-	-	0.8 1.2
<p>S + CH₃CH₂CH=CH₂ + cy-(CH₃CH₂CH₂)CHCH₂B Sulfur atom + 1-Pentene Z2 KER/PAB</p>	2			298	0.1(+12)	-	-	
<p>NOTE: Recommended k.</p>	2							

CHEMICAL REACTIONS

Chemical Reaction	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f
<p>S + CH₃CH₂C(CH₃)=CH₂ + cy-(CH₃CH₂)C(CH₃)CH₂θ Sulfur atom + 1-butene, 2-methyl- ZA SIRZOG</p> <p>NOTE: k/k_{ref}: 0.78exp(+1424/T)</p> <p>k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂θ Conventional photolysis method. Z2 KERZPAR</p> <p>NOTE: Recommended k.</p>	2			298-450	-	-	-	
<p>S + CH₃CH=C(CH₃)₂ + cy-(CH₃)CHC(CH₃)₂θ Sulfur atom + 2-butene, 2-methyl- ZA SIRZOG</p> <p>NOTE: k/k_{ref}: 0.51exp(+1515/T)</p> <p>k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂θ Conventional photolysis method. Z2 KERZPAR</p> <p>NOTE: Recommended k.</p>	2			298	7.4(+13)	-	-	
<p>S + (CH₃)₂C=C(CH₃)₂ + cy-(CH₃)₂CC(CH₃)₂θ Sulfur atom + 2-butene, 2,3-dimethyl- ZA CONZVAN</p> <p>NOTE: Lower limit k. Flash photolysis method. ZA SIRZOG</p> <p>NOTE: k/k_{ref}: 0.50exp(+1670/T)</p> <p>k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂θ Conventional photolysis method. Z2 KERZPAR</p> <p>NOTE: Recommended k.</p>	2			298	6.5(+13)	-	-	
<p>S + (CH₃)₂C=C(CH₃)₂ + cy-(CH₃)₂CC(CH₃)₂θ Sulfur atom + 2-butene, 2,3-dimethyl- ZA CONZVAN</p> <p>NOTE: Lower limit k. Flash photolysis method. ZA SIRZOG</p> <p>NOTE: k/k_{ref}: 0.50exp(+1670/T)</p> <p>k_{ref}: S + CH₂=CH₂ + cy-CH₂CH₂θ Conventional photolysis method. Z2 KERZPAR</p> <p>NOTE: Recommended k.</p>	2		56.0	298	-	-	-	0.9 1.1
<p>S + (CH₃)₂C=C(CH₃)₂ + products Sulfur atom + 2-butene, 2,3-dimethyl- ZA DAVZKLE</p> <p>S₂ + O + S + SO</p> <p>Sulfur dimer + Oxygen atom Z3 BENZGOL</p> <p>NOTE: Semi-empirical evaluation.</p>	2			252-500	2.8(+12)	0	-650±115	0.6 1.4
<p>S₂ + H + θ + SH Sulfur dimer + Oxygen atom Z5 BENZGOL</p> <p>NOTE: Semi-empirical evaluation.</p>	2				6.3(+11)	0.5	0	
<p>S₂ + H + θ + SH Sulfur dimer + Oxygen atom Z5 BENZGOL</p> <p>NOTE: Semi-empirical evaluation.</p>	2				7.9(+12)	0.5	8355	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F
$S_2 + S + S + S_2$ Sulfur dimer + Sulfur atom Z5 BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
$S_2 + S_2 + M + S_4 + M$ Sulfur dimer Z2 LANZOLD Z3 LANZOLD NOTE: Given with caution.	3 3	CO ₂ CO ₂		293 293	9.1(+17) 3.6(+18)	- -	- -	0.1 10.
$S_2 + N + S + NS$ Sulfur dimer + Nitrogen atom Z5 BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	4000	
$S_2 + C + S + CS$ Sulfur dimer + Carbon atom Z5 BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
$SO + O + O + SO$ Sulfur monoxide + Oxygen atom Z5 BENZOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
$SO + O + S + O_2$ Sulfur monoxide + Oxygen atom Z5 BENZOL NOTE: Semi-empirical evaluation.	2				2.0(+11)	0.5	2770	
$SO + O + M + SO_2 + M$ Sulfur monoxide + Oxygen atom Z1 MIYAZAKA Z6 KAUZDRY NOTE: Recommended k.	3 3	Ar		298 298	7.3(+16) 6.7(+13)	- -	- -	0.9 1.1 0.7 1.3
$SO + O_2 + SO_2 + O$ Sulfur monoxide + Oxygen molecule Z6 KAUZDRY NOTE: Recommended k.	2			440-2100	4.5(+11)	0	3250±590	0.3 1.7
$SO + O_3 (v=n) + SO_2^* + O_2$ Sulfur monoxide + Ozone Z4 KAUZDRY NOTE: $k_{ref} = SO + O_3 + SO_2^* + O_2$	2		2.4	300	-	-	-	0.0 1.3

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k _f factors F
SO + C + S + CO Sulfur monoxide + Carbon atom Z5 UNZGOL NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
SO ₂ + O + SO + O ₂ Sulfur dioxide + Oxygen atom Z6 GAD/DRY NOTE: Recommended k ₁ = Kk ₋₁	2			440-2100	1.3(+14)	-0.5	9980	0.3 1.7
SO ₂ + O + M → SO ₃ + M Sulfur dioxide + Oxygen atom Z4 AIKZPII Z5 WSSZREUR	3	N ₂ O		299-392	3.3(+16)	0	1000±200	
	3	He		240-415	3.3(+16)	0	1400±50	0.8 1.2
	3	He		297	3.0(+14)	-	-	0.9 1.1
NOTE: M _{eff} : He(1.0)	3	SO ₂		297	2.9(+15)	-	-	0.7 1.3
M _{eff} : SO ₂ (9.5)	3	N ₂		297	7.2(+14)	-	-	0.9 1.1
M _{eff} : N ₂ (2.4)	3	Ar		299-400	1.1(+16)	0	1010±150	
Z9 AIKZPII	3	N ₂		300	5.0(+14)	-	-	0.8 1.2
Z8 WSSZREUR	3	SO ₂		299	3.4(+15)	-	-	0.7 1.3
	3			1685	7.4(+14)	-	-	
SO ₂ * + O ₂ + products Sulfur dioxide + Oxygen molecule Z0 PARZUEI NOTE: k _{ref} : SO ₂ * + ¹ SO ₂ , or SO ₂ (SO ₂ * is a singlet formed on absorption).	2		0.05	298	1.3(+8)	-	-	
¹ SO ₂ + O ₂ + products Sulfur dioxide + Oxygen molecule Z0 PARZUEI NOTE: k _{ref} : ¹ SO ₂ + SO ₂ + products (¹ SO ₂ is a fluorescent singlet).	2		0.29	298	-	-	-	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f F
SO ₂ * (J ₁) + O ₂ + products Sulfur dioxide + Oxygen molecule Z0 PAR/WHI	2		0.36	298	-	-	-	
NOTE: k _{ref} : SO ₂ * (J ₁) + SO ₂ + products								
SO ₂ + O ₃ + SO ₃ + O ₂ Sulfur dioxide + Ozone Z4 DAV/PAU	2			300	(6.0(+1))	-	-	
NOTE: Upper limit k.								
SO ₂ + H + M + HSO ₂ + M Sulfur dioxide + Hydrogen atom Z6 FAU/DRY	3			1660-2120	5.1(+15)	-	-	0.5 1.5
NOTE: Recommended k.								
SO ₂ + OH(v=9) + HSO ₃ Sulfur dioxide + Hydroxyl free radical Z2 HOR/COI	2			298	>1.4(+10)	-	-	0.8 1.2
NOTE: Lower limit k. (Unreported I assumed to be 298K.)								
SO ₂ + OH + M + HOSO ₂ + M Sulfur dioxide + Hydroxyl free radical Z4 LUX/23	2			294	3.6(+11)	-	-	0.9 1.1
NOTE: Evaluation. Rate constant expressed as k(M) with M = N ₂ + O ₂ at 1 atm.								
Z5 CAS/DAY	2	N ₂		298	3.6(+11)	-	-	
NOTE: Limiting high-pressure k (760 torr).	3	N ₂		298	5.8(+16)	-	-	
k ₀ (low pressure, (20 torr). Z5 GOR/MUL	2	H ₂ O		435	1.1(+12)	-	-	0.9 1.1
NOTE: In an atmosphere of water vapor. Z5 HAR/MAY	3	Ar		298	1.6(+17)	-	-	0.7 1.3
Z6 AIR/PERE	3	N ₂		290	2.6(+17)	-	-	0.9 1.1
NOTE: At 760 torr. Limiting high-pressure k. k ₀ (low-pressure k). Z7 CAS/TON	2	Ar		298	4.0(+11)	-	-	0.9 1.1
Z7 CAS/TON	2	Ar		298	5.0(+11)	-	-	
NOTE: Limiting high-pressure k (760 torr). k ₀ (low-pressure k).	3	Ar		298	5.9(+16)	-	-	0.8 1.2
Z7 CAS/TON	2	N ₂		297	3.6(+11)	-	-	
NOTE: Limiting high-pressure k (760 torr). k ₀ (low-pressure k).	3	N ₂		297	5.8(+16)	-	-	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F
<p>k_0 (low pressure). On the basis of k_0 (297) and E_a experimental values.</p> <p>k_0 (low-pressure k). Alternative T-dependent expression. Z2 DAY/RAV NOTE: Unreported T assumed to be 290K.</p> <p>$SO_2 + HO_2 \rightarrow SO_3 + OH$ Sulfur dioxide + hydroperoxyl free radical Z3 DAY/RAV NOTE: Evaluation. Z4 LEO</p> <p>NOTE: Evaluation. Ratio data versus k_{ref} for reaction $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$ Z2 MUR/ZEL NOTE: Upper limit k.</p> <p>$SO_2 + HO_2 \rightarrow$ products Sulfur dioxide + hydroperoxyl free radical Z2 BRZ/AM NOTE: Upper limit k.</p> <p>$SO_2 + HO_2 + M \rightarrow HO_2SO_2 + M$ Sulfur dioxide + hydroperoxyl free radical Z2 MUR/ZEL NOTE: Upper limit k.</p> <p>$SO_2 + SO_2^*(^1A_1) + SO^*(^3\Sigma^-) + SO_3$ Sulfur dioxide Z3 GUN/CAL</p> <p>$SO_2 + SO_2^*(^3B_1) + SO + SO_3$ Sulfur dioxide Z3 MUR/ZEL NOTE: In an atmosphere of water vapor. (Approximate k).</p> <p>$SO_2 + SO_2^*(^3A_1) + SO^*(^3\Sigma^-) + SO_3$ Sulfur dioxide Z5 CHU/CAL</p>	3 3 2 2 2 2 3 2 2	N ₂ N ₂ N ₂ He		253-297 253-297 298 300 300 298 300 298 298 298	5.0(+14) 2.5(+29) 5.4(+11) 5.2(+8) 5.2(+8) (1.2(+7)) (6.0(+5)) (1.5(+17)) 2.2(+12) 2.0(+14) 4.2(+10)	0 -5.1 - - - - - - - -	-1410 0 - - - - - - - -	0.8 1.3 0.8 1.2 0.9 1.2 0.8 1.2 0.9 1.1

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f
$SO_2 + NO_2 + SO_3 + NO$ Sulfur dioxide + Nitrogen oxide (NO ₂) Z1 ARN/CUL ZZ EBEZCAL NOTE: Extended validity of k reported in 71 ARN/CUL (above), up to 2000K.	2			703-1193	6.3(+12)	0	13950	
$SO_2 + NO_2^* + products$ Sulfur dioxide + Nitrogen oxide (NO ₂) Z0 IMA/PRE NOTE: At 50 torr.	2			430-1850	6.3(+12)	0	16000	
$SO_2 + NO_3 + SO_3 + NO_2$ Sulfur dioxide + Nitrogen oxide (NO ₂) Z5 DAVZCAL NOTE: Upper limit k.	2			298	0.2(+10)	-	-	
$SO_2 + N_2O_5 + SO_3 + N_2O_4$ Sulfur dioxide + Nitrogen oxide (N ₂ O ₄) Z5 DAVZCAL NOTE: Upper limit k.	2			300	(4.2(+3))	-	-	
$SO_2 + CO + SO + CO_2$ Sulfur dioxide + Carbon monoxide Z3 CER/UEI NOTE: k _{ref} = 5.0 x 10 ⁻³ (at 2537 A°) k/k _{ref} = 5.0 x 10 ⁻³ (at 2537 A°) k/k _{ref} = 1.5 x 10 ⁻³ (at 3130 A°)	2			300	(2.5(+1))	-	-	
$SO_2^* + CO + SO + CO_2$ Sulfur dioxide + Carbon monoxide Z3 CER/UEI NOTE: k _{ref} = 2.2 x 10 ⁻⁵ (3130 to 3261 A°) (SO ₂ [*] is a vibrationally excited singlet).	2			300	-	-	-	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F
<p>SO₂ ** + CO + SO + CO₂ Sulfur dioxide + Carbon monoxide Z3 SCH/HEI</p> <p>NOTE: k_{ref} SO₂ ** + SO₂ k_{ref} = 1.8x10⁻⁵ (2537 to 3261 A°) (SO₂ ** is a chemically active triplet).</p>	2			300	-	-	-	0.7 1.4
<p>SO₂ + CO + M + products Sulfur dioxide + Carbon monoxide Z1 HAU/ICE</p> <p>NOTE: At 27-170 torr pressure.</p>	2	Ar		1770-2453	2.7(+12)	0	24300±600	0.8 1.3
<p>SO₂ + CH₃ + N + CH₃SO₂ + M Sulfur dioxide + Methyl free radical Z3 JAM/KER</p> <p>NOTE: Limiting high-pressure k.</p>	2			298	1.8(+11)	-	-	0.9 1.1
<p>SO₂ + CH₃O₂ + CH₃O₂SO₂ Sulfur dioxide + Methylloxy free radical Z2 SAN/6IM Z2 SIM/UEI</p> <p>NOTE: k_{ref} NO + CH₃O₂ + NO₂ + CH₃O.</p>	2		0.0025	298 296	4.9(+9)	-	-	0.9 1.1 0.8 1.2
<p>SO₂ + CH₃O₂ + products Sulfur dioxide + Methylloxy free radical Z2 SAN/UC9</p> <p>NOTE: Best k estimate, based on apparent rate constant (k_{app} ≈ 2k).</p>	2			296	3.2(+9)	-	-	0.8 1.2
<p>SO₂ + CH₂=CH + products Sulfur dioxide + Ethyne Z1 CIE/NOB</p> <p>NOTE: Given with caution.</p>	2			1550-2150	3.2(+10)	0.5	20535	
<p>SO₂ ** + CH₂=C=CH₂ + products Sulfur dioxide + 1,2-Propadiene Z0 BAR/UEI</p> <p>NOTE: k_{ref} SO₂ ** + CH₂=C=CH₂ + C₃H₄ + other products (SO₂ ** is a non-emitting triplet).</p>	2		4.0	298	-	-	-	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f F
$\text{SO}_2^*(^3P_1) + \text{cis-CH}_3\text{CH=CHCH}_3 +$ $(\text{cis-CH}_3\text{CH=CHCH}_3 \cdot \text{SO}_2)^*$ Sulfur dioxide + cis-2-Pentene ZI DEMZCAL	2			294	1.3(+14)	-	-	0.9 1.1
$\text{SO}_2^*(^3P_1) + \text{trans-CH}_3\text{CH=CHCH}_3 +$ $(\text{trans-CH}_3\text{CH=CHCH}_3 \cdot \text{SO}_2)^*$ Sulfur dioxide + trans-2-Pentene ZI DEMZCAL	2			294	1.2(+14)	-	-	0.9 1.1
$\text{SO}_2^*(^1P_1) + (\text{CH}_3)_3\text{CH} + \text{products}$ Sulfur dioxide + Propane, 2-methyl- ZI SU ZCAL NOTE: Evaluation.	2			298	8.4(+12)	-	-	
$\text{SO}_2^*(^3P_1) + (\text{CH}_3)_3\text{CH} + \text{products}$ Sulfur dioxide + Propane, 2-methyl- ZI SU ZCAL NOTE: Evaluation.	2			298	8.7(+11)	-	-	
$\text{SO}_2^*(^3P_1) + \text{cis-CH}_3\text{CH}_2\text{CH=CHCH}_3 +$ $(\text{SO}_2 \cdot \text{CH}_3\text{CH}_2\text{CH=CHCH}_3)^*$ Sulfur dioxide + cis-2-Pentene ZI SU ZCAL	2			295	6.3(+13)	-	-	0.8 1.2
$\text{SO}_2^*(^3P_1) + \text{trans-CH}_3\text{CH}_2\text{CH=CHCH}_3 +$ $(\text{SO}_2 \cdot \text{CH}_3\text{CH}_2\text{CH=CHCH}_3)^*$ Sulfur dioxide + trans-2-Pentene ZI SU ZCAL	2			295	1.0(+14)	-	-	0.7 1.3
$\text{SO}_2 + \text{M} + \text{SO} + \text{O} + \text{M}$ Sulfur dioxide ZI SU ZCAL	2	Ar		2800-3800	8.0(+15)	0	54350	0.7 1.3
$\text{SO}_3 + \text{O} + \text{SO}_2 + \text{O}_2$ Sulfur trioxide + Oxygen atom ZI SU ZCAL NOTE: k determined in H_2O flame.	2			1100-1400	6.5(+14)	0	5435	
$\text{SO}_3 + \text{O} + \text{SO}_2 + \text{O}_2$ Sulfur trioxide + Oxygen atom ZI SU ZCAL NOTE: k determined in CO_2 flame.	2			900-1600	2.8(+14)	0	6040	
$\text{SO}_3 + \text{O} + \text{SO}_2 + \text{O}_2$ Sulfur trioxide + Oxygen atom ZI SU ZCAL NOTE: k determined in CO_2 flame.	2			300-500	1.5(+8)	0	500	
$\text{SO}_3 + \text{O} + \text{SO}_2 + \text{O}_2$ Sulfur trioxide + Oxygen atom ZI SU ZCAL NOTE: k determined in CO_2 flame.	2			1685	1.5(+11)	-	-	

CHEMICAL REACTIONS

Chemical Reaction	n	M	k _r /k _r ref	T/K	A	B	E/R (ln K)	k factors f
SO ₃ + O + M → SO ₂ + O ₂ + M Sulfur trioxide + Oxygen atom Z5 WES/DLII	3	He		290-507	5.0(+16)	0	-705	0.9 1.1
NOTE: M _{eff} = He(1.0)	3	He		290	7.3(+17)	-	-	0.9 1.1
M _{eff} = SO ₃ (10.0) Upper limit ratio.	3	SO ₃		290	(7.3(+18))	-	-	0.9 1.1
M _{eff} = N ₂ (1.4)	3	N ₂		290	1.0(+18)	-	-	0.9 1.1
SO ₃ + H ₂ O → H ₂ SO ₄ Sulfur trioxide + Water Z5 CAS/PAY	2			290	5.5(+11)	-	-	0.8 1.2
SO ₃ + SO → SO ₂ + SO ₂ Sulfur trioxide + Sulfur monoxide Z4 CIVZ/GAL	2			290	1.2(+9)	-	-	0.4 1.6
SO ₃ + N + SO ₂ → NO Sulfur trioxide + Nitrogen atom Z2 JAC/WIN Z5 WES/DLII	2			300	3.0(+8)	-	-	-
NOTE: Upper limit k.	2			290	(6.0(+6))	-	-	-
SO ₃ + M + SO ₂ → O + M Sulfur trioxide Z2 ASI/GSA	2	Ar		1700-2500	3.2(+15)	0	31900±300	0.6 1.6
S ₂ O + O → SO + SO Sulfur oxide(S ₂ O) + Oxygen atom Z4 SIK/OLY	2			290	9.0(+11)	-	-	0.9 1.1
NOTE: Evaluation.	2			290	6.3(+11)	0.5	4000	-
SH + O → S + OH Mercapto free radical + Oxygen atom Z5 WEN/GOL	2			295	6.3(+11)	0.5	0	-
NOTE: Semi-empirical evaluation.	2			295	9.6(+13)	-	-	0.7 1.3

CHEMICAL REACTIONS

Chemical Reaction	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f
SH + C → S + CH Hydrogen sulfide + Carbon atom Z5 HEN/SOL	2				4.0(+11)	0.5	6090	
NOTE: Semi-empirical evaluation.								
H ₂ S + O → SH + OH								
Hydrogen sulfide + Oxygen atom Z6 HUY/ZIM	2			263-495	4.4(+12)	0	1660±50	0.9 1.1
Z6 HUY/ZIM	2			263-495	4.4(+12)	0	1660±50	0.8 1.2
O ₂ S + O → SO + OD								
Hydrogen sulfide(O ₂ S) + Oxygen atom Z6 HUY/ZIM	2			298-450	6.3(+12)	0	2145±155	0.5 1.5
H ₂ S + O → products								
Hydrogen sulfide + Oxygen atom Z6 HUY/ZIM	2			281-497	1.5(+13)	0	1920±45	0.9 1.1
NOTE: k based on editor's least square fit of 6 given experimental points.								
Z6 HUY/ZIM	2			297-502	1.6(+13)	0	2171±202	0.5 1.5
H ₂ S + O ₃ → SO ₂ + H ₂ O								
Hydrogen sulfide + Ozone Z5 HUY/ZIM	2			298	(1.2(+4)	-	-	
NOTE: Upper limit k. Unreported T assumed to be 298K.								
Z5 HUY/ZIM	2			293-343	4.9(+10)	0	3420	
NOTE: Estimated k.								
Z5 HUY/ZIM	2			290-343	1.6(+12)	0	2620±600	0.2 6.3
Z5 HUY/ZIM	2			298	4.0(+2)	-	-	0.1 10.0
NOTE: Recommended k.								
H ₂ S + H → SH + H ₂								
Hydrogen sulfide + Hydrogen atom Z1 KUR/ZPEI	2			190-464	7.8(+12)	0	860±30	0.9 1.1
Z2 ROM/ZSCH	2			290	2.3(+11)	-	-	0.8 1.3
Z3 HUY/ZIM	2			298	5.0(+11)	-	-	
Z6 HUY/ZIM	2			190-470	7.8(+12)	0	860±50	0.5 1.5
NOTE: Recommended k.								
H ₂ S + OH → SH + H ₂ O								
Hydrogen sulfide + Hydroxyl free radical Z5 HUY/ZIM	2			298-885	1.4(+13)	0	443	
Z4 HUY/ZIM	2			298	1.9(+12)	-	-	0.8 1.2
Z6 HUY/ZIM	2			298-900	6.3(+12)	0	200±150	0.7 1.3
NOTE: k factors changing to f = 0.5 and F = 1.5 at 900K. Recommended k.								
Z6 HUY/ZIM	2			297-427	3.1(+12)	0	-	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f
H ₂ S + OH + products (overall) Hydrogen sulfide + Hydroxyl free radical Z5 HCN/COI NOTE: Approximate k.	2			300	5.2(+12)	-	-	
H ₂ S + OH(v=9) + products Z5 HCN/COI Hydrogen sulfide + Hydroxyl free radical Z5 HCN/COI NOTE: Lower limit k. Unreported T assumed to be 298K.	2			298	>1.5(+11)	-	-	0.6 1.4
H ₂ S + CH ₃ + SH + CH ₄ Hydrogen sulfide + Methyl free radical Z5 KER/PAR NOTE: Tentative k value.	2			300-600	2.0(+11)	0	2065±150	0.4 2.5
H ₂ S + H + SH + H + H Hydrogen sulfide Z5 HCN/COI Z5 HCN/COI	2	Ar		2380-3000	1.3(+16)	0	46300	
	2	Ar		2700-3800	2.0(+13)	0	37300±960	0.7 1.5
CS + O + S + CO Carbon monosulfide free radical + Oxygen atom Z1 HCN/SHI NOTE: Evaluation.	2			298	0.4(+12)	-	-	
	2				6.3(+11)	0.5	0	
NOTE: Semi-empirical evaluation.	2			300	1.3(+13)	-	-	0.8 1.2
NOTE: Unreported T assumed to be 300K.	2		0.1	298	-	-	-	
CS + O + S + CO(v=n) Carbon monosulfide free radical + Oxygen atom Z5 HCN/COI NOTE: k _{ref} CS + O + S + CO(v=13) Ratio increasing from 0.1 to 0.9 between v=7 and v=12, then decreasing to 0.3 from v=14 to v=15. Unreported T assumed to be 290K.	2			305	1.2(+13)	-	-	0.9 1.1
	2			300	1.4(+13)	-	-	0.8 1.2
CS + O + SH + C Carbon monosulfide free radical + Oxygen atom Z5 HCN/COI NOTE: Semi-empirical evaluation.	2				1.6(+12)	0.5	28940	
CS + H + S + CH Carbon monosulfide free radical + Hydrogen atom Z5 HCN/COI NOTE: Semi-empirical evaluation.	2				1.3(+13)	0.5	50930	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f
CS + H + SH + C Carbon monosulfide free radical + Hydrogen atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				2.0(+13)	0.5	48870	
CS + S + S + CS Carbon monosulfide free radical + Sulfur atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
CS + S + C + S ₂ Carbon monosulfide free radical + Sulfur atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				1.6(+12)	0.5	40463	
CS + S + M + CS ₂ + H Carbon monosulfide free radical + Sulfur atom ZS BEN/60L NOTE: k ₁ = Kk ₋₁ Recommended k.	3			1800-3700	8.7(+13)	0	4370	0.5 1.5
CS + N + S + CN Carbon monosulfide free radical + Nitrogen atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				1.3(+12)	0.5	1160	
CS + N + C + NS Carbon monosulfide free radical + Nitrogen atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				4.0(+12)	0.5	37200	
CS + C + S + C ₂ Carbon monosulfide free radical + Carbon atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				5.0(+11)	0.5	20435	
CS + C + C + CS Carbon monosulfide free radical + Carbon atom ZS BEN/60L NOTE: Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
CS ₂ + O + CS + SO Carbon disulfide + Oxygen atom ZS BEN/60L NOTE: Recommended k.	2			278	1.4(+12)	-	-	0.9 1.1
	2			210-293	1.7(+13)	0	645±35	0.9 1.1
	2			200-1000	2.2(+13)	0	700	0.7 1.3

Chemical Reactions	n	M k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f
<p>CO₂ + O → SO + CO Carbon oxide sulfide + Oxygen atom Z1 REF Z1 REF/SIM Z4 REF/SII Z5 REF/III Z6 REF/DRY</p> <p>NOTE: k factors changing to, f = 0.3 and F = 3.0 above 300K. Recommended k.</p>	2		300-523	9.8(+12)	0	2265	
	2		300-523	9.8(+12)	0	2265	0.9 1.1
	2		263-502	9.9(+12)	0	2167±20	0.8 1.2
	2		239-404	1.2(+13)	0	2150±35	0.5 1.5
	2		190-1200	1.6(+13)	0	2250±250	
<p>CO₂ + O*(¹D) → SO + CO Carbon oxide sulfide + Oxygen atom Z5 OZONE</p> <p>NOTE: k_{ref} O₂ + O*(¹D) → O₂*(¹T_g) + O</p> <p>NOTE: Evaluation.</p>	2	4.1	300	-	-	-	
	2		300	1.8(+14)	-	-	
<p>CO₂ + H → CO + SH Carbon oxide sulfide + Hydrogen atom Z2 ROW/SCH Z5 ISM/YOK Z6 ROW/DRY</p> <p>NOTE: Recommended k.</p>	2		298	1.3(+10)	-	-	0.8 1.3
	2		300-525	9.1(+12)	0	1965±105	0.9 1.1
	2		298	1.3(+10)	-	-	0.8 1.3
	2		298-478	9.8(+13)	0	2775±40	0.9 1.1
	2		261-500	5.5(+12)	0	1940±55	0.8 1.2
<p>CO₂ + OH → products Carbon oxide sulfide + Hydroxyl free radical Z0 AIR/PEQ</p> <p>NOTE: Upper limit k.</p>	2		299	(4.2(+9)	-	-	
	2		430	(1.2(+10)	-	-	
	2		296	3.4(+10)	-	-	
<p>CO₂ + OH(v=9) → products Carbon oxide sulfide + Hydroxyl free radical Z5 OZONE</p> <p>NOTE: Unreported F assumed to be 298K.</p>	2		298	1.5(+10)	-	-	0.4 1.6
<p>CO₂ + S → CO + S₂ Carbon oxide sulfide + Sulfur atom Z6 JAK/ZAMJ</p> <p>NOTE: Evaluation.</p>	2		290	1.1(+10)	-	-	
	2		233-245	9.2(+11)	0	1825±60	0.9 1.1
	2		230-2600	1.7(+12)	0	2050±330	0.3 3.0

CHEMICAL REACTIONS

Chemical Reactions	n	M	k/k _{ref}	T/K	A	B	E/R (ln K)	k factors f
$CO_2 + S^*(1D) \rightarrow CO + S_2$ Carbon oxide sulfide + Sulfur atom Z2 LILZDA6 NOTE: k _{ref} : $CH_2=CH_2 + S^*(1D) \rightarrow$ products	2		1.5	300	-	-	-	
$CO_2 + CO_3 \rightarrow CO + CO_3^*$ Carbon oxide sulfide + Methyl-d ₃ free radical Z2 JAK/AHM NOTE: Evaluation.	2			354-490	3.8(+11)	0	5710±175	0.6 1.0
$CO_2 + CN \rightarrow SCN + CO$ Carbon oxide sulfide + Cyanogen free radical Z2 BDDZLSA NOTE: Lower limit k.	2			295	>1.8(+13)	-	-	
$CO_2 + M \rightarrow$ products Carbon oxide sulfide ZA IBA NOTE: k measured in shock tube. Unspecified, high T range.	2				8.3(+14)	0	31700±650	
$CH_3^* + CH_2=CH \rightarrow CH_3SCH=CH^*$ Methylthio free radical + Ethene Z2 KERZPAR NOTE: Recommended k.	2			298-333	7.9(+7)	-	-	
$CH_3^* + CH_2=CH_2 \rightarrow CH_3SCH_2CH_2^*$ Methylthio free radical + Ethene Z2 KERZPAR NOTE: Recommended k.	2			298	4.8(+8)	-	-	
$CH_3^* + cy-CH_2CH_2S \rightarrow CH_3S^* + CH_2=CH_2$ Methylthio free radical + Thirane Z2 JAK/AHM NOTE: Approximate k.	2			304-478	3.2(+11)	0	4430	
$CH_3^* + CH_3CH=CHCH_3 \rightarrow CH_3CH(SCH_3)CH^*()CH_3$ Methylthio free radical + 2-Butene Z2 KERZPAR NOTE: cis-trans equilibrium-weighted k.	2			298-333	1.6(+9)	-	-	
$CH_3SH + CH_3^* \rightarrow SH$ Methanethiol Z2 BENZON NOTE: Critical evaluation.	1			1005-1102	3.2(+15)	0	38550	

CHEMICAL REACTIONS

Chemical Reaction	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{SH} + \text{O} + \text{CH}_3 + \text{HS}(\text{O}) + \text{CH}_3\text{S}(\text{O}) + \text{H} + \text{CH}_3\text{S}$ + CH_3O Methanethiol + Oxygen atom Z6 SIK/CRG Z11 SIK/ZKQJ	2 2			360 254-495	1.1(+12) 1.1(+12)	- -	- -	
NOTE: Non-linear Arrhenius behavior. Within the given T range, k increasing from 1.1×10^{12} at 254K to $2.6 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 495K.								
$\text{CH}_3\text{SH} + \text{CH}_3 + \text{CH}_2\text{SH} + \text{CH}_4$ Methanethiol + Methyl free radical Z6 KER/POB	2			303	1.2(+8)	-	-	0.5 2.0
NOTE: Recommended k.								
$\text{CD}_3\text{SH} + \text{CH}_3 + \text{CD}_3\text{S} + \text{CH}_4$ Methane-d ₃ -thiol + Methyl free radical Z6 KER/POB	2			400-500	1.1(+11)	0	2065±500	0.5 2.0
NOTE: Recommended k.								
$\text{CD}_3\text{SH} + \text{CH}_3 + \text{CD}_2\text{SH} + \text{CH}_3\text{D}$ Methane-d ₃ -thiol + Methyl free radical Z6 KER/POB	2			400-500	7.6(+10)	0	4200±250	0.5 2.0
NOTE: Recommended k.								
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{O} + \text{CH}_2=\text{CH}_2 + \text{SO}$ Thirane + Oxygen atom Z6 LEE/ZIFJ	2			260-424	8.1(+12)	0	10±20	0.9 1.1
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{H} + \text{CH}_2=\text{CH}_2 + \text{SH}$ Thirane + Hydrogen atom Z6 YOK/ZQJH	2			300-425	5.7(+13)	0	978±00	0.9 1.1
$\text{cy-CH}_2\text{SCH}_2 + \text{H} + \text{cy-CH}_2\text{SCH} + \text{H}_2$ Thirane + Hydrogen atom Z6 LEE	2			298	7.1(+11)	-	-	0.6 1.2
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{S} + \text{CH}_2=\text{CH}_2 + \text{S}_2$ Thirane + Sulfur atom Z1 SIK/ZOG	2			298-450	-	-	-	
NOTE: k/k _{ref} = 0.3exp(+906/T) k _{ref} = $\text{CH}_2=\text{CH}_2 + \text{S} + \text{cy-CH}_2\text{CH}_2\text{S}$ Conventional photolysis method. Z3 RUC/DAVI	2			298-355	2.7(+13)	0	0	0.9 1.1

CHEMICAL REACTIONS

Chemical Reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CH}_3 + \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{S} \cdot$ Thiirane + Methyl free radical Z6 JAKZAMM	2			304-478	7.1(+10)	0	3370±400	0.3 3.3
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CD}_3 + \text{CH}_2=\text{CH}_2 + \text{CD}_3\text{S} \cdot$ Thiirane + Methyl-d ₃ free radical Z6 JAKZAMM	2			303-477	5.9(+10)	0	3270±500	0.2 4.4
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CD}_3 + \text{cy-CH}_2\text{CH}(\text{O})\text{S} + \text{CD}_3\text{H}$ Thiirane + Methyl-d ₃ free radical Z6 JAKZAMM	2			303-477	2.2(+11)	0	4800±500	0.3 4.0
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{CH}_3\text{S} \cdot + \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{S}_2$ Thiirane + Methylthio free radical Z6 JAKZAMM	2			300-500	2.2(+11)	0	4800±500	0.5 2.0
$\text{CH}_3\text{SCH}_2 + \text{CH}_4 + (\text{CH}_3)_2\text{S} + \text{CH}_3$ Methyl (methylthio)- free radical + Methane Z6 ABIZELE	2			304-478	3.2(+11)	0	4430	
$\text{CH}_3\text{SCH}_2 + \text{CH}_4 + (\text{CH}_3)_2\text{S} + \text{CH}_3$ Methyl (methylthio)- free radical + Methane Z6 ABIZELE	2			393-518	6.3(+11)	0	7662	
$\text{CH}_3\text{SCH}_2\text{SH} + \text{CH}_2=\text{CH}_2 + \text{H}_2\text{S}$ Ethanethiol Z6 BENZON	1			785-930	1.0(+13)	0	25900	
$\text{CH}_3\text{SCH}_2\text{SH} + \text{CH}_3\text{CH}_2 \cdot + \text{SH}$ Ethanethiol Z6 BENZON	1			785-938	6.3(+15)	0	36336	
$\text{CH}_3\text{SCH}_2\text{SH} + \text{O} + \text{CH}_3\text{CH}_2 \cdot + \text{HS}(\text{O}) \cdot + \text{CH}_3\text{CH}_2\text{S}(\text{O}) \cdot + \text{H}$ Ethanethiol + Oxygen atom Z6 BLOZGRA	2			300	1.7(+12)	-	-	
$\text{CH}_3\text{SCH}_2\text{SH} + \text{O} + \text{CH}_3\text{CH}_2 \cdot + \text{HS}(\text{O}) \cdot + \text{CH}_3\text{CH}_2\text{S}(\text{O}) \cdot + \text{H}$ Ethanethiol + Oxygen atom Z6 BLOZGRA	2			257-495	1.9(+12)	-	-	

NOTE: Evaluation.

NOTE: Evaluation.

NOTE: Recommended k.

NOTE: Approximate k.

NOTE: Evaluation based on k₋₁ and thermodynamic data.

NOTE: Critical evaluation.

NOTE: Critical evaluation.

NOTE: Non-linear Arrhenius behavior. Within the given T range, k increasing from 1.9x10¹² at 257K to 3.2x10¹² cm³mol⁻¹s⁻¹ at 495K.

E/R (k factors)

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F
$\text{CH}_3\text{CH}_2\text{SH} + \text{CH}_3 \rightarrow \text{products}$ Ethanethiol + Methyl free radical Z6 BERZFOR				300	3.5(+17)	-	-	0.5 2.0
NOTE: Tentative k.								
$(\text{CH}_3)_2\text{S} + \text{O} \rightarrow \text{CH}_3\text{S}(\text{O}) + \text{CH}_3$ Methane, thiohis., + Oxygen atom Z6 BERZFOR	2			250-424	0.6(+12)	0	-360±16	0.9 1.1
Z6 BERZFOR				300	3.0(+13)	-	-	
Z6 BERZFOR				252-493	3.0(+13)	-	-	
NOTE: Possible non-linear Arrhenius behavior within the given T range, k decreasing from 3.0×10^{13} at 252K to 2.2×10^{13} $\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$ at 493K.								
$(\text{CH}_3)_2\text{S} + \text{O} \rightarrow \text{products}$ Methane, thiohis., + Oxygen atom Z4 CADZVIC	2			300	3.3(+11)	-	-	
$(\text{CH}_3)_2\text{S} + \text{O}_3 \rightarrow \text{PRODUCTS}$ Methane, thiohis., + Ozone Z0 BERZFOR	2			296	<5.0(+15)	-	-	
NOTE: Upper limit k.								
$(\text{CH}_3)_2\text{S} + \text{H} \rightarrow \text{CH}_3\text{SH} + \text{CH}_3$ Methane, thiohis., + Hydrogen atom Z2 YORKZIR	2			300-472	1.7(+13)	0	1320±44	1.0 1.2
$(\text{CH}_3)_2\text{S} + \text{H} \rightarrow \text{CH}_3\text{SCH}_2 + \text{H}_2$ Methane, thiohis., + Hydrogen atom Z6 BERZFOR				300	9.0(+10)	-	-	0.7 1.3
$(\text{CH}_3)_2\text{S} + \text{OH} \rightarrow \text{PRODUCTS}$ Methane, thiohis., + Hydroxyl free radical Z0 BERZFOR	2			300	5.9(+12)	-	-	0.9 1.1
NOTE: Recommended k.								
$(\text{CH}_3)_2\text{S} + \text{CH}_3 \rightarrow \text{CH}_3\text{SCH}_2 + \text{CH}_4$ Methane, thiohis., + Methyl free radical Z0 BERZFOR	2			299-430	3.3(+12)	0	-179±150	
Z0 BERZFOR				273-426	3.7(+12)	0	134±135	0.6 1.4
$\text{CH}_3\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{CH}_3$ Methane, sulfonyhis. Z0 BERZFOR	2			393-510	4.2(+11)	0	4613±02	0.8 1.2
NOTE: Critical evaluation								
$\text{CH}_3\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{CH}_3$ Methane, sulfonyhis. Z0 BERZFOR	1			783-913	2.0(+14)	0	30500	

CHEMICAL REACTIONS

Chemical Reaction	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{CH}_3 \rightarrow \text{cy-CH}_2\text{CH}(\text{CH}_2\text{CH}_2\text{S}) + \text{CH}_4$ Infrared and Methyl free radical Z6 KR/PGR NOTE: Tentative k.	2			300-450	3.2(+11)	0	4630±750	
$\text{cy-(CH}_3\text{)CCH}_2\text{S} + \text{S} \rightarrow \text{CH}_3\text{CH=CH}_2 + \text{S}_2$ Infrared, methyl-, and Sulfur atom Z1 SIR/OCZ NOTE: k/k _{ref} = 0.4exp(1057/T)	2			290-450	-	-	-	
$\text{cy-(CH}_3\text{)CCH}_2\text{S} + \text{S} \rightarrow \text{CH}_3\text{CH=CH}_2 + \text{CH}_3\text{S}$ Infrared, methyl-, and Methyl free radical Z2 IAK/ALM NOTE: Evaluation.	2			339-435	2.1(+11)	0	3750±830	1.1 8.3
$\text{cy-(CH}_3\text{)CCH}_2\text{S} + \text{CH}_3 \rightarrow \text{cy-(CH}_2\text{)CCH}_2\text{S} + \text{CH}_4$ Infrared, methyl-, and Methyl free radical Z2 IAK/ALM NOTE: Evaluation.	2			339-435	1.0(+11)	0	4160±440	1.3 3.0
$(\text{CH}_3)_2\text{CSH} + \text{CH}_3 \rightarrow \text{products}$ 2-Propenethiol and Methyl free radical Z6 KR/PGR NOTE: Tentative k.	2			303	4.1(+7)	-	-	
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{H} \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH}$ Infrared, tetrahydro-, and Hydrogen atom Z0 HOR/NIS NOTE: At 5 torr.	2			295-576	8.5(+12)	0	1010	
$\text{CH}_3\text{C(S)SCCH}_2\text{CH}_3 + \text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CH}_2$ Ethane(dithioic) acid ethyl ester Z0 ALA/NIS NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger	1			629	1.8(-3)	-	-	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{H}_2\text{S}$ Propanethiol and Hydrogen atom Z0 HOR/NIS NOTE: At 5 torr.	1			651-716	9.2(+12)	0	22730	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{H}_2$ Propanethiol and Hydrogen atom Z0 HOR/NIS NOTE: At 5 torr.	1			295-576	1.6(+12)	0	1120	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{H}_2$ Propanethiol and Hydrogen atom Z0 HOR/NIS NOTE: At 5 torr.	1			295-576	1.5(+13)	0	1600	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f
$(CH_3)_3CSH + (CH_3)_2C=CH_2 + H_2S$ <u>Z6 KERNZORN</u> NOTE: Critical evaluation.	1			950-1230	2.5(+13)	0	27830	
$(CH_3)_3CSH + CH_3 + (CH_3)_3CS + CH_2C(CH_3)_2SH + CH_4$ <u>Z6 KERNZORN</u> NOTE: tentative k.	2			303	5.9(+7)	-	-	
$CH_2=C(CH_3)SO_2CH_3 + CH_2=C(CH_3)CH_2 + CH_3SO_2$ <u>Z6 KERNZORN</u> NOTE: Critical evaluation.	1			573-633	5.0(+12)	0	20030	
$CH_3SO(O)OC(O)CH_3 + CH_3SH + CO_2 + CH_2=CH_2$ <u>Z6 KERNZORN</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	1.0(-4)	-	-	
$CH_3OC(O)SCH_2CH_3 + CH_3OH + COB + CH_2=CH_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			490-550	1.8(+12)	0	23500	
$CH_3OC(O)SCH(CH_3)_2 + CH_3OH + COB + CH_3CH=CH_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	7.8(-7)	-	-	
$CH_3OC(O)SCH(CH_3)_2 + CH_3OH + COB + CH_3CH=CH_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			490-550	1.2(+13)	0	27800	
$CH_3SC(O)OC(CH_3)_2 + CH_3SH + CO_2 + CH_3CH=CH_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	4.6(-5)	-	-	
$CH_3SC(O)OC(CH_3)_2 + CH_3SH + CO_2 + CH_3CH=CH_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			440-480	8.4(+12)	0	25000	
$CH_3SC(O)OC(CH_3)_3 + CH_3SH + CO_2 + CH_2=C(CH_3)_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	9.4(-3)	-	-	
$CH_3SC(O)OC(CH_3)_3 + CH_3SH + CO_2 + CH_2=C(CH_3)_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			547-584	6.7(+11)	0	20060	
$CH_3SC(O)OC(CH_3)_3 + CH_3SH + CO_2 + CH_2=C(CH_3)_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	4.2(-1)	-	-	
$CH_3SC(O)OC(CH_3)_3 + CH_3SH + CO_2 + CH_2=C(CH_3)_2$ <u>Z6 ALAZRIG</u> NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			479-502	5.4(+10)	0	16000	

CHEMICAL REACTIONS	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors F
$\text{CH}_3\text{OC}(\text{O})\text{SC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2$ Carbonothioic acid S-(1,1,1-dimethylethyl) O-methyl ester ZI ALAZIIG	1			629	1.2(-3)	-	-	
NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			370-420	1.4(+12)	0	21800	
$\text{CH}_3\text{C}(\text{S})\text{SCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3 + \text{CH}_4 + \text{C}_2\text{H}_4 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ Ethane(dithioic) acid butyl ester ZI ALAZIIG	1			629	3.3(-3)	-	-	
NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			651-716	1.2(+13)	0	22500	
$\text{CH}_3\text{C}(\text{S})\text{SCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 + \text{CH}_4 + \text{C}_2\text{H}_4 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ + cis-, and trans- $\text{CH}_3\text{CH}=\text{CHCH}_3$ Ethane(dithioic) acid 1-methylpropyl ester ZI ALAZIIG	1			629	7.4(-2)	-	-	
NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			504-639	6.7(+12)	0	20210	
$\text{CH}_3\text{C}(\text{S})\text{SC}(\text{CH}_3)_3 + \text{CH}_4 + \text{C}_2\text{H}_4 + (\text{CH}_3)_2\text{C}=\text{CH}_2$ Ethane(dithioic) acid 1,1-dimethylethyl ester ZI ALAZIIG	1			629	3.1(-1)	-	-	
NOTE: k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			448-502	1.1(+13)	0	19600	

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

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

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

EQUIVALENT THIRD ORDER RATE CONSTANTS

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

See note to Table for Second Order Rate Constants

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