

Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)

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Prepared for

Morgantown Energy Technology Center
Department of Energy
Morgantown, WV 26505

and

Office of Standard Reference Data
National Bureau of Standards
Washington, DC 20234



U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, Secretary
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, Director

Issued May 1982

Library of Congress Cataloging in Publication Data

Westley, Francis

Tables of rate constants for gas phase chemical reactions of sulfur compounds (1971-1980)

(NSRDS-NBS ; 72)

"Issued May 1982."

1. Chemical reaction, Rate of—Tables. 2. Sulphur compounds—Tables. I. Morgantown Energy Technology Center. II. United States. National Bureau of Standards. Office of Standard Reference Data. III. Title. IV. Series.

QC100.U573 no. 72 [QD502]

602'.18s

82-2094

[546'.7232]

AACR2

NSRDS-NBS 72

Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 72, 42 pages (May 1982)

CODEN: NSRDAP

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Foreword

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

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

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

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

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



ERNEST AMBLER, *Director*

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Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)

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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 19 unimolecular, 208 bimolecular, and 13 termolecular reactions totaling 240 distinct chemical reactions. There are 441 rate constants associated with these reactions, distributed as follows: 30 for first order reactions, 377 for second order reactions, and 34 for third order reactions. The kinetic data were compiled from 145 experimental papers and 8 critical reviews published between 1971 and 1980.

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

1. Introduction

This publication consists of a table of rate constants for reactions of inorganic and organic sulfur compounds in the gas phase, as well as of their reactions with other substrates. The table is a compilation of rate constants given in 145 experimental papers and 8 critical reviews published between 1971 and 1980. Its purpose is to provide the kineticist and combustion modeler with a comprehensive and easy-to-use source of kinetic data for chemical processes involving sulfur compounds. The table gives 441 distinct reaction rate constants from the above mentioned sources. A list of references including the 153 papers, arranged alphabetically by author for each separate year, is appended at the end of the table.

The table includes a limited number of reactions involving excited states like S*(¹D) and SO₂*; however, no attempt was made to cover all the papers from the literature dealing with such excited species. The reader interested in the reaction kinetics of electronically excited species is encouraged to consult Keith Schofield's excellent review: "Critically Evaluated Rate Constants for Gaseous Reactions of Several Electronically Excited Species," *J. Phys. Chem. Ref. Data* **8**, 723 (1979).

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, 18

bimolecular reactions and 1 termolecular reaction involve 2 sulfur-containing reactants. For that reason, these 19 reactions are listed twice, the second time with the order of the sulfur-containing reactants reversed, e.g., COS + S → CO + S₂ is also listed as S + COS → S₂ + CO. As a result, the total number of tabulated entries is 460, although the real number of distinct entries is only 441. The arrangement of the tables and the standard order of chemical compounds are described in detail in the next section "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, cm³mol⁻¹s⁻¹, and cm⁶mol⁻²s⁻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 go to all of them. In particular, I wish to thank Dr. Robert F. Hampson, Jr., Director of the Chemical Kinetics Data Center, for his more than helpful suggestions and constant guidance; Dr. John T. Herron, Chief of the

Chemical Kinetics Division, and Dr. Wing Tsang, of the Chemical Kinetics Division, for their encouragement; Dr. Bert R. Staples, Manager of the Electrolyte Data Center, for assistance in computer formatting; Mrs. Bettijoyce Molino and Mrs. Carla G. Messina from the Office of Standard Reference Data for applying the OMNIDATA and GPSDIC programs to photocompose the present tables; Mrs. Janice L. Jones for typing the original text with particular care; and Mrs. Miriam Oland from the Technical Information and Publications Division for retyping the text for photocomposition.

2. Guidelines for the User

General

As pointed out above, the presentation of the kinetic data in this publication is an attempt to simplify and standardize them. Units for rate constants used in this table are the cubic centimeter, the mole, and the second. The uncertainties given in this table are derived from the error limits specified by the author of the original paper or critical review. These have been converted to a standard format, as described below. 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 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.

Uncertainty limits expressed in the form of lower and upper k factors, f and F , respectively, are used in this 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 publication¹ and will not be repeated here.

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

Arrangement of the Table

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 $k = AT^n \exp(-E/RT)$, and the uncertainty limits expressed as k factors f and F .

The bibliography includes the full references for the 145 experimental papers and 8 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 is as follows:

Column 1, the chemical reaction indicating both the reactants and the products. In the same column, under each chemical reaction, the names of the reactants are given. The chemical nomenclature adopted is the one used in the Chemical Substance Indexes of Chemical Abstracts. Alternative names are not given. The chemical names of the products are not given. The line with chemical names is indented with respect to the line above it. Under the chemical names, the short reference 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 the first three letters of each author's name. 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.

Recommended values for rate constants or ratios are indicated in parentheses after the short reference, e.g., 76 BAU/DRY (Recommended k); 72 KER/PAR (Recommended ratio).

The last line of column 1, placed under the line including the short reference, 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 the first order reactions	s^{-1}
2	for the second order reactions	$cm^3 mol^{-1} s^{-1}$
3	for third order reactions	$cm^6 mol^{-2} s^{-1}$

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, H₂O, N₂, N₂O, SO₂, SO₃, CO₂. For the reaction SO₂ + OH + M → HOSO₂ + M, the third body, a mixture of N₂ and O₂, 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 $k = AT^n \exp(-E/RT)$. A is expressed as a number less than 10 followed by the exponent in parentheses, 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 $k = AT^n \exp(-E/RT)$. 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.

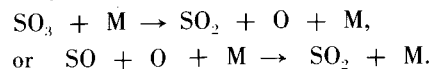
Column 8, with the heading E/R, indicates the value of E/R for the equation $k = AT^n \exp(-E/RT)$. Since E is the activation energy in cal mol⁻¹ and R the gas constant with a value of 1.987 cal mol⁻¹ K⁻¹, it follows that the units of E/R are kelvins. The values given in column 5 for E/R may vary from 0 to over 100,000 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): $f k_0 < k < F k_0$. 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 270-3.² 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 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 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 these reactions, M will always be placed after all other reactions, e.g.,



² Wagman, D. D., Evans, W. H., Parker, V. B., Halow, I., Bailey, S. M., and Schumm, R. H., "Selected Values of Chemical Thermodynamic Properties," NBS Tech. Note 270-3, pp. 5, 16, 22 (1968).

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., $\text{SO}_2 + \text{HO}_2 \rightarrow \text{products}$.

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: CH_4 , CH_3CH_3 , $\text{CH}_3\text{CH}_2\text{CH}_3$. Unsaturated hydrocarbons are written 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 parentheses 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 parentheses 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 a dot.

Acknowledgment

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

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
S + O ₂ → SO + O <i>Sulfur atom + Oxygen molecule</i>									
71 FAI/VAN	2			298	1.7(+12)	-	-	0.9	1.1
72 DAV/KLE1	2			252-423	1.3(+12)	0	0±50	0.8	1.2
72 DON/LIT	2			295	1.0(+12)	-	-	0.8	1.2
75 CLY/TOW	2			298	9.0(+11)	-	-	0.8	1.2
79 CLY/WHI	2			296-410	1.0(+12)	0	-153±108	0.7	1.4
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			230-400	1.2(+12)	0	0±100	0.7	1.4
S + O ₃ → SO + O ₂ <i>Sulfur atom + Ozone</i>									
75 CLY/TOW	2			298	7.2(+12)	-	-	0.7	1.3
80 BAU/COX (Recommended k).	2			298	7.2(+12)	-	-	0.5	2.0
S + H ₂ → SH + H <i>Sulfur atom + Hydrogen molecule</i>									
76 BAU/DRY (Recommended k). k ₁ = Kk ₋₁ .	2			298	1.3(-1)	-	-	0.5	1.5
75 BEN/GOL Semi-empirical evaluation.	2				2.5(+12)	0.5	13640		
S*(¹ D) + H ₂ → products <i>Sulfur atom + Hydrogen molecule</i>									
72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products.	2		0.22	300	-	-	-		
S + OH → SO + H <i>Sulfur atom + Hydroxyl free radical</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
79 JOU/LEB	2			298	4.0(+13)	-	-	0.8	1.2
S + OH → SH + O <i>Sulfur atom + Hydroxyl free radical</i>									
75 BEN/GOL Semi-empirical evaluation.	2				1.3(+12)	0.5	12700		
S + S + M → S ₂ + M <i>Sulfur atom</i>									
79 NIC/AMO	3			295	4.3(+18)	-	-	0.8	1.2
S + S ₂ → S ₂ + S <i>Sulfur atom + Sulfur dimer</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S + SO → S ₂ + O <i>Sulfur atom + Sulfur monoxide</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	11500		
S + SO → SO + S <i>Sulfur atom + Sulfur monoxide</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S + SH → S ₂ + H <i>Sulfur atom + Mercapto free radical</i>									
73 SCH	2			295	2.4(+13)	-	-		
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
79 NIC/AMO Upper limit k.	2			295	<3.0(+12)	-	-		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
S + SH → SH + S <i>Sulfur atom + Mercapto free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	4000		
S + N ₂ → NS + N <i>Sulfur atom + Nitrogen molecule</i> 75 BEN/GOL Semi-empirical evaluation.	2				4.0(+12)	0.5	55200		
S*(¹ D) + N ₂ → products <i>Sulfur atom + Nitrogen molecule</i> 72/LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ + products	2		0.062	300	-	-	-		
S + NO → SO + N <i>Sulfur atom + Nitrogen oxide(NO)</i> 75 BEN/GOL Semi-empirical evaluation.	2				4.0(+11)	0.5	17260		
S + NO → NS + O <i>Sulfur atom + Nitrogen oxide(NO)</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.0(+12)	0.5	17365		
S*(¹ D) + NO → products <i>Sulfur atom + Nitrogen oxide(NO)</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products	2		0.68		-	-	-		
S + NO + M → SNO + M <i>Sulfur atom + Nitrogen oxide(NO)</i> 78 VAN/OBI Limiting high-pressure k.	2	CO ₂		298	9.3(+12)	-	-	0.8	1.2
78 VAN OBI k _v (low pressure).	3	CO ₂		298	1.9(+17)	-	-		
S + NO ₂ → SO + NO <i>Sulfur atom + Nitrogen oxide(NO₂)</i> 75 CLY/TOW	2			298	3.7(+13)	-	-	0.8	1.2
79 CLY/WHY	2			296-410	3.0(+13)	0	-84±60	0.8	1.2
S*(¹ D) + N ₂ O → NS + NO <i>Sulfur atom + Nitrogen oxide(N₂O)</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products (Approximate ratio).	2		0.1	300	-	-	-		
S + NH → SH + N <i>Sulfur atom + Imdogen free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	4000		
S*(¹ D) + CO → products <i>Sulfur atom + Carbon monoxide</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products	2		0.19	300	-	-	-		
S*(¹ D) + CO ₂ → products <i>Sulfur atom + Carbon dioxide</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products	2		0.24	300	-	-	-		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
S*(¹ D) + CH ₄ → CH ₃ SH <i>Sulfur atom + Methane</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products 80 ADD/DON	2		0.076	300	-	-	-		
	2			295	1.1(+14)	-	-	0.7	1.3
S + CS → CS + S <i>Sulfur atom + Carbon monosulfide free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S + CS → S ₂ + C <i>Sulfur atom + Carbon monosulfide free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.6(+12)	0.5	40463		
S + CS + M → CS ₂ + M <i>Sulfur atom + Carbon monosulfide free radical</i> 76 BAU/DRY (Recommended k). k ₁ = Kk ₋₁ .	3			1800-3700	8.7(+13)	0	-4370	0.5	1.5
S + CS ₂ → S ₂ + CS <i>Sulfur atom + Carbon disulfide</i> 76 BAU/DRY (Recommended k).	2			298	3.9(+11)	-	-	0.5	1.5
S + COS → S ₂ + CO <i>Sulfur atom + Carbon oxide sulfide</i> 72 JAK/AHM Evaluation. 74 KLE/DAV 76 BAU/DRY (Recommended k).	2			298	1.1(+10)	-	-		
	2			233-245	9.2(+11)	0	1825±60	0.9	1.1
	2			230-2600	1.7(+12)	0	2050±230	0.3	3.0
S*(¹ D) + COS → S ₂ + CO <i>Sulfur atom + Carbon oxide sulfide</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products 79 ADD/BYR 79 SHE/SAF k _{ref} : S*(¹ D) + COS → S(³ P) + COS (Optimization). 80 ADD/DON	2		1.5	300	-	-	-	0.7	1.3
	2			290	7.2(+13)	-	-	0.8	1.3
	2		2.4	298	-	-	-		
	2			295	1.8(+14)	-	-	0.7	1.3
S + CN → CS + N <i>Sulfur atom + Cyanogen free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S + C ₂ → CS + C <i>Sulfur atom + Carbon dimer</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S + CH≡CH → cy-CH=CHS <i>Sulfur atom + Ethyne</i> 71 STR/O'C k/k _{ref} : 6.2exp(-1007/T). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method. 72 KER/PAR (Recommended k).	2			298-450	-	-	-		
	2			298	1.7(+11)	-	-		
S + CH≡CH → products <i>Sulfur atom + Ethyne</i> 78 VAN/SAF	2			298-484	3.4(+13)	0	1510±200	0.4	1.6

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
S + CD≡CD → products <i>Sulfur atom + Ethyne-d₂</i> 78 VAN/SAF	2			298	2.3(+11)	-	-	0.8	1.2
S*(¹ D) + CH ₂ =CH ₂ → CH ₂ =CHSH <i>Sulfur atom + Ethene</i> 79 SHE/SAF Optimization.	2			298	4.2(+13)	-	-		
S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S <i>Sulfur atom + Ethene</i> 71 CON/VAN Flash photolysis method.	2			298	9.0(+11)	-	-	0.9	1.1
71 STR/O'C k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2		1.0	298-450	-	-	-		
72 DAV/KLE2	2			218-442	4.3(+12)	0	795 ± 40	0.9	1.1
72 KER/PAR (Recommended k).	2			298	8.1(+11)	-	-		
S*(¹ D) + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S* <i>Sulfur atom + Ethene</i> 79 SHE/SAF Optimization.	2			298	3.8(+13)	-	-		
S + CD ₂ =CH ₂ → cy-CD ₂ CH ₂ S <i>Sulfur atom + Ethene-1,1-d₂</i> 71 STR/O'C k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2		1.07	298-450	-	-	-		
S + cis-CHD=CHD → cy-CHDCHDS <i>Sulfur atom + cis-Ethene-1,2-d₂</i> 71 STR/O'C k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2		1.04	298-450	-	-	-		
S + CD ₂ =CD ₂ → cy-CD ₂ CD ₂ S <i>Sulfur atom + Ethene-d₄</i> 71 STR/O'C k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2		1.14	298-450	-	-	-		
S*(¹ D) + CH ₃ CH ₃ → products <i>Sulfur atom + Ethane</i> 72 LIT/DAL k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → products	2		0.17	300	-	-	-		
S + cy-CH ₂ CH ₂ S → S ₂ + CH ₂ =CH ₂ <i>Sulfur atom + Thiirane</i> 71 STR/O'C k/k _{ref} : 8.3exp(+906/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
73 KLE/DAVI	2			298-355	2.7(+13)	0	0	0.9	1.1
S + CH ₃ C≡CH → cy-(CH ₃)C=CHS <i>Sulfur atom + 1-Propyne</i> 71 STR/O'C k/k _{ref} : 6.2exp(-453/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	1.1(+12)	-	-		
S + CH ₃ C≡CH → products <i>Sulfur atom + Propyne</i> 78 VAN/SAF	2			298-449	2.0(+13)	0	453 ± 100	0.4	1.6

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
S + CH ₃ CH=CH ₂ → cy-(CH ₃)CHCH ₂ S <i>Sulfur atom + Propene</i>									
71 CON/VAN Flash photolysis method.	2			298	6.0(+12)	-	-	0.8	1.2
71 STR/O'C k/k _{ref} : 1.0exp(+574/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	5.8(+12)	-	-		
72 KER/PAR (Recommended ratio). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		6.9	298	-	-	-		
73 KLE/DAV2	2			214-500	3.6(+12)	0	190±45	0.2	5.2
S*(¹ D) + CH ₃ CH=CH ₂ → cy-(CH ₃)CHCH ₂ S <i>Sulfur atom + Propene</i>									
72 KER/PAR (Recommended ratio). k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		1.7	300	-	-	-		
S + cy-(CH ₃)CHCH ₂ S → S ₂ + CH ₃ CH=CH ₂ <i>Sulfur atom + Thiirane, methyl-</i>									
71 STR/O'C k/k _{ref} : 8.4exp(+1057/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
S + CH ₃ CH ₂ C≡CH → products <i>Sulfur atom + 1-Butyne</i>									
78 VAN/SAF	2			298	3.3(+12)	-	-	0.9	1.1
S + CH ₃ C≡CCH ₃ → cy-(CH ₃)C=C(CH ₃)S <i>Sulfur atom + 2-Butyne</i>									
71 STR/O'C k/k _{ref} : 2.7exp(+654/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	1.9(+13)	-	-		
S + CH ₃ C≡CCH ₃ → products <i>Sulfur atom + 2-Butyne</i>									
78 VAN/SAF	2			298	1.6(+13)	-	-	0.9	1.1
S + CH ₂ =CHCH=CH ₂ → cy-(CH ₂ =CH)CHCH ₂ S <i>Sulfur atom + 1,3-Butadiene</i>									
71 STR/O'C k/k _{ref} : 2.4exp(+1027/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	6.0(+13)	-	-		
S + CH ₃ CH ₂ CH=CH ₂ → cy-(CH ₃ CH ₂)CHCH ₂ S <i>Sulfur atom + 1-Butene</i>									
71 CON/VAN Flash photolysis method.	2			298	9.0(+12)	-	-	0.9	1.1
71 STR/O'C k/k _{ref} : 0.75exp(+866/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR	2			298	9.3(+12)	-	-		
72 KER/PAR (Recommended ratio). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		10.0	298	-	-	-		
73 KLE/DAV2	2			216-475	4.5(+12)	0	180±45	0.1	4.0

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
S + cis-CH ₃ CH=CHCH ₃ → cy-(CH ₃)CHCH(CH ₃)S <i>Sulfur atom + cis-2-Butene</i> 71 STR/O'C k/k _{ref} : 0.53exp(+1050/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	1.4(+13)	-	-		
72 KER/PAR (Recommended ratio). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		16.0	298	-	-	-		
S + cis-CH ₃ CH=CHCH ₃ → products <i>Sulfur atom + cis-2-Butene</i> 73 DAV/KLE	2			219-500	2.8(+12)	0	-116±45	0.9	1.1
S + trans-CH ₃ CH=CHCH ₃ → cy-(CH ₃)CHCH(CH ₃)S <i>Sulfur atom + trans-2-Butene</i> 71 CON/VAN Flash photolysis method.	2			298	1.2(+13)	-	-	0.8	1.2
71 STR/O'C k/k _{ref} : 0.65exp(+1010/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	1.4(+13)	-	-		
72 KER/PAR (Recommended ratio). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		20.0	298	-	-	-		
S + (CH ₃) ₂ C=CH ₂ → cy-(CH ₃) ₂ CCH ₂ S <i>Sulfur atom + 1-Propene, 2-methyl-</i> 71 CON/VAN Flash photolysis method.	2			298	3.6(+13)	-	-	0.9	1.1
71 STR/O'C k/k _{ref} : 0.97exp(+1190/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	4.0(+13)	-	-		
72 KER/PAR (Recommended ratio). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		50.0	298	-	-	-		
S*(¹ D) + (CH ₃) ₂ C=CH ₂ → cy-(CH ₃) ₂ CCH ₂ S <i>Sulfur atom + 1-Propene, 2-methyl-</i> 72 KER/PAR (Recommended ratio). k _{ref} : S*(¹ D) + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		3.5	300	-	-	-		
S + CH ₃ CH ₂ C≡CCH ₃ → products <i>Sulfur atom + 2-Pentyne</i> 78 VAN/SAF	2			298	1.8(+13)	-	-	0.8	1.2
S + CH ₃ CH ₂ CH ₂ CH=CH ₂ → cy-(CH ₃ CH ₂ CH ₂)CHCH ₂ S <i>Sulfur atom + 1-Pentene</i> 72 KER/PAR (Recommended k).	2			298	8.1(+12)	-	-		
S + CH ₃ CH ₂ C(CH ₃)=CH ₂ → cy-(CH ₃ CH ₂)C(CH ₃)CH ₂ S <i>Sulfur atom + 1-Butene, 2-methyl-</i> 71 STR/O'C k/k _{ref} : 0.78exp(+1424/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	7.4(+13)	-	-		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
S + CH ₃ CH=C(CH ₃) ₂ → cy-(CH ₃)CH[C(CH ₃) ₂]S <i>Sulfur atom + 2-Butene, 2-methyl-</i> 71 STR/O'C k/k _{ref} : 0.51exp(+1515/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	6.5(+13)	-	-		
72 KER/PAR (Recommended ratio). k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S	2		56.0	298	-	-	-		
S + (CH ₃) ₂ C=C(CH ₃) ₂ → cy-[(CH ₃) ₂]CC[(CH ₃) ₂]S <i>Sulfur atom + 2-Butene, 2,3-dimethyl-</i> 71 CON/VAN Lower limit k. Flash photolysis method.	2			298	>6.2(+13)	-	-	0.9	1.1
71 STR/O'C k/k _{ref} : 0.50exp(+1690/T) k _{ref} : S + CH ₂ =CH ₂ → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
72 KER/PAR (Recommended k).	2			298	8.5(+13)	-	-		
S + (CH ₃) ₂ C=C(CH ₃) ₂ → products <i>Sulfur atom + 2-Butene, 2,3-dimethyl-</i> 73 DAV/KLE	2			252-500	2.8(+12)	0	-650±115	0.6	1.4
S ₂ + O → S + SO <i>Sulfur dimer + Oxygen atom</i> 73 SCH Approximate k. Given with caution.	2			1050	4.2(+12)	-	-		
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S ₂ + H → S + SH <i>Sulfur dimer + Hydrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				7.9(+12)	0.5	8355		
S ₂ + S → S + S ₂ <i>Sulfur dimer + Sulfur atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S ₂ + S ₂ + M → S ₄ + M <i>Sulfur dimer</i> 72 LAN/OLD 73 LAN/OLD Given with caution.	3	CO ₂		293	9.1(+17)	-	-	0.1	10.
	3	CO ₂		293	3.6(+18)	-	-		
79 NIC/AMO	3			295	8.0(+18)	-	-	0.9	1.1
S ₂ + N → S + NS <i>Sulfur dimer + Nitrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	4000		
S ₂ + C → S + CS <i>Sulfur dimer + Carbon atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
S ₂ + M → S + S + M <i>Sulfur dimer</i> 80 HIG/SAI	2	Ar		4500-6000	4.8(+13)	0	38750		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SO + O → O + SO <i>Sulfur monoxide + Oxygen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
SO + O → S + O ₂ <i>Sulfur monoxide + Oxygen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				2.0(+11)	0.5	2770		
SO + O + M → SO ₂ + M <i>Sulfur monoxide + Oxygen atom</i> 71 MIY/TAKI 76 BAU/DRY (Recommended k).	3	Ar		298	7.3(+16)	-	-	0.9	1.1
	3			298	6.7(+13)	-	-	0.7	1.3
SO + O ₂ → SO ₂ + O <i>Sulfur monoxide + Oxygen molecule</i> 72 BRE/MIL Upper limit k.	2			297	<5.0(+7)	-	-		
80 BAU/COX (Recommended k). k factors apply at 298k only.	2			300-1000	3.6(+11)	0	3300±500	0.3	3.2
SO + O ₃ → SO ₂ + O ₂ <i>Sulfur monoxide + Ozone</i> 80 BAU/COX (Recommended k). k factors apply at 298K only.	2			220-300	1.5(+12)	0	1100±400	0.5	2.0
80 ROB/SMI	2			296	5.2(+10)	-	-	0.8	1.2
SO + O ₃ (v=n) → SO ₂ * + O ₂ <i>Sulfur monoxide + Ozone</i> 74 KAL/BRA k _{ref} : SO + O ₃ → SO ₂ * + O ₂	2		2.4	300	-	-	-	0.8	1.3
SO + H → O + SH <i>Sulfur monoxide + Hydrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	19930		
SO + H → S + OH <i>Sulfur monoxide + Hydrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				4.0(+12)	0.5	11200		
SO + OH → SO ₂ + H <i>Sulfur monoxide + Hydroxyl free radical</i> 73 SCH (Recommended k). 79 JOU/LEB	2			298	3.3(+13)	-	-	0.5	2.0
	2			298	5.1(+13)	-	-	0.8	1.2
SO + S → O + S ₂ <i>Sulfur monoxide + Sulfur atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	11500		
SO + S → S + SO <i>Sulfur monoxide + Sulfur atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SO + SO → SO ₂ + S <i>Sulfur monoxide</i>									
72 BRE/MIL Upper limit k.	2			297	<3.0(+10)	-	-		
73 SCH Upper limit k.	2			300	<1.8(+9)	-	-		
73 SCH Upper limit k.	2			1000	<1.2(+11)	-	-		
75 CHU/CAL	2			298	5.0(+8)	-	-	0.2	1.8
SO + SO + M → (SO) ₂ + M <i>Sulfur monoxide</i>									
80 HER/HUI 2 - 8 torr.	3			298	1.6(+17)	-	-		
SO + SO ₃ → SO ₂ + SO ₂ <i>Sulfur monoxide + Sulfur trioxide</i>									
75 CHU/CAL	2			298	1.2(+9)	-	-	0.4	1.6
SO + (SO) ₂ → SO ₂ + S ₂ O <i>Sulfur monoxide + Sulfur monoxide dimer</i>									
80 HER/HUI 2 - 8 torr.	2			298	2.0(+10)	-	-		
SO + N → O + NS <i>Sulfur monoxide + Nitrogen atom</i>									
75 BEN/GOL Semi-empirical evaluation.	2				1.6(+12)	0.5	8254		
SO + N → S + NO <i>Sulfur monoxide + Nitrogen atom</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	4000		
SO + NO ₂ → SO ₂ + NO <i>Sulfur monoxide + Nitrogen oxide(NO₂)</i>									
71 CUP/GLA k _{ref} : O + NO ₂ → O ₂ + NO	2		1.6	300	-	-	-		
71 MIY/TAK2	2			298	1.2(+16)	-	-	0.9	1.1
80 BAU/COX (Recommended k).	2			298	8.4(+12)	-	-	0.5	2.0
80 CLY/MAC	2			295	8.2(+12)	-	-	0.9	1.1
SO + C → O + CS <i>Sulfur monoxide + Carbon atom</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
SO + C → S + CO <i>Sulfur monoxide + Carbon atom</i>									
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
SO + M → S + O + M <i>Sulfur monoxide</i>									
78 AST/GLA Rate constant expressed as k[Ar].	2	Ar		5700-7200	1.6(+14)	0	55330±3610	0.3	4.0
SO ₂ + O → SO + O ₂ <i>Sulfur dioxide + Oxygen atom</i>									
76 BAU/DRY (Recommended k). k ₁ = Kk ₋₁ .	2			440-2100	1.3(+14)	-0.5	9980	0.3	1.7
80 GRI/REE	2			2630-3570	4.0(+12)	0	9210	0.9	1.1
80 SLA/GRI	2			3500	3.8(+11)	-	-	0.9	1.1

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
SO ₂ + O + M → SO ₃ + M <i>Sulfur dioxide + Oxygen atom</i> 73 SCH M = Ar, O ₂ , N ₂ , He. k factors are larger at other temperatures.	3			250–1000	3.6(+14)	0	-500	0.5	2.0
74 ATK/PIT3	3	N ₂ O		299–392	3.3(+16)	0	1000±200		
75 WES/DEH2	3	He		248–415	3.9(+16)	0	1400±50	0.8	1.2
75 WES DEH2 M _{eff} : He(1.0)	3	He		297	3.0(+14)	-	-	0.9	1.1
75 WES DEH2 M _{eff} : SO ₂ (9.5)	3	SO ₂		297	2.9(+15)	-	-	0.7	1.3
75 WES DEH2 M _{eff} : N ₂ (2.4)	3	N ₂		297	7.2(+14)	-	-	0.9	1.1
78 ATK/PIT4	3	Ar		299–400	1.1(+16)	0	1010±150		
78 ATK/PIT4	3	N ₂		300	5.0(+14)	-	-	0.8	1.2
78 ATK PIT4	3	SO ₂		299	3.4(+15)	-	-	0.7	1.3
79 MER/LEV	3			1685	7.4(+14)	-	-		
80 BAU/COX (Recommended k). k factors apply at 298K only.	3	N ₂		200–400	1.5(+16)	0	1000±200	0.5	2.
80 BAU/COX (Recommended k). k factors apply at 298K only.	3	Ar		200–2500	5.4(+28)	-3.75	2650±200	0.5	2.0
SO ₂ + O ₂ ^(1Δ_g) → SO ₃ + O <i>Sulfur dioxide + Oxygen molecule</i> 76 DUM	2			298	1.3(+8)	-	-		
SO ₂ [*] + O ₂ → products <i>Sulfur dioxide + Oxygen molecule</i> 78 PAR/HEI k _{ref} : SO ₂ [*] → ¹ SO ₂ , or SO ₂ (SO ₂ [*] is a singlet formed on absorption).	2		0.05	298	-	-	-		
¹ SO ₂ + O ₂ → products <i>Sulfur dioxide + Oxygen molecule</i> 78 PAR/HEI k _{ref} : ¹ SO ₂ + SO ₂ → products (¹ SO ₂ is a fluorescent singlet).	2		0.29	298	-	-	-		
SO ₂ ^(3B₁) + O ₂ → products <i>Sulfur dioxide + Oxygen molecule</i> 78 PAR/HEI k _{ref} : SO ₂ ^(3B₁) + SO ₂ → products	2		0.36	298	-	-	-		
SO ₂ + O ₃ → SO ₃ + O ₂ <i>Sulfur dioxide + Ozone</i> 74 DAV/PRU Upper limit k.	2			300	<6.0(+1)	-	-		
SO ₂ + H + M → HSO ₂ + M <i>Sulfur dioxide + Hydrogen atom</i> 76 BAU/DRY (Recommended k).	3			1660–2120	5.1(+15)	-	-	0.5	1.5
SO ₂ + OH → products <i>Sulfur dioxide + Hydroxyl free radical</i> 80 COX/DER	2			297	4.0(+11)	-	-	0.8	1.2
SO ₂ + OH(v=9) → HSO ₃ <i>Sulfur dioxide + Hydroxyl free radical</i> 72 WOR/COL Lower limit k. Unreported T assumed to be 298K.	2			298	>1.4(+10)	-	-	0.8	1.2

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SO ₂ + OH + M → HOSO ₂ + M <i>Sulfur dioxide + Hydroxyl free radical</i>									
74 COX2 Evaluation. Rate constant expressed as k[M] with M = N ₂ + O ₂ at 1 atm.	2			294	3.6(+11)	-	-	0.9	1.1
75 CAS/DAV Limiting high-pressure k (760 torr).	2	N ₂		298	3.6(+11)	-	-		
75 CAS/DAV k _o (low pressure: <20 torr).	3	N ₂		298	5.8(+16)	-	-		
75 GOR/MULI In an atmosphere of water vapor.	2	H ₂ O		435	1.1(+12)	-	-	0.9	1.1
75 HAR/WAY	3	Ar		298	1.6(+17)	-	-	0.7	1.3
75 HAR/WAY	3	N ₂		298	2.6(+17)	-	-	0.9	1.1
76 ATK/PER3 At 760 torr.	2	Ar		298	4.0(+11)	-	-	0.9	1.1
76 ATK/PER3 Limiting high-pressure k.	2	Ar		298	5.0(+11)	-	-		
76 ATK/PER3 k _o (low-pressure k).	3	Ar		298	5.9(+16)	-	-	0.8	1.2
77 CAS/TAN Limiting high-pressure k (760 torr).	2	N ₂		297	3.6(+11)	-	-		
77 CAS/TAN k _o (low-pressure k).	3	N ₂		297	5.8(+16)	-	-		
77 CAS/TAN k _o (low-pressure). On the basis of k _o (297) and E _a experimental values.	3	N ₂		253-297	5.0(+14)	0	-1410		
77 CAS/TAN k _o (low-pressure k). Alternative T-dependent expression.	3	N ₂		253-297	2.5(+29)	-5.1	0		
79 DAV/RAV Total pressure 1 atm. (extrapolated value).	2	N ₂		298	5.4(+11)	-	-	0.8	1.3
80 BAU/COX (Recommended k). k _o (low-pressure k). k factors apply at 298K only.	3	N ₂		200-400	1.7(+24)	-2.9	0	0.5	2.0
80 BAU/COX (Recommended k). Limiting high-pressure k. k factors apply at 298K only.	2			200-400	1.2(+12)	0	0	0.4	2.5
80 HAR/ATK Total pressure 650 torr.	2	Ar		298-424	7.0(+9)	0	-1193±150	0.7	1.5
80 HAR/ATK Total pressure 650 torr.	2	SF ₆		298-424	7.6(+10)	0	-753±150	0.7	1.
80 HAR/ATK Total pressure 650 torr.	2	N ₂		298-424	2.4(+10)	0	-956		
SO ₂ + HO ₂ → SO ₃ + OH <i>Sulfur dioxide + Hydroperoxyl free radical</i>									
73 PAY/STI Evaluation.	2			300	5.2(+8)	-	-	0.8	1.2
74 LLO Evaluation. Ratio data versus k _{ref} for reaction HO ₂ + HO ₂ → H ₂ O ₂ + O ₂	2			300	5.2(+8)	-	-	0.9	1.2
79 BUR/CLI Upper limit k.				298	<1.2(+7)	-	-		
SO ₂ + HO ₂ → products <i>Sulfur dioxide + Hydroperoxyl free radical</i>									
79 GRA/WIN Upper limit k.	2			300	<6.0(+5)	-	-		
SO ₂ + HO ₂ + M → HO ₂ SO ₂ + M <i>Sulfur dioxide + Hydroperoxyl free radical</i>									
79 BUR/CLI Upper limit k.	3	He		298	<1.5(+14)	-	-		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SO ₂ + SO ₂ *(¹ B ₁) → SO*(¹ Δ _g , ³ Σ ⁻) + SO ₃ <i>Sulfur dioxide</i> 75 CHU/CAL	2			298	2.2(+12)	-	-	0.8	1.2
SO ₂ + SO ₂ *(³ B ₁) → SO + SO ₃ <i>Sulfur dioxide</i> 78 MAR/REI In an atmosphere of water vapor. (Approximate k).	2			298	2.0(+14)	-	-		
SO ₂ + SO ₂ *(³ B ₁) → SO*(¹ Σ ⁻) + SO ₃ <i>Sulfur dioxide</i> 75 CHU/CAL	2			298	4.2(+10)	-	-	0.9	1.1
SO ₂ + NO ₂ → SO ₃ + NO <i>Sulfur dioxide + Nitrogen oxide(NO₂)</i> 71 ARM/CUL 77 FRE/PAL Extended validity of k reported in 71 ARM/CUL (above), up to 2000K.	2 2			703-1193 430-1850	6.3(+12) 6.3(+12)	0 0	13950 16000		
SO ₂ + NO ₂ * → products <i>Sulfur dioxide + Nitrogen oxide(NO₂)</i> 78 IWA/PRE At 50 torr.	2			298	8.2(+10)	-	-		
SO ₂ + NO ₃ → SO ₃ + NO ₂ <i>Sulfur dioxide + Nitrogen oxide(NO₃)</i> 75 DAU/CAL Upper limit k.	2			300	<4.2(+3)	-	-		
SO ₂ + N ₂ O ₅ → SO ₃ + N ₂ O ₄ <i>Sulfur dioxide + Nitrogen oxide(N₂O₅)</i> 75 DAU/CAL Upper limit k.	2			300	<2.5(+1)	-	-		
¹ SO ₂ * + CO → SO + CO ₂ <i>Sulfur dioxide + Carbon monoxide</i> 73 CEH/HEI k _{ref} : ¹ SO ₂ * + SO ₂ → products. k/k _{ref} = 5.0x10 ⁻³ (at 2537 A°) 73 CEH HEI k/k _{ref} = 1.5x10 ⁻³ (at 3130 A°)	2 2			300 300	- -	- -	- -		
SO ₂ * + CO → SO + CO ₂ <i>Sulfur dioxide + Carbon monoxide</i> 73 CEH/HEI k _{ref} : SO ₂ * → products k/k _{ref} = 2.2x10 ⁻⁵ (3130 to 3261 A°) (SO ₂ * is a vibrationally excited singlet).	2			300	-	-	-		
SO ₂ ** + CO → SO + CO ₂ <i>Sulfur dioxide + Carbon monoxide</i> 73 CEH/HEI k _{ref} : SO ₂ ** → SO ₂ k _{ref} = 1.8x10 ⁻⁵ (2537 to 3261 A°) (SO ₂ ** is a chemically active triplet).	2			300	-	-	-	0.7	1.4
SO ₂ + CO + M → products <i>Sulfur dioxide + Carbon monoxide</i> 71 BAU/JEF At 27-170 torr pressure.	2	Ar		1770-2453	2.7(+12)	0	24300±600	0.8	1.3

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
SO ₂ + CH ₃ + M → CH ₃ SO ₂ + M <i>Sulfur dioxide + Methyl free radical</i> 73 JAM/KER Limiting high-pressure k.	2			298	1.8(+11)	-	-	0.9	1.1
SO ₂ + CH ₃ O ₂ → CH ₃ O ₂ SO ₂ <i>Sulfur dioxide + Methylendioxy free radical</i> 79 SAN/SIM 79 SIM/HEI k _{ref} : NO + CH ₃ O ₂ → NO ₂ + CH ₃ O	2 2		0.0025	298 296	4.9(+9) -	- -	- -	0.9 0.8	1.1 1.2
SO ₂ + CH ₃ O ₂ → products <i>Sulfur dioxide + Methylendioxy free radical</i> 79 KAN/MCQ Best k estimate, based on apparent rate constant (k _{app} 2k).	2			296	3.2(+9)	-	-	0.8	1.2
SO ₂ + CH≡CH → products <i>Sulfur dioxide + Ethyne</i> 71 FIF/MOR Given with caution.	2			1550-2150	3.2(+10)	0.5	20535		
SO ₂ ** + CH ₂ =C=CH ₂ → products <i>Sulfur dioxide + 1,2-Propadiene</i> 78 PAR/HEI k _{ref} : SO ₂ ** + CH ₂ =C=CH ₂ → CO + other products (SO ₂ ** is a non-emitting triplet).	2		4.0	298	-	-	-		
SO ₂ *(³ B ₁) + cis-CH ₃ CH=CHCH ₃ → [cis-CH ₃ CH=CHCH ₃ ,SO ₂]* <i>Sulfur dioxide + cis-2-Butene</i> 74 DEM/CAL	2			294	1.3(+14)	-	-	0.9	1.1
SO ₂ *(³ B ₁) + trans-CH ₃ CH=CHCH ₃ → [trans-CH ₃ CH=CHCH ₃ ,SO ₂]* <i>Sulfur dioxide + trans-2-Butene</i> 74 DEM/CAL	2			294	1.2(+14)	-	-	0.9	1.1
SO ₂ *(¹ B ₁) + (CH ₃) ₂ CH → products <i>Sulfur dioxide + Propane, 2-methyl-</i> 78 SU/CAL Evaluation.	2			298	8.4(+12)	-	-		
SO ₂ *(³ B ₁) + (CH ₃) ₂ CH → products <i>Sulfur dioxide + Propane, 2-methyl-</i> 78 SU/CAL Evaluation.	2			298	8.7(+11)	-	-		
SO ₂ *(³ B ₁) + cis-CH ₃ CH ₂ CH=CHCH ₃ → [SO ₂ ,CH ₃ CH ₂ CH=CHCH ₃]* <i>Sulfur dioxide + cis-2-Pentene</i> 76 WAM	2			295	6.3(+13)	-	-	0.8	1.2
SO ₂ *(³ B ₁) + trans-CH ₃ CH ₂ CH=CHCH ₃ → [SO ₂ ,CH ₃ CH ₂ CH=CHCH ₃]* <i>Sulfur dioxide + trans-2-Pentene</i> 76 WAM	2			295	1.0(+14)	-	-	0.7	1.3

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SO ₂ + M → SO + O + M									
<i>Sulfur dioxide</i>									
75 KIE	2	Kr		2900–5200	1.7(+16)	0	56370±2000	0.6	1.6
78 AST/GLA	2	Ar		3700–6500	4.0(+14)	0	53890±2170	0.5	2.0
Rate constant expressed as k[Ar].									
78 JUS/RIM	2	Ar		2500–3400	2.9(+16)	0	58590±2270	0.5	2.2
79 GRI/REE	2	Ar		2800–3880	8.0(+15)	0	54355	0.7	1.3
80 SAI/YOK	2	Ar		4300–6200	3.5(+14)	0	52805		
80 TYA/BAB	2	Ar		4000–6000	3.3(+15)	0	54150		
80 TYA BAB	2	SO ₂		4000–6000	5.0(+14)	0	33520		
SO ₃ + O → SO ₂ + O ₂									
<i>Sulfur trioxide + Oxygen atom</i>									
71 MER/LEV	2			1100–1400	6.5(+14)	0	5435		
k determined in H ₂ S flame.									
71 MER/LEV	2			900–1600	2.8(+14)	0	6040		
k determined in COS flame.									
72 JAC/WIN	2			300–500	1.5(+8)	0	500		
73 SCH	2			1480–1550	2.8(+14)	0	6040		
Given with caution.									
79 MER/LEV	2			1685	1.5(+11)	-	-		
SO ₃ + O + M → SO ₂ + O ₂ + M									
<i>Sulfur trioxide + Oxygen atom</i>									
75 WES/DEH1	3	He		298–507	5.0(+16)	0	-785	0.9	1.1
75 WES DEH1	3	He		298	7.3(+17)	-	-	0.9	1.1
M _{eff} : He(1.0)									
75 WES DEH1	3	SO ₃		298	<7.3(+18)	-	-		
M _{eff} : SO ₃ (<10.0). Upper limit ratio.									
75 WES DEH1	3	N ₂		298	1.0(+18)	-	-	0.9	1.1
M _{eff} : N ₂ (1.4)									
SO ₃ + H ₂ O → H ₂ SO ₄									
<i>Sulfur trioxide + Water</i>									
75 CAS/DAV	2			298	5.5(+11)	-	-	0.8	1.2
SO ₃ + SO → SO ₂ + SO ₂									
<i>Sulfur trioxide + Sulfur monoxide</i>									
75 CHU/CAL	2			298	1.2(+9)	-	-	0.4	1.6
SO ₃ + N → SO ₂ + NO									
<i>Sulfur trioxide + Nitrogen atom</i>									
72 JAC/WIN	2			300	3.0(+8)	-	-		
75 WES/DEH1	2			298	<6.0(+6)	-	-		
Upper limit k.									
SO ₃ + M → SO ₂ + O + M									
<i>Sulfur trioxide</i>									
78 AST/GLA	2	Ar		1700–2500	3.2(+15)	0	31880±1320	0.6	1.6
Rate constant expressed as k[Ar].									
79 AST/GLA	2	Ar		1700–2500	3.2(+15)	0	31900±300	0.6	1.6
S ₂ O + O → SO + SO									
<i>Sulfur oxide(S₂O) + Oxygen atom</i>									
74 STE/ALV	2			298	9.0(+11)	-	-	0.9	1.1
Evaluation.									
SH + O → S + OH									
<i>Mercapto free radical + Oxygen atom</i>									
73 SCH	2			298–2500	2.3(+11)	0.67	956		
Theoretical estimate.									
75 BEN/GOL	2				6.3(+11)	0.5	4000		
Semi-empirical evaluation.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SH + O → SO + H <i>Mercapto free radical + Oxygen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
75 CUP/GLA	2			295	9.6(+13)	-	-	0.7	1.3
SH + H → S + H ₂ <i>Mercapto free radical + Hydrogen atom</i> 72 LAN/OLD	2			293	<6.0(+12)	-	-		
73 BRA/TRU	2			298	2.5(+13)	-	-		
75 CUP/GLA	2			298	1.5(+13)	-	-	0.7	1.3
76 BAU/DRY (Recommended k).	2			298	1.5(+13)	-	-	0.5	1.5
79 NIC/AMO	2			295	1.3(+13)	-	-	0.8	1.2
SH + H → H + SH <i>Mercapto free radical + Hydrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
SH + S → H + S ₂ <i>Mercapto free radical + Sulfur atom</i> 73 SCH	2			295	2.4(+13)	-	-		
75 BEN/GOL Semi-empirical evaluation	2				6.3(+11)	0.5	0		
79 NIC/AMO Upper limit k.	2			295	<3.0(+12)	-	-		
SH + S → S + SH <i>Mercapto free radical + Sulfur atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	4000		
SH + SH → H ₂ + S ₂ <i>Mercapto free radical</i> 73 SCH Estimated upper limit k.	2			295	<3.0(+10)	-	-		
SH + SH → H ₂ S + S <i>Mercapto free radical</i> 72 LAN/OLD Upper limit k.	2			293	<1.8(+13)	-	-		
73 BRA/TRU	2			298	7.8(+12)	-	-		
76 BAU/DRY (Recommended k).	2			295	7.8(+12)	-	-	0.5	1.5
79 NIC/AMO	2			295	1.9(+13)	-	-	0.9	1.1
SH + N → H + NS <i>Mercapto free radical + Nitrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	403		
SH + N → S + NH <i>Mercapto free radical + Nitrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	9060		
SH + NO → products <i>Mercapto free radical + Nitrogen oxide(NO)</i> 73 BRA/TRU	2			298	6.3(+11)	-	-		
SH + C → H + CS <i>Mercapto free radical + Carbon atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
SH + C → S + CH <i>Mercapto free radical + Carbon atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				4.0(+11)	0.5	6090		
H ₂ S + O → SH + OH <i>Hydrogen sulfide + Oxygen atom</i> 73 SCH 76 WHY/TIM 78 WHY/TIM 80 BAU/COX (Recommended k). k factors apply at 298K only.	2 2 2 2			200-350 263-495 263-495 250-500	3.8(+11) 4.4(+12) 4.4(+12) 4.3(+12)	0 0 0 0	920±45 1660±50 1660±50 1660±150	0.5 0.9 0.8 0.8	2.0 1.1 1.2 1.3
D ₂ S + O → SD + OD <i>Hydrogen sulfide(D₂S) + Oxygen atom</i> 76 WHY/TIM	2			298-450	6.3(+12)	0	2145±155	0.5	1.5
H ₂ S + O → products <i>Hydrogen sulfide + Oxygen atom</i> 78 SLA/BAL k based on editor's least square fit of 6 given experimental points. 79 SIN/IRW	2 2			281-497 297-502	1.5(+13) 1.6(+13)	0 0	1920±45 2171±202	0.8 0.5	1.2 1.5
H ₂ S + O ₃ → SO ₂ + H ₂ O <i>Hydrogen sulfide + Ozone</i> 75 BEC/INO Upper limit k. Unreported T assumed to be 298K. 75 GLA/TOB1 Estimated k. 75 GLA/TOB2 75 BAU/DRY (Recommended k).	2 2 2 2			298 293-343 298-343 298	<1.2(+4) 4.9(+10) 1.6(+12) 4.0(+2)	- 0 0 -	- 3420 2620±600 -	- - 0.2 0.1	- - 6.3 10.0
H ₂ S + H → SH + H ₂ <i>Hydrogen sulfide + Hydrogen atom</i> 71 KUR/PET 72 ROM/SCH 73 BRA/TRU 76 BAU/DRY (Recommended k). 79 NIC/AMO 80 HUS/SLA	2 2 2 2 2 2			190-464 298 298 190-470 295 300	7.8(+12) 2.3(+11) 5.0(+11) 7.8(+12) 5.0(+11) 5.2(+11)	0 - - 0 - -	860±30 - - 860±50 - -	0.9 0.8 - 0.5 0.9 0.9	1.1 1.3 - 1.5 1.1 1.1
D ₂ S + D → SD + D ₂ <i>Hydrogen sulfide(D₂S) + Deuterium atom</i> 80 HUS/SLA	2			300	4.8(+11)	-	-	0.9	1.1
H ₂ S + OH → SH + H ₂ O <i>Hydrogen sulfide + Hydroxyl free radical</i> 73 WES/DEH3 74 STU 76 BAU/DRY (Recommended k). k factors changing to: f = 0.5 and F = 1.5 at 900K. 76 PER/ATK1 80 BAU/COX (Recommended k). k factors apply at 298K only.	2 2 2 2 2			298-885 298 298-900 297-427 250-400	1.4(+13) 1.9(+12) 6.3(+12) 3.1(+12) 6.6(+12)	0 - 0 0 0	443 - 200±150 0 225±225	0.8 0.7 0.9 0.8	1.2 1.3 - 1.1 1.3
H ₂ S + OH → products (overall) <i>Hydrogen sulfide + Hydroxyl free radical</i> 72 NIK/MORI Approximate k. 80 COX/SHE	2 2			300 297	5.2(+12) 3.0(+12)	- -	- -	0.9	1.1

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
H ₂ S + OH(v=9) → products <i>Hydrogen sulfide + Hydroxyl free radical</i> 72 WOR/COL 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 ₃ <i>Hydrogen sulfide + Methyl free radical</i> 76 KER/PAR Tentative k value.	2			300-600	2.0(+11)	0	2065±150	0.4	2.5
H ₂ S + M → SH + H + M <i>Hydrogen sulfide</i> 76 HIG/SAI 77 BOW/DOD	2 2	Ar Ar		2380-3000 2700-3800	1.3(+16) 2.0(+13)	0 0	46300 37300±960	0.7	1.5
CS + O → S + CO <i>Carbon monosulfide free radical + Oxygen atom</i> 71 HAN/SMI Evaluation.	2			298	8.4(+12)	-	-		
73 SCH Approximate k.	2			298	8.4(+12)	-	-	0.5	2.0
73 SCH Approximate k.	2			900	9.0(+13)	-	-	0.5	2.0
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
77 LIL/RIC	2			150-300	1.6(+14)	0	760±140	0.8	1.2
78 KOL Unreported T assumed to be 300K.	2			300	1.3(+13)	-	-	0.8	1.2
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			150-300	1.6(+14)	0	760±250	0.8	1.3
CS + O → S + CO(v=n) <i>Carbon monosulfide free radical + Oxygen atom</i> 72 HAN/RID 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 298K.	2		0.1	298	-	-	-		
75 SLA/GRAI	2			305	1.2(+13)	-	-	0.9	1.1
76 BID/BRE	2			300	1.4(+13)	-	-	0.8	1.2
CS + O → SO + C <i>Carbon monosulfide free radical + Oxygen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.6(+12)	0.5	28940		
CS + O ₂ → SO + CO <i>Carbon monosulfide free radical + Oxygen molecule</i> 73 SCH Estimated upper limit k.	2			298	<1.8(+6)	-	-		
CS + O ₂ → COS + O <i>Carbon monosulfide free radical + Oxygen molecule</i> 73 SCH Estimated upper limit k.	2			298	<1.8(+6)	-	-		
CS + H → S + CH <i>Carbon monosulfide free radical + Hydrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.3(+13)	0.5	50930		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
CS + H → SH + C <i>Carbon monosulfide free radical + Hydrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				2.0(+13)	0.5	48870		
CS + S → S + CS <i>Carbon monosulfide free radical + Sulfur atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
CS + S → C + S ₂ <i>Carbon monosulfide free radical + Sulfur atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.6(+12)	0.5	40463		
CS + S + M → CS ₂ + M <i>Carbon monosulfide free radical + Sulfur atom</i> 76 BAU/DRY (Recommended k). k ₁ = Kk ₋₁	3			1800-3700	8.7(+13)	0	-4370	0.5	1.5
CS + N → S + CN <i>Carbon monosulfide free radical + Nitrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.3(+12)	0.5	1160		
CS + N → C + NS <i>Carbon monosulfide free radical + Nitrogen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				4.0(+12)	0.5	37200		
CS + C → S + C ₂ <i>Carbon monosulfide free radical + Carbon atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				5.0(+11)	0.5	20435		
CS + C → C + CS <i>Carbon monosulfide free radical + Carbon atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
CS ₂ + O → CO + S ₂ <i>Carbon disulfide + Oxygen atom</i> 79 HSU/SHA	2			298	3.5(+10)	-	-	0.9	1.1
CS ₂ + O → CS + SO <i>Carbon disulfide + Oxygen atom</i> 71 TAK	2			298	1.4(+12)	-	-	0.9	1.1
75 WEI/TIM	2			218-293	1.7(+13)	0	645±35	0.9	1.1
76 BAU/DRY (Recommended k).	2			200-1000	2.2(+13)	0	700	0.7	1.3
CS ₂ + O → COS + S <i>Carbon disulfide + Oxygen atom</i> 73 SCH Approximate k.	2			1100	1.2(+12)	-	-		
74 SLA/GIL k _{ref} : CS ₂ + O → products	2		0.093	302	-	-	-		
76 BAU/DRY (Recommended k).	2			302	2.2(+11)	-	-	0.5	1.5
77 GRA/GUT k _{ref} : CS ₂ + O → products within the given T range, the k/k _{ref} ratio decreases from 0.098±0.004 at 249K to 0.081±0.007 at 500K.	2		0.098	249-500	-	-	-		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
CS ₂ + O → COS + S —continued 77 GRA GUT Within the given T range, k increases from 1.7x10 ¹¹ at 249K to 5.5x10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ at 500K.	2			249-500	1.7(+11)	-	-	0.9	1.2
CS ₂ + O → products <i>Carbon disulfide + Oxygen atom</i> 74 SLA/GIL	2			302	2.4(+12)	-	-		
74 GRA/GUT Non-linear Arrhenius behavior. Within the given T range, k increases from 1.7x10 ¹² at 249K to 6.7x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 500K.	2			249-500	1.7(+12)	-	-	0.9	1.1
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			200-500	3.5(+13)	0	700±100	0.6	1.6
CS ₂ + OH → products <i>Carbon disulfide + Hydroxyl free radical</i> 78 ATK/PER1 Upper limit k.	2			300	<4.2(+10)	-	-		
78 ATK PER1 Upper limit k.	2			425	<6.0(+10)	-	-		
78 KUR2	2			296	1.1(+11)	-	-	0.8	1.2
80 BAU/COX (Recommended k). Upper limit k.	2			298	<1.2(+11)	-	-		5.0
80 COX/SHE	2			297	2.6(+11)	-	-	0.7	1.3
80 IYE/ROW Upper limit k.	2			298	<1.8(+9)	-	-		
80 WIN/SHA Upper limit k.	2			251	<6.0(+9)	-	-		
80 WIN SHA Upper limit k.	2			297	<9.0(+8)	-	-		
80 WIN SHA Upper limit k.	2			363	<9.6(+8)	-	-		
CS ₂ + S → CS + S ₂ <i>Carbon disulfide + Sulfur atom</i> 76 BAU/DRY (Recommended k).	2			298	3.9(+11)	-	-	0.5	1.5
CS ₂ + M → CS + S + M <i>Carbon disulfide</i> 76 BAU/DRY (Recommended k).	2	Ar		1800-3700	2.6(+15)	0	38960±9000	0.5	1.5
80 SAI/TOR	2	Ar		2000-2900	2.5(+14)	0	37240		
CS ₂ + M → products <i>Carbon disulfide</i> 74 TRA k measured in shock tube. Unspecified high T range.	2				6.8(+14)	0	36000±700		
COS + O → SO + CO <i>Carbon oxide sulfide + Oxygen atom</i> 71 KRE	2			300-523	9.8(+12)	0	2265		
71 KRE/SIM	2			300-523	9.8(+12)	0	2265		
72 BRE/MIL	2			297	7.2(+9)	-	-	0.8	1.2
74 KLE/STI	2			263-502	9.9(+12)	0	2167±28	0.9	1.1
75 WEI/TIM	2			239-404	1.2(+13)	0	2150±35	0.8	1.2
76 MAN/BRA (Recommended k). k factors changing to: f = 0.3 and F = 3.0 above 300K.	2			296	8.4(+9)	-	-	0.9	1.1
78 YOS/SAI	2			298	7.1(+9)	-	-	0.9	1.1
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			220-600	1.6(+13)	0	2250±150	0.6	1.6
80 ROB/SMI	2			296	1.0(+10)	-	-	0.9	1.1

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
COS + O*(¹ D) → SO + CO <i>Carbon oxide sulfide + Oxygen atom</i>									
75 GAU/SNE	2		4.1	300	-	-	-		
k _{ref} : O ₂ + O*(¹ D) → O ₂ *(¹ Σ _g ⁺) + O									
75 GAU SNE	2			300	1.8(+14)	-	-		
Evaluation.									
COS + H → CO + SH <i>Carbon oxide sulfide + Hydrogen atom</i>									
72 ROM/SCH	2			298	1.3(+10)	-	-	0.8	1.3
75 TSU/YOK	2			300-525	9.1(+12)	0	1965±185	0.9	1.1
76 BAU/DRY (Recommended k).	2			298	1.3(+10)	-	-	0.8	1.3
76 LEE	2			298-478	9.8(+13)	0	2775±40	0.9	1.1
77 LEE/STI	2			261-500	5.5(+12)	0	1940±55	0.8	1.2
COS + OH → products <i>Carbon oxide sulfide + Hydroxyl free radical</i>									
78 ATK/PER1	2			299	<4.2(+9)	-	-		
Upper limit k.									
78 ATK PER1	2			430	<1.2(+10)	-	-		
Upper limit k.									
78 KUR2	2			296	3.4(+10)	-	-		
80 BAU/COX (Recommended k).	2			298	<3.6(+10)	-	-		5.0
Upper limit k.									
80 COX/SHE	2			297	<2.4(+10)	-	-		
Upper limit k.									
COS + OH(v=9) → products <i>Carbon oxide sulfide + Hydroxyl free radical</i>									
72 WOR/COL	2			298	1.5(+10)	-	-	0.4	1.6
Unreported T assumed to be 298K.									
COS + S → CO + S ₂ <i>Carbon oxide sulfide + Sulfur atom</i>									
72 JAK/AHM	2			298	1.1(+10)	-	-		
Evaluation.									
74 KLE/DAV	2			233-245	9.2(+11)	0	1825±60	0.9	1.1
76 BAU/DRY (Recommended k).	2			230-2600	1.7(+12)	0	2050±230	0.3	3.0
COS + S*(¹ D) → CO + S ₂ <i>Carbon oxide sulfide + Sulfur atom</i>									
72 LIT/DAL	2		1.5	300	-	-	-		
k _{ref} : CH ₂ =CH ₂ + S*(¹ D) → products									
78 SHE/SAF	2		2.4	298	-	-	-		
k _{ref} : COS + S*(¹ D) → COS + S(³ P)									
Optimization.									
79 ADD/BYR	2			290	7.2(+13)	-	-	0.8	1.3
80 ADD/DON	2			295	1.8(+14)	-	-	0.7	1.3
COS + CD ₃ → CO + CD ₃ S <i>Carbon oxide sulfide + Methyl-d₃ free radical</i>									
72 JAK/AHM	2			354-490	3.8(+11)	0	5710±175	0.6	1.8
Evaluation.									
COS + CN → SCN + CO <i>Carbon oxide sulfide + Cyanogen free radical</i>									
79 ADD/LEI	2			295	>1.8(+13)	-	-		
Lower limit k.									
COS + M → products <i>Carbon oxide sulfide</i>									
74 TRA	2				8.3(+14)	0	31700±650		
k measured in shock tube.									
Unspecified, high T range.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
CH ₃ S + CH≡CH → CH ₃ SCH=CH <i>Methylthio free radical + Ethyne</i> 72 KER/PAR (Recommended k).	2			298-333	7.9(+7)	-	-		
CH ₃ S + CH ₂ =CH ₂ → CH ₃ SCH ₂ CH ₂ <i>Methylthio free radical + Ethene</i> 72 KER/PAR (Recommended k).	2			298	4.8(+8)	-	-		
CH ₃ S + cy-CH ₂ CH ₂ S → CH ₃ S ₂ + CH ₂ =CH ₂ <i>Methylthio free radical + Thiirane</i> 72 JAK/AHM Approximate k.	2			304-478	3.2(+11)	0	4430		
CH ₃ S + CH ₃ CH=CHCH ₃ → CH ₃ CH(SCH ₃)CH(CH ₃) <i>Methylthio free radical + 2-Butene</i> 72 KER/PAR cis-trans equilibrium-weighted k.	2			298-333	1.6(+9)	-	-		
CH ₃ SH → CH ₃ + SH <i>Methanethiol</i> 70 BEN/O'N Critical evaluation.	1			1005-1102	3.2(+15)	0	38550		
CH ₃ SH + O → products <i>Methanethiol + Oxygen atom</i> 76 SLA/GRA 78 KIR/VET 78 SLA/BAL Non-linear Arrhenius behavior. Within the given T range, k increasing from 1.1x10 ¹² at 254K to 2.6x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 495K.	2 2 2			300 300-661 254-495	1.1(+12) 8.5(+12) 1.1(+12)	- 0 -	- -625±36 -	0.9	1.1
CH ₃ SH + OH → products <i>Methanethiol + Hydroxyl free radical</i> 80 COX/SHE	2			297	5.4(+13)	-	-	0.9	1.1
CH ₃ SH + CH ₃ → CH ₂ SH + CH ₄ <i>Methanethiol + Methyl free radical</i> 76 KER/PAR (Recommended k).	2			303	1.2(+8)	-	-	0.5	2.0
CD ₃ SH + CH ₃ → CD ₃ S + CH ₄ <i>Methane-d₃-thiol + Methyl free radical</i> 76 KER/PAR (Recommended k).	2			400-500	1.1(+11)	0	2065±500	0.5	2.0
CD ₃ SH + CH ₃ → CD ₂ SH + CH ₃ D <i>Methane-d₃-thiol + Methyl free radical</i> 76 KER/PAR (Recommended k). 76 KER/PAR (Recommended k).	2 2			400-500 400-500	7.6(+10) 1.1(+11)	0 0	4200±250 2065±500	0.5 0.5	2.0 2.0
CD ₃ SH + CH ₃ → CD ₂ SH + CH ₃ D <i>Methane-d₃-thiol + Methyl free radical</i> 76 KER/PAR (Recommended k).	2			400-500	7.6(+10)	0	4200±250	0.5	2.0
cy-CH ₂ CH ₂ S* → CH ₂ =CHSH <i>Thiirane</i> 79 SHE/SAF	1			298	5.0(+10)	-	-		
cy-CH ₂ CH ₂ S + O → CH ₂ =CH ₂ + SO <i>Thiirane + Oxygen atom</i> 76 LEE/TIM	2			268-424	8.1(+12)	0	18±20	0.9	1.1

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
cy-CH ₂ CH ₂ S + O ₃ → CH ₂ =CH ₂ + other products <i>Thiirane + Ozone</i> 80 MAR/HER 8 torr. pressure.	2			296	<1.0(+4)	-	-		
cy-CH ₂ CH ₂ S + H → CH ₂ =CH ₂ + SH <i>Thiirane + Hydrogen atom</i> 75 YOK/AHM	2			300-425	5.7(+13)	0	978±88	0.9	1.1
cy-CH ₂ SCH ₂ + H → cy-CH ₂ SCH + H ₂ <i>Thiirane + Hydrogen atom</i> 76 LEE	2			298	7.1(+11)	-	-	0.8	1.2
cy-CH ₂ CH ₂ S + S → CH ₂ =CH ₂ + S ₂ <i>Thiirane + Sulfur atom</i> 71 STR/O'C k/k _{ref} : 8.3exp(+906/T) k _{ref} : CH ₂ =CH ₂ + S → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
73 KLE/DAVI	2			298-355	2.7(+13)	0	0	0.9	1.1
cy-CH ₂ CH ₂ S + CH ₃ → CH ₂ =CH ₂ + CH ₃ S <i>Thiirane + Methyl free radical</i> 72 JAK/AHM	2			304-478	7.1(+10)	0	3370±400	0.3	3.3
cy-CH ₂ CH ₂ S + CD ₃ → CH ₂ =CH ₂ + CD ₃ S <i>Thiirane + Methyl-d₃ free radical</i> 72 JAK/AHM Evaluation.	2			303-477	5.9(+10)	0	3270±500	0.2	4.4
cy-CH ₂ CH ₂ S + CD ₃ → cy-CH ₂ CH(CD ₃)S + CD ₃ H <i>Thiirane + Methyl-d₃ free radical</i> 72 JAK/AHM Evaluation.	2			303-477	2.2(+11)	0	4800±500	0.3	4.0
76 KER/PAR (Recommended k).	2			300-500	2.2(+11)	0	4800±500	0.5	2.0
cy-CH ₂ CH ₂ S + CH ₃ S → CH ₂ =CH ₂ + CH ₃ S ₂ <i>Thiirane + Methylthio free radical</i> 72 JAK/AHM Approximate k.	2			304-478	3.2(+11)	0	4430		
CH ₃ SCH ₂ + CH ₄ → (CH ₃) ₂ S + CH ₃ <i>Methyl, (methylthio)-, free radical + Methane</i> 76 ART/LEE Evaluation based on k ₋₁ and thermodynamic data.	2			393-518	6.3(+11)	0	7662		
CH ₃ CH ₂ SH → CH ₂ =CH ₂ + H ₂ S <i>Ethanethiol</i> 70 BEN/O'N Critical evaluation.	1			785-938	1.0(+13)	0	25900		
CH ₃ CH ₂ SH → CH ₃ CH ₂ + SH <i>Ethanethiol</i> 70 BEN/O'N Critical evaluation.	1			785-938	6.3(+15)	0	36336		
CH ₃ CH ₂ SH + O → products <i>Ethanethiol + Oxygen atom</i> 76 SLA/GRA 78 KIR/VET 78 SLA/BLA	2			300	1.7(+12)	-	-		
	2			304-421	5.8(+12)	0	-391±18	0.9	1.1
	2			257-495	1.9(+12)	-	-		
Non-linear Arrhenius behavior. Within the given T range, k increasing from 1.9x10 ¹² at 257K to 3.2x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 495K.									

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors	
								f	F
CH ₃ CH ₂ SH + CH ₃ → products <i>Ethaneithiol + Methyl free radical</i> 76 KER/PAR Tentative k.	2			303	3.5(+7)	-	-	0.5	2.0
(CH ₃) ₂ S + O → CH ₃ S(O) + CH ₃ <i>Methane, thiobis-, + Oxygen atom</i> 76 LEE/TIM 76 SLA/GRA 78 SLA/BAL Possible non-linear Arrhenius behavior. Within the given T range, k decreasing from 3.8x10 ¹³ at 252K to 2.2x10 ¹³ cm ³ mol ⁻¹ s ⁻¹ at 493K.	2 2 2			268-424 300 252-493	8.6(+12) 3.8(+13) 3.8(+13)	0 - -	-366±16 - -	0.9	1.1
(CH ₃) ₂ S + O → products <i>Methane, thiobis-, + Oxygen atom</i> 80 LEE/TANI	2			272-472	7.7(+12)	0	-404±30	0.9	1.1
(CH ₃) ₂ S + O → products <i>Methane, thiobis-, + Oxygen atom</i> 74 CAD/WIC	2			300	3.3(+11)	-	-		
(CH ₃) ₂ S + O ₃ → products <i>Methane, thiobis-, + Ozone</i> 78 MAR/HER Upper limit k.	2			296	<5.0(+5)	-	-		
(CH ₃) ₂ S + H → CH ₃ SH + CH ₃ <i>Methane, thiobis-, + Hydrogen atom</i> 79 YOK/STR 80 YOK/STR Indirect measurement.	2 2			300-472 300-472	1.7(+13) 1.7(+13)	0 0	1320±44 1319±44	0.8 0.8	1.2 1.2
(CH ₃) ₂ S + H → CH ₃ SCH ₂ + H ₂ <i>Methane, thiobis-, + Hydrogen atom</i> 76 LEE	2			300	9.0(+10)	-	-	0.7	1.3
(CH ₃) ₂ S + OH → products <i>Methane, thiobis-, + Hydroxyl free radical</i> 78 ATK/PER1 78 ATK PER1 78 KURI (Recommended k). 80 COX/SHE	2 2 2 2			300 299-430 273-426 297	5.9(+12) 3.3(+12) 3.7(+12) 5.5(+12)	- 0 0 -	- -179±150 134±135 -	0.9 0.6 0.8	1.1 1.4 1.2
(CH ₃) ₂ S + CH ₃ → CH ₃ SCH ₂ + CH ₄ <i>Methane, thiobis-, + Methyl free radical</i> 76 ART/LEE	2			393-518	4.2(+11)	0	4613±82	0.8	1.2
CH ₃ SSCH ₃ + O → products <i>Disulfide, dimethyl-, + Oxygen atom</i> 80 LEE/TAN2	2			270-329	1.3(+14)	0	0	0.9	1.1
CH ₃ SSCH ₃ + H → CH ₃ S + CH ₃ SH <i>Disulfide, dimethyl-, + Hydrogen atom</i> 80 EKW/JOD	2			298-428	5.7(+12)	0	-50±50	0.8	1.2
CH ₃ SSCH ₃ + OH → products <i>Disulfide, dimethyl-, + Hydroxyl free radical</i> 80 COX/SHE	2			297	1.3(+14)	-	-	0.6	1.4
CH ₃ SO ₂ CH ₃ → CH ₃ SO ₂ + CH ₃ <i>Methane, sulfonylbis-</i> 70 BEN/O'N Critical evaluation.	1			783-913	2.0(+14)	0	30500		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
cy-CH ₂ CH ₂ CH ₂ S + CH ₃ → cy-CH ₂ CH(CH ₂)S + CH ₄ <i>Thietane + Methyl free radical</i> 76 KER/PAR Tentative k.	2			300-450	3.2(+11)	0	4630 ± 750		
cy-(CH ₃)CHCH ₂ S + S → CH ₃ CH=CH ₂ + S ₂ <i>Thiirane, methyl-, + Sulfur atom</i> 71 STR/O'C k/k _{ref} : 8.4exp(+1057/T) k _{ref} : CH ₂ =CH ₂ + S → cy-CH ₂ CH ₂ S Conventional photolysis method.	2			298-450	-	-	-		
cy-(CH ₃)CHCH ₂ S + CH ₃ → CH ₃ CH=CH ₂ + CH ₃ S <i>Thiirane, methyl-, + Methyl free radical</i> 72 JAK/AHM Evaluation.	2			339-435	2.1(+11)	0	3750 ± 830	0.1	8.3
cy-(CH ₃)CHCH ₂ S + CH ₃ → cy-[(CH ₂)CHCH ₂]S + CH ₄ <i>Thiirane, methyl-, + Methyl free radical</i> 72 JAK/AHM	2			339-435	1.0(+11)	0	4160 ± 440	0.3	3.0
CH ₃ CH ₂ CH ₂ SH + O → products <i>1-Propanethiol + Oxygen atom</i> 78 KIR/VET	2			303-421	8.3(+12)	0	-494 ± 22	0.9	1.1
(CH ₃) ₂ CHSH + CH ₃ → products <i>2-Propanethiol + Methyl free radical</i> 76 KER/PAR Tentative k.	2			303	4.1(+7)	-	-		
cy-CH ₂ CH ₂ CH ₂ CH ₂ S + H → CH ₂ CH ₂ CH ₂ CH ₂ SH <i>Thiophene, tetrahydro-, + Hydrogen atom</i> 78 HOR/NIS At 5 torr.	2			295-576	8.5(+12)	0	1010		
CH ₃ C(S)SCH ₂ CH ₃ → CH ₄ + CS ₂ + CH ₂ =CH ₂ <i>Ethane(dithioic) acid ethyl ester</i> 78 ALA/BIG 78 ALA BIG k based on reported ΔH [†] and ΔS [†] .	1 1			629 651-716	1.8(-3) 9.2(+12)	- 0	- 22730		
CH ₃ CH ₂ CH ₂ CH ₂ SH + O → products <i>1-Butanethiol + Oxygen atom</i> 78 KIR/VET	2			306-419	5.8(+12)	0	-321 ± 19	0.9	1.1
CH ₃ CH ₂ CH ₂ CH ₂ SH + H → CH ₃ CH ₂ CH ₂ CH ₂ + H ₂ S <i>1-Butanethiol + Hydrogen atom</i> 78 HOR/NIS At 5 torr.	2			295-576	1.6(+12)	0	1120		
CH ₃ CH ₂ CH ₂ CH ₂ SH + H → CH ₃ CH ₂ CH ₂ CH ₂ S + H ₂ <i>1-Butanethiol + Hydrogen atom</i> 78 HOR/NIS At 5 torr.	2			295-576	1.3(+13)	0	1600		
(CH ₃) ₂ CSH → (CH ₃) ₂ C=CH ₂ + H ₂ S <i>2-Propanethiol, 2-methyl-</i> 70 BEN/O'N Critical evaluation.	1			950-1230	2.5(+13)	0	27830		
(CH ₃) ₂ CSH + CH ₃ → (CH ₃) ₂ CS + CH ₂ C(CH ₃) ₂ SH + CH ₄ <i>2-Propanethiol, 2-methyl-, + Methyl free radical</i> 76 KER/PAR Tentative k.	2			303	5.9(+7)	-	-		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_2=\text{CHCH}_2\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2\cdot + \text{CH}_3\text{SO}_2\cdot$ <i>1-Propene, 3-methylsulfonyl-</i> 70 BEN/O'N Critical evaluation.	1			573-633	5.0(+12)	0	28030		
$\text{CH}_3\text{SC(O)OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ <i>Carbonothioic acid O-ethyl S-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	1.0(-4)	-	-		
$\text{CH}_3\text{SC(O)OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{SH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ <i>Carbonothioic acid O-ethyl S-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			490-550	1.8(+12)	0	23500		
$\text{CH}_3\text{OC(O)SCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_2=\text{CH}_2$ <i>Carbonothioic acid S-ethyl O-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	7.8(-7)	-	-		
$\text{CH}_3\text{OC(O)SCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_2=\text{CH}_2$ <i>Carbonothioic acid S-ethyl O-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			490-550	1.2(+13)	0	27800		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{O} \rightarrow \text{products}$ <i>1-Pentanethiol + Oxygen atom</i> 78 KIR/VET	2			302-409	6.2(+12)	0	-328±19	0.9	1.1
$\text{CH}_3\text{OC(O)SCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ <i>Carbonothioic acid O-methyl S-(1-methylethyl) ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	4.6(-5)	-	-		
$\text{CH}_3\text{OC(O)SCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ <i>Carbonothioic acid O-methyl S-(1-methylethyl) ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			440-480	8.4(+12)	0	25000		
$\text{CH}_3\text{SC(O)OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{SH} + \text{CO}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ <i>Carbonothioic acid S-methyl O-(1-methylethyl) ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger . (Evacuated sealed tube method).	1			629	9.4(-3)	-	-		
$\text{CH}_3\text{SC(O)OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{SH} + \text{CO}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ <i>Carbonothioic acid S-methyl O-(1-methylethyl) ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			547-584	6.7(+11)	0	20060		
$\text{CH}_3\text{SC(O)OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{SH} + \text{CO}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2$ <i>Carbonothioic acid O-(1,1-dimethylethyl) S-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger . (Inhibited sealed tube method).	1			629	4.2(-1)	-	-		
$\text{CH}_3\text{SC(O)OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{SH} + \text{CO}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2$ <i>Carbonothioic acid O-(1,1-dimethylethyl) S-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			479-502	5.4(+10)	0	16080		
$\text{CH}_3\text{OC(O)SC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_2=\text{C}(\text{CH}_3)_2$ <i>Carbonothioic acid S-(1,1-dimethylethyl) O-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	1.2(-3)	-	-		
$\text{CH}_3\text{OC(O)SC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_2=\text{C}(\text{CH}_3)_2$ <i>Carbonothioic acid S-(1,1-dimethylethyl) O-methyl ester</i> 79 ALA/BIG 79 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			370-420	1.4(+12)	0	21800		
$\text{CH}_3\text{C(S)SCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow$ $\text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ <i>Ethane(dithioic) acid butyl ester</i> 78 ALA/BIG 78 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	3.3(-3)	-	-		
$\text{CH}_3\text{C(S)SCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow$ $\text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ + cis-, and trans- $\text{CH}_3\text{CH}=\text{CHCH}_3$ <i>Ethane(dithioic) acid 1-methylpropyl ester</i> 78 ALA/BIG 78 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			651-716	1.2(+13)	0	22500		
$\text{CH}_3\text{C(S)SCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow$ $\text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ + cis-, and trans- $\text{CH}_3\text{CH}=\text{CHCH}_3$ <i>Ethane(dithioic) acid 1-methylpropyl ester</i> 78 ALA/BIG 78 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	7.4(-2)	-	-		
$\text{CH}_3\text{C(S)SCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow$ $\text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_3$ + cis-, and trans- $\text{CH}_3\text{CH}=\text{CHCH}_3$ <i>Ethane(dithioic) acid 1-methylpropyl ester</i> 78 ALA/BIG 78 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			584-639	6.7(+12)	0	20210		

Table of Arrhenius parameters for gas phase chemical reactions of sulfur compounds — Continued

Chemical reactions	n	M	k/k _{ref}	T/K	A	B	E/R (in K)	k factors f F	
$\text{CH}_3\text{C}(\text{S})\text{SC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + \text{CS}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$ <i>Ethane(dithioic acid 1,1-dimethylethyl ester)</i> 78 ALA/BIG 78 ALA BIC k based on reported ΔH^\ddagger and ΔS^\ddagger	1 1			629 448-502	3.1(-1) 1.1(+13)	- 0	- 19600		
$(\text{CH}_3)_3\text{CSC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{S} + (\text{CH}_3)_3\text{SH}$ $+ (\text{CH}_3)_3\text{SH}$ <i>Propane, 2,2'-thiobis[2-methyl-</i> 80 MAR/BAR	1			633-686	1.3(+15)	0	27545±962	0.5	2.0
$(\text{CH}_3)_3\text{CSSC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{other products}$ <i>Disulfide, bis(1,1-dimethylethyl)-</i> 76 MAR/BAR In a stirred-flow system.	1			603-673	4.0(+14)	0	22130±480	0.4	2.5
76 MAR BAR In a static system.	1			519-573	4.0(+13)	0	21290±240	0.6	1.6

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Appendix: Conversion Tables

Equivalent second order rate constants

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

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under column B and multiply the old value by it, e.g. to convert cm³ molecule⁻¹ s⁻¹ to m³ mol⁻¹ s⁻¹ multiply by 6.023 × 10¹⁷.

Table adapted from High Temperature Reaction Rate Data No. 5, The University, Leeds (1970).

Equivalent third order rate constants

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

See note to table for second order rate constants.

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET <i>(See instructions)</i>	1. PUBLICATION OR REPORT NO. NSRDS-NBS 72	2. Performing Organ. Report No.	3. Publication Date May 1982
4. TITLE AND SUBTITLE Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)			
5. AUTHOR(S) Francis Westley			
6. PERFORMING ORGANIZATION <i>(If joint or other than NBS, see instructions)</i> NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234		7. Contract/Grant No.	8. Type of Report & Period Covered N/A
9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS <i>(Street, City, State, ZIP)</i> Morgantown Energy Technology Center and Office of Standard Reference Data Department of Energy Morgantown, WV 26505 National Bureau of Standards Washington, DC 20234			
10. SUPPLEMENTARY NOTES Library of Congress Catalog Card Number: 82-2094 <input type="checkbox"/> Document describes a computer program; SF-185, FIPS Software Summary, is attached.			
11. ABSTRACT <i>(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)</i> 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, S ₂ , SO, SO ₂ , SO ₃ , S ₂ O, SH, H ₂ S, CS, CS ₂ , COS, CH ₃ S•, CH ₃ SH, cy-CH ₂ CH ₂ S•, CH ₃ SCH ₂ • and a number of thiols, thioethers, and thioesters, with other compounds. The table includes 19 unimolecular, 208 bimolecular, and 13 termolecular reactions totaling 240 distinct chemical reactions. There are 441 rate constants associated with these reactions, distributed as follows: 30 for first order reactions, 377 for second order reactions, and 34 for third order reactions. The kinetic data were compiled from 145 experimental papers and 8 critical reviews published between 1971 and 1980.			
12. KEY WORDS <i>(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)</i> Arrhenius parameters; chemical kinetics; combustion; decomposition; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur			
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