

A11102 146357

NAT'L INST OF STANDARDS & TECH R.I.C.



A1102146357

Westley, Francis/Tables of rate constant
QC100 .U573 V72:1982 C.2 NBS-PUB-C 1982



NSRDS-NBS 72

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards



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

QC

100

.U573

No. 72

1982

C.2

NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards¹ was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the Nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the Nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, and the Institute for Computer Sciences and Technology.

THE NATIONAL MEASUREMENT LABORATORY provides the national system of physical and chemical and materials measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; conducts materials research leading to improved methods of measurement, standards, and data on the properties of materials needed by industry, commerce, educational institutions, and Government; provides advisory and research services to other Government agencies; develops, produces, and distributes Standard Reference Materials; and provides calibration services. The Laboratory consists of the following centers:

Absolute Physical Quantities² — Radiation Research — Chemical Physics — Analytical Chemistry — Materials Science

THE NATIONAL ENGINEERING LABORATORY provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

Applied Mathematics — Electronics and Electrical Engineering² — Manufacturing Engineering — Building Technology — Fire Research — Chemical Engineering²

THE INSTITUTE FOR COMPUTER SCIENCES AND TECHNOLOGY conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following centers:

Programming Science and Technology — Computer Systems Engineering.

¹Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Washington, DC 20234.

²Some divisions within the center are located at Boulder, CO 80303.

NOV 9 1982

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

NSRDS-NBS

Francis Westley

Chemical Kinetics Division
Center for Chemical Physics
National Bureau of Standards
Washington, DC 20234

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

© 1982 by the Secretary of Commerce on Behalf of the United States Government

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.

A handwritten signature in dark ink, reading "Ernest Ambler." The signature is fluid and cursive, with the first name "Ernest" and the last name "Ambler" clearly distinguishable.

ERNEST AMBLER, *Director*

Contents

	Page
Foreword	iii
1. Introduction	1
2. Guidelines for the User	2
Table of Arrhenius Parameters for Chemical Reactions of Sulfur Compounds	5
Reactions of:	
S (Sulfur atom)	5
S ₂ (Sulfur dimer)	11
SO (Sulfur monoxide)	12
SO ₂ (Sulfur dioxide)	13
SO ₃ (Sulfur trioxide)	18
S ₂ O (Sulfur oxide)	18
SH (Mercapto free radical)	18
H ₂ S (Hydrogen sulfide)	20
CS (Carbon monosulfide free radical)	21
CS ₂ (Carbon disulfide)	22
COS (Carbon oxide sulfide)	23
CH ₃ S· (Methylthio free radical)	25
CH ₃ SH (Methanethiol)	25
cy-CH ₂ CH ₂ S (Thiirane)	25
CH ₃ SCH ₂ · (Methyl, (methylthio)-, free radical)	26
CH ₃ CH ₂ SH (Ethanethiol)	26
(CH ₃) ₂ S (Methane, thiobis-)	27
CH ₃ SSCH ₃ (Disulfide, dimethyl-)	27
CH ₃ SO ₂ CH ₃ (Methane, sulfonylbis-)	27
cy-CH ₂ CH ₂ CH ₂ S (Thietane)	28
cy-(CH ₃)CHCH ₂ S (Thiirane, methyl-)	28
CH ₃ CH ₂ CH ₂ SH (1-Propanethiol)	28
(CH ₃) ₂ CHSH (2-Propanethiol)	28
cy-CH ₂ CH ₂ CH ₂ CH ₂ S (Thiophene, tetrahydro-)	28
CH ₃ C(S)SCH ₂ CH ₃ (Ethane(dithioic) acid ethyl ester)	28
CH ₃ CH ₂ CH ₂ CH ₂ SH (1-Butanethiol)	28
(CH ₃) ₃ CSH (2-Propanethiol, 2-methyl-)	28
CH ₂ =CHCH ₂ SO ₂ CH ₃ (1-Propene, 3-methylsulfonyl)	29
CH ₃ SC(O)OCH ₂ CH ₃ (Carbonothioic acid O-ethyl S-methyl ester)	29
CH ₃ OC(O)SCH ₂ CH ₃ (Carbonothioic acid S-ethyl O-methyl ester)	29
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ SH (1-Pentanethiol)	29
CH ₃ OC(O)SCH(CH ₃) ₂ (Carbonothioic acid O-methyl S-(1-methylethyl) ester)	29
CH ₃ SC(O)OCH(CH ₃) ₂ (Carbonothioic acid S-methyl O-(1-methylethyl) ester)	29
CH ₃ (SC(O)OC(CH ₃) ₂ (Carbonothioic acid O-(1,1-dimethyl ethyl) S-methyl ester)	29
CH ₃ OC(O)SC(CH ₃) ₃ (Carbonothioic acid S-(1,1-dimethyl ethyl) O-methyl ester)	29
CH ₃ C(S)SCH ₂ CH ₂ CH ₂ CH ₃ (Ethane(dithioic) acid butyl ester)	29
CH ₃ C(S)SCH(CH ₃)CH ₂ CH ₃ (Ethane(dithioic) acid 1-methyl-propyl ester)	29
CH ₃ C(S)SC(CH ₃) ₃ (Ethane(dithioic) acid, 1,1-dimethyl ethyl ester)	30
(CH ₃) ₄ CSC(CH ₃) ₃ (Propane, 2,2'-thiobis[2-methyl]-)	30
(CH ₃) ₃ CSSC(CH ₃) ₃ (Disulfide, bis[1,1-dimethylethyl]-)	30
3. Bibliography	31
Appendix: Conversion Tables	36

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

Francis Westley

Chemical Kinetics Division, Center for Chemical Physics, National Bureau of Standards, Washington, DC 20234

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.

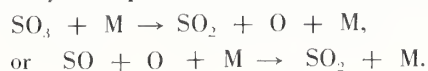
Column 8, with the heading *E/R*, indicates the value of *E/R* for the equation $k = AT^n \exp(-E/RT)$. Since *E* is the activation energy in cal mol⁻¹ and *R* the gas constant with a value of 1.987 cal mol⁻¹ K⁻¹, it follows that the units of *E/R* are kelvins. The values given in column 5 for *E/R* 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, L., 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, $\text{HO}_2\cdot$, SH, NH, CH, $\text{CH}_2\cdot$, $\text{CH}_3\cdot$, 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
$S + O_2 \rightarrow SO + O$ <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
$S + O_3 \rightarrow SO + O_2$ <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
$S + H_2 \rightarrow SH + H$ <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	
$S^*(^1D) + H_2 \rightarrow \text{products}$ <i>Sulfur atom + Hydrogen molecule</i>								
72 LIT/DAL k _{ref} : $S^*(^1D) + CH_2=CH_2 \rightarrow \text{products}$.	2		0.22	300	–	–	–	
$S + OH \rightarrow SO + H$ <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
$S + OH \rightarrow SH + O$ <i>Sulfur atom + Hydroxyl free radical</i>								
75 BEN/GOL Semi-empirical evaluation.	2				1.3(+12)	0.5	12700	
$S + S + M \rightarrow S_2 + M$ <i>Sulfur atom</i>								
79 NIC/AMO	3			295	4.3(+18)	–	–	0.8 1.2
$S + S_2 \rightarrow S_2 + S$ <i>Sulfur atom + Sulfur dimer</i>								
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
$S + SO \rightarrow S_2 + O$ <i>Sulfur atom + Sulfur monoxide</i>								
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	11500	
$S + SO \rightarrow SO + S$ <i>Sulfur atom + Sulfur monoxide</i>								
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0	
$S + SH \rightarrow S_2 + H$ <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. 78 VAN OBI k ₀ (low pressure).	2	CO ₂		298	9.3(+12)	—	—	0.8	1.2
	3	CO ₂		298	1.9(+17)	—	—		
S + NO ₂ → SO + NO <i>Sulfur atom + Nitrogen oxide(NO₂)</i> 75 CLY/TOW 79 CLY/WHY	2			298	3.7(+13)	—	—	0.8	1.2
	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 + Imidogen 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	
$S^*(^1D) + CH_4 \rightarrow CH_3SH$ <i>Sulfur atom + Methane</i> 72 LIT/DAL $k_{ref}: S^*(^1D) + CH_2=CH_2 \rightarrow \text{products}$ 80 ADD/DON	2		0.076	300	—	—	—		
	2			295	1.1(+14)	—	—	0.7	1.3
$S + CS \rightarrow CS + S$ <i>Sulfur atom + Carbon monosulfide free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
$S + CS \rightarrow S_2 + C$ <i>Sulfur atom + Carbon monosulfide free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				1.6(+12)	0.5	40463		
$S + CS + M \rightarrow CS_2 + M$ <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
$S + CS_2 \rightarrow S_2 + CS$ <i>Sulfur atom + Carbon disulfide</i> 76 BAU/DRY (Recommended k).	2			298	3.9(+11)	—	—	0.5	1.5
$S + COS \rightarrow S_2 + CO$ <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
$S^*(^1D) + COS \rightarrow S_2 + CO$ <i>Sulfur atom + Carbon oxide sulfide</i> 72 LIT/DAL $k_{ref}: S^*(^1D) + CH_2=CH_2 \rightarrow \text{products}$ 79 ADD/BYR 79 SHE/SAF $k_{ref}: S^*(^1D) + COS \rightarrow S(^3P) + COS$ (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
$S + CN \rightarrow CS + N$ <i>Sulfur atom + Cyanogen free radical</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
$S + C_2 \rightarrow CS + C$ <i>Sulfur atom + Carbon dimer</i> 75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	0		
$S + CH\equiv CH \rightarrow cy-CH=CHS$ <i>Sulfur atom + Ethyne</i> 71 STR/O'C $k/k_{ref}: 6.2\exp(-1007/T)$. $k_{ref}: S + CH_2=CH_2 \rightarrow cy-CH_2CH_2S$ Conventional photolysis method. 72 KER/PAR (Recommended k).	2			298–450	—	—	—		
	2			298	1.7(+11)	—	—		
$S + CH\equiv CH \rightarrow \text{products}$ <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 ₃ 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 ₃ =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/DAV1	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	3	CO ₂		293	9.1(+17)	–	–	0.1	10.
73 LAN/OLD Given with caution.	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 3	Ar		298 298	7.3(+16) 6.7(+13)	— —	— —	0.9 0.7	1.1 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 2			298 298	3.3(+13) 5.1(+13)	— —	— —	0.5 0.8	2.0 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 _{ref} : He(1.0)	3	He		297	3.0(+14)	–	–	0.9 1.1
75 WES DEH2 M _{ref} : SO ₂ (9.5)	3	SO ₂		297	2.9(+15)	–	–	0.7 1.3
75 WES DEH2 M _{ref} : 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 (¹ Δ _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 *(³ B ₁) + O ₂ → products <i>Sulfur dioxide + Oxygen molecule</i> 78 PAR/HEI k _{ref} : SO ₂ *(³ B ₁) + 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
$\text{SO}_2 + \text{OH} + \text{M} \rightarrow \text{HOSO}_2 + \text{M}$ <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 ₀ (low pressure: <20 torr).	3	N ₂		298	5.8(+16)	—	—	
75 GOR/MUL1 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 ₀ (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 ₀ (low-pressure k).	3	N ₂		297	5.8(+16)	—	—	
77 CAS/TAN k ₀ (low-pressure). On the basis of k ₀ (297) and E _a experimental values.	3	N ₂		253–297	5.0(+14)	0	–1410	
77 CAS/TAN k ₀ (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 ₀ (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	
$\text{SO}_2 + \text{HO}_2 \rightarrow \text{SO}_3 + \text{OH}$ <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)	—	—	
$\text{SO}_2 + \text{HO}_2 \rightarrow \text{products}$ <i>Sulfur dioxide + Hydroperoxyl free radical</i>								
79 GRA/WIN Upper limit k.	2			300	<6.0(+5)	—	—	
$\text{SO}_2 + \text{HO}_2 + \text{M} \rightarrow \text{HO}_2\text{SO}_2 + \text{M}$ <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	
$\text{SO}_2 + \text{SO}_2^*(^1\text{B}_1) \rightarrow \text{SO}^*(^1\Delta_g, ^3\Sigma^-) + \text{SO}_3$ <i>Sulfur dioxide</i> 75 CHU/CAL	2			298	2.2(+12)	—	—	0.8	1.2
$\text{SO}_2 + \text{SO}_2^*(^3\text{B}_1) \rightarrow \text{SO} + \text{SO}_3$ <i>Sulfur dioxide</i> 78 MAR/REI In an atmosphere of water vapor. (Approximate k).	2			298	2.0(+14)	—	—		
$\text{SO}_2 + \text{SO}_2^*(^3\text{B}_1) \rightarrow \text{SO}^*(^3\Sigma^-) + \text{SO}_3$ <i>Sulfur dioxide</i> 75 CHU/CAL	2			298	4.2(+10)	—	—	0.9	1.1
$\text{SO}_2 + \text{NO}_3 \rightarrow \text{SO}_3 + \text{NO}$ <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		
$\text{SO}_2 + \text{NO}_2^* \rightarrow \text{products}$ <i>Sulfur dioxide + Nitrogen oxide(NO₂)</i> 78 IWA/PRE At 50 torr.	2			298	8.2(+10)	—	—		
$\text{SO}_2 + \text{NO}_3 \rightarrow \text{SO}_3 + \text{NO}_2$ <i>Sulfur dioxide + Nitrogen oxide(NO₂)</i> 75 DAU/CAL Upper limit k.	2			300	<4.2(+3)	—	—		
$\text{SO}_2 + \text{N}_2\text{O}_5 \rightarrow \text{SO}_3 + \text{N}_2\text{O}_4$ <i>Sulfur dioxide + Nitrogen oxide(N₂O₅)</i> 75 DAU/CAL Upper limit k.	2			300	<2.5(+1)	—	—		
$^1\text{SO}_2^* + \text{CO} \rightarrow \text{SO} + \text{CO}_2$ <i>Sulfur dioxide + Carbon monoxide</i> 73 CEH/HEI $k_{\text{ref}}: ^1\text{SO}_2^* + \text{SO}_2 \rightarrow \text{products}$ $k/k_{\text{ref}} = 5.0 \times 10^{-3}$ (at 2537 Å)	2			300	—	—	—		
73 CEH/HEI $k/k_{\text{ref}} = 1.5 \times 10^{-3}$ (at 3130 Å)	2			300	—	—	—		
$\text{SO}_2^* + \text{CO} \rightarrow \text{SO} + \text{CO}_2$ <i>Sulfur dioxide + Carbon monoxide</i> 73 CEH/HEI $k_{\text{ref}}: \text{SO}_2^* \rightarrow \text{products}$ $k/k_{\text{ref}} = 2.2 \times 10^{-5}$ (3130 to 3261 Å) (SO ₂ [*] is a vibrationally excited singlet).	2			300	—	—	—		
$\text{SO}_2^{**} + \text{CO} \rightarrow \text{SO} + \text{CO}_2$ <i>Sulfur dioxide + Carbon monoxide</i> 73 CEH/HEI $k_{\text{ref}}: \text{SO}_2^{**} \rightarrow \text{SO}_2$ $k_{\text{ref}} = 1.8 \times 10^{-5}$ (2537 to 3261 Å) (SO ₂ ^{**} is a chemically active triplet).	2			300	—	—	—	0.7	1.4
$\text{SO}_2 + \text{CO} + \text{M} \rightarrow \text{products}$ <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
$\text{SO}_2 + \text{CH}_3 + \text{M} \rightarrow \text{CH}_3\text{SO}_2 + \text{M}$ <i>Sulfur dioxide + Methyl free radical</i> 73 JAM/KER Limiting high-pressure k.	2			298	1.8(+11)	—	—	0.9 1.1
$\text{SO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O}_2\text{SO}_2$ <i>Sulfur dioxide + Methylldioxy free radical</i> 79 SAN/SIM 79 SIM/HEI $k_{\text{ref}}: \text{NO} + \text{CH}_3\text{O}_2 \rightarrow \text{NO}_2 + \text{CH}_3\text{O}$	2 2		0.0025	298 296	4.9(+9) —	— —	— —	0.9 1.1 0.8 1.2
$\text{SO}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{products}$ <i>Sulfur dioxide + Methylldioxy 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
$\text{SO}_2 + \text{CH}\equiv\text{CH} \rightarrow \text{products}$ <i>Sulfur dioxide + Ethyne</i> 71 FIF/MOR Given with caution.	2			1550–2150	3.2(+10)	0.5	20535	
$\text{SO}_2^{**} + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow \text{products}$ <i>Sulfur dioxide + 1,2-Propadiene</i> 78 PAR/HEI $k_{\text{ref}}: \text{SO}_2^{**} + \text{CH}_2=\text{C}=\text{CH}_2 \rightarrow$ $\text{CO} + \text{other products}$ (SO_2^{**} is a non-emitting triplet).	2		4.0	298	—	—	—	
$\text{SO}_2(^3\text{B}_1) + \text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow$ $[\text{cis-CH}_3\text{CH}=\text{CHCH}_3\text{SO}_2]^*$ <i>Sulfur dioxide + cis-2-Butene</i> 74 DEM/CAL	2			294	1.3(+14)	—	—	0.9 1.1
$\text{SO}_2(^3\text{B}_1) + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow$ $[\text{trans-CH}_3\text{CH}=\text{CHCH}_3\text{SO}_2]^*$ <i>Sulfur dioxide + trans-2-Butene</i> 74 DEM/CAL	2			294	1.2(+14)	—	—	0.9 1.1
$\text{SO}_2(^1\text{B}_1) + (\text{CH}_3)_2\text{CH} \rightarrow \text{products}$ <i>Sulfur dioxide + Propane, 2-methyl-</i> 78 SU /CAL Evaluation.	2			298	8.4(+12)	—	—	
$\text{SO}_2(^3\text{B}_1) + (\text{CH}_3)_2\text{CH} \rightarrow \text{products}$ <i>Sulfur dioxide + Propane, 2-methyl-</i> 78 SU /CAL Evaluation.	2			298	8.7(+11)	—	—	
$\text{SO}_2(^3\text{B}_1) + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow$ $[\text{SO}_2\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3]^*$ <i>Sulfur dioxide + cis-2-Pentene</i> 76 WAM	2			295	6.3(+13)	—	—	0.8 1.2
$\text{SO}_2(^3\text{B}_1) + \text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow$ $[\text{SO}_2\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3]^*$ <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
$\text{SO}_2 + \text{M} \rightarrow \text{SO} + \text{O} + \text{M}$ <i>Sulfur dioxide</i>								
75 KIE	2	Kr		2900–5200	1.7(+16)	0	56370±2000	0.6 1.6
78 AST/GLA Rate constant expressed as k[Ar].	2	Ar		3700–6500	4.0(+14)	0	53890±2170	0.5 2.0
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	
$\text{SO}_3 + \text{O} \rightarrow \text{SO}_2 + \text{O}_2$ <i>Sulfur trioxide + Oxygen atom</i>								
71 MER/LEV k determined in H ₂ S flame.	2			1100–1400	6.5(+14)	0	5435	
71 MER/LEV k determined in COS flame.	2			900–1600	2.8(+14)	0	6040	
72 JAC/WIN	2			300–500	1.5(+8)	0	500	
73 SCH Given with caution.	2			1480–1550	2.8(+14)	0	6040	
79 MER/LEV	2			1685	1.5(+11)	–	–	
$\text{SO}_3 + \text{O} + \text{M} \rightarrow \text{SO}_2 + \text{O}_2 + \text{M}$ <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 M _{eff} : He(1.0)	3	He		298	7.3(+17)	–	–	0.9 1.1
75 WES DEH1 M _{eff} : SO ₃ (<10.0). Upper limit ratio.	3	SO ₃		298	<7.3(+18)	–	–	
75 WES DEH1 M _{eff} : N ₂ (1.4)	3	N ₂		298	1.0(+18)	–	–	0.9 1.1
$\text{SO}_3 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{SO}_4$ <i>Sulfur trioxide + Water</i>								
75 CAS/DAV	2			298	5.5(+11)	–	–	0.8 1.2
$\text{SO}_3 + \text{SO} \rightarrow \text{SO}_2 + \text{SO}_2$ <i>Sulfur trioxide + Sulfur monoxide</i>								
75 CHU/CAL	2			298	1.2(+9)	–	–	0.4 1.6
$\text{SO}_3 + \text{N} \rightarrow \text{SO}_2 + \text{NO}$ <i>Sulfur trioxide + Nitrogen atom</i>								
72 JAC/WIN	2			300	3.0(+8)	–	–	
75 WES/DEH1 Upper limit k.	2			298	<6.0(+6)	–	–	
$\text{SO}_3 + \text{M} \rightarrow \text{SO}_2 + \text{O} + \text{M}$ <i>Sulfur trioxide</i>								
78 AST/GLA Rate constant expressed as k[Ar].	2	Ar		1700–2500	3.2(+15)	0	31880±1320	0.6 1.6
79 AST/GLA	2	Ar		1700–2500	3.2(+15)	0	31900±300	0.6 1.6
$\text{S}_2\text{O} + \text{O} \rightarrow \text{SO} + \text{SO}$ <i>Sulfur oxide(S₂O) + Oxygen atom</i>								
74 STE/ALV Evaluation.	2			298	9.0(+11)	–	–	0.9 1.1
$\text{SH} + \text{O} \rightarrow \text{S} + \text{OH}$ <i>Mercapto free radical + Oxygen atom</i>								
73 SCH Theoretical estimate.	2			298–2500	2.3(+11)	0.67	956	
75 BEN/GOL Semi-empirical evaluation.	2				6.3(+11)	0.5	4000	

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 73 BRA/TRU 75 CUP/GLA 76 BAU/DRY (Recommended k). 79 NIC/AMO	2 2 2 2 2			293 298 298 298 295	<6.0(+12) 2.5(+13) 1.5(+13) 1.5(+13) 1.3(+13)	— — — — —	— — — — —	0.7 0.5 0.8	1.3 1.5 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 75 BEN/GOL Semi-empirical evaluation 79 NIC/AMO Upper limit k.	2 2 2			295 295	2.4(+13) 6.3(+11) <3.0(+12)	— 0.5 —	— 0 —		
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. 73 BRA/TRU 76 BAU/DRY (Recommended k). 79 NIC/AMO	2 2 2 2			293 298 295 295	<1.8(+13) 7.8(+12) 7.8(+12) 1.9(+13)	— — — —	— — — —	0.5 0.9	1.5 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	2			200–350	3.8(+11)	0	920±45	0.5 2.0
76 WHY/TIM	2			263–495	4.4(+12)	0	1660±50	0.9 1.1
78 WHY/TIM	2			263–495	4.4(+12)	0	1660±50	0.8 1.2
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			250–500	4.3(+12)	0	1660±150	0.8 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.	2			281–497	1.5(+13)	0	1920±45	0.8 1.2
79 SIN/IRW	2			297–502	1.6(+13)	0	2171±202	0.5 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.	2			298	<1.2(+4)	–	–	
75 GLA/TOB1 Estimated k.	2			293–343	4.9(+10)	0	3420	
75 GLA/TOB2	2			298–343	1.6(+12)	0	2620±600	0.2 6.3
75 BAU/DRY (Recommended k).	2			298	4.0(+2)	–	–	0.1 10.0
H ₂ S + H → SH + H ₂ <i>Hydrogen sulfide + Hydrogen atom</i> 71 KUR/PET	2			190–464	7.8(+12)	0	860±30	0.9 1.1
72 ROM/SCH	2			298	2.3(+11)	–	–	0.8 1.3
73 BRA/TRU	2			298	5.0(+11)	–	–	
76 BAU/DRY (Recommended k).	2			190–470	7.8(+12)	0	860±50	0.5 1.5
79 NIC/AMO	2			295	5.0(+11)	–	–	0.9 1.1
80 HUS/SLA	2			300	5.2(+11)	–	–	0.9 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	2			298–885	1.4(+13)	0	443	
74 STU	2			298	1.9(+12)	–	–	0.8 1.2
76 BAU/DRY (Recommended k). k factors changing to: f = 0.5 and F = 1.5 at 900K.	2			298–900	6.3(+12)	0	200±150	0.7 1.3
76 PER/ATK1	2			297–427	3.1(+12)	0	0	0.9 1.1
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			250–400	6.6(+12)	0	225±225	0.8 1.3
H ₂ S + OH → products (overall) <i>Hydrogen sulfide + Hydroxyl free radical</i> 72 NIK/MOR1 Approximate k.	2			300	5.2(+12)	–	–	
80 COX/SHE	2			297	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	
$\text{H}_2\text{S} + \text{OH}(v=9) \rightarrow \text{products}$ <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
$\text{H}_2\text{S} + \text{CH}_3 \rightarrow \text{SH} + \text{CH}_3$ <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
$\text{H}_2\text{S} + \text{M} \rightarrow \text{SH} + \text{H} + \text{M}$ <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
$\text{CS} + \text{O} \rightarrow \text{S} + \text{CO}$ <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	2			300	$1.3(+13)$	—	—	0.8	1.2
Unreported T assumed to be 300K.									
80 BAU/COX (Recommended k). k factors apply at 298K only.	2			150–300	$1.6(+14)$	0	760 ± 250	0.8	1.3
$\text{CS} + \text{O} \rightarrow \text{S} + \text{CO}(v=n)$ <i>Carbon monosulfide free radical + Oxygen atom</i> 72 HAN/RID $k_{\text{ref}}: \text{CS} + \text{O} \rightarrow \text{S} + \text{CO}(v=13)$ 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/GRA1	2			305	$1.2(+13)$	—	—	0.9	1.1
76 BID/BRE	2			300	$1.4(+13)$	—	—	0.8	1.2
$\text{CS} + \text{O} \rightarrow \text{SO} + \text{C}$ <i>Carbon monosulfide free radical + Oxygen atom</i> 75 BEN/GOL Semi-empirical evaluation.	2				$1.6(+12)$	0.5	28940		
$\text{CS} + \text{O}_2 \rightarrow \text{SO} + \text{CO}$ <i>Carbon monosulfide free radical + Oxygen molecule</i> 73 SCH Estimated upper limit k.	2			298	$<1.8(+6)$	—	—		
$\text{CS} + \text{O}_2 \rightarrow \text{COS} + \text{O}$ <i>Carbon monosulfide free radical + Oxygen molecule</i> 73 SCH Estimated upper limit k.	2			298	$<1.8(+6)$	—	—		
$\text{CS} + \text{H} \rightarrow \text{S} + \text{CH}$ <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/PERI Upper limit k.	2			300	<4.2(+10)	–	–		
78 ATK PERI 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	
$\text{COS} + \text{O}^*(^1\text{D}) \rightarrow \text{SO} + \text{CO}$ <i>Carbon oxide sulfide + Oxygen atom</i> 75 GAU/SNE $k_{\text{ref}}: \text{O}_2 + \text{O}^*(^1\text{D}) \rightarrow \text{O}_2^*(^1\Sigma_g^+) + \text{O}$ 75 GAU SNE Evaluation.	2		4.1	300	—	—	—		
	2			300	1.8(+14)	—	—		
$\text{COS} + \text{H} \rightarrow \text{CO} + \text{SH}$ <i>Carbon oxide sulfide + Hydrogen atom</i> 72 ROM/SCH 75 TSU/YOK 76 BAU/DRY (Recommended k). 76 LEE 77 LEE/STI	2			298	1.3(+10)	—	—	0.8	1.3
	2			300–525	9.1(+12)	0	1965±185	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
$\text{COS} + \text{OH} \rightarrow \text{products}$ <i>Carbon oxide sulfide + Hydroxyl free radical</i> 78 ATK/PER1 Upper limit k. 78 ATK PER1 Upper limit k. 78 KUR2 80 BAU/COX (Recommended k). Upper limit k. 80 COX/SHE Upper limit k.	2			299	<4.2(+9)	—	—		
	2			430	<1.2(+10)	—	—		
	2			296	3.4(+10)	—	—		
	2			298	<3.6(+10)	—	—		5.0
	2			297	<2.4(+10)	—	—		
$\text{COS} + \text{OH}(v=9) \rightarrow \text{products}$ <i>Carbon oxide sulfide + Hydroxyl free radical</i> 72 WOR/COL Unreported T assumed to be 298K.	2			298	1.5(+10)	—	—	0.4	1.6
$\text{COS} + \text{S} \rightarrow \text{CO} + \text{S}_2$ <i>Carbon oxide sulfide + Sulfur atom</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
$\text{COS} + \text{S}^*(^1\text{D}) \rightarrow \text{CO} + \text{S}_2$ <i>Carbon oxide sulfide + Sulfur atom</i> 72 LIT/DAL $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S}^*(^1\text{D}) \rightarrow \text{products}$ 78 SHE/SAF $k_{\text{ref}}: \text{COS} + \text{S}^*(^1\text{D}) \rightarrow \text{COS} + \text{S}(^3\text{P})$ Optimization. 79 ADD/BYR 80 ADD/DON	2		1.5	300	—	—	—		
	2		2.4	298	—	—	—		
	2			290	7.2(+13)	—	—	0.8	1.3
	2			295	1.8(+14)	—	—	0.7	1.3
$\text{COS} + \text{CD}_3 \rightarrow \text{CO} + \text{CD}_3\text{S}$ <i>Carbon oxide sulfide + Methyl-d₃ free radical</i> 72 JAK/AHM Evaluation.	2			354–490	3.8(+11)	0	5710±175	0.6	1.8
$\text{COS} + \text{CN} \rightarrow \text{SCN} + \text{CO}$ <i>Carbon oxide sulfide + Cynogen free radical</i> 79 ADD/LEI Lower limit k.	2			295	>1.8(+13)	—	—		
$\text{COS} + \text{M} \rightarrow \text{products}$ <i>Carbon oxide sulfide</i> 74 TRA k measured in shock tube. Unspecified, high T range.	2				8.3(+14)	0	31700±650		

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	
$\text{CH}_3\text{S} + \text{CH}\equiv\text{CH} \rightarrow \text{CH}_3\text{SCH}=\text{CH}$ <i>Methylthio free radical + Ethyne</i> 72 KER/PAR (Recommended k).	2			298–333	7.9(+7)	–	–		
$\text{CH}_3\text{S} + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{SCH}_2\text{CH}_2$ <i>Methylthio free radical + Ethene</i> 72 KER/PAR (Recommended k).	2			298	4.8(+8)	–	–		
$\text{CH}_3\text{S} + \text{cy-CH}_2\text{CH}_2\text{S} \rightarrow \text{CH}_3\text{S}_2 + \text{CH}_2=\text{CH}_2$ <i>Methylthio free radical + Thiirane</i> 72 JAK/AHM Approximate k.	2			304–478	3.2(+11)	0	4430		
$\text{CH}_3\text{S} + \text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}(\text{SCH}_3)\text{CH}(\text{CH}_3)$ <i>Methylthio free radical + 2-Butene</i> 72 KER/PAR cis–trans equilibrium–weighted k.	2			298–333	1.6(+9)	–	–		
$\text{CH}_3\text{SH} \rightarrow \text{CH}_3 + \text{SH}$ <i>Methanethiol</i> 70 BEN/O'N Critical evaluation.	1			1005–1102	3.2(+15)	0	38550		
$\text{CH}_3\text{SH} + \text{O} \rightarrow \text{products}$ <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 1.1×10^{12} at 254K to $2.6 \times 10^{12} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ 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
$\text{CH}_3\text{SH} + \text{OH} \rightarrow \text{products}$ <i>Methanethiol + Hydroxyl free radical</i> 80 COX/SHE	2			297	5.4(+13)	–	–	0.9	1.1
$\text{CH}_3\text{SH} + \text{CH}_3 \rightarrow \text{CH}_2\text{SH} + \text{CH}_4$ <i>Methanethiol + Methyl free radical</i> 76 KER/PAR (Recommended k).	2			303	1.2(+8)	–	–	0.5	2.0
$\text{CD}_3\text{SH} + \text{CH}_3 \rightarrow \text{CD}_2\text{S} + \text{CH}_4$ <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
$\text{CD}_3\text{SH} + \text{CH}_3 \rightarrow \text{CD}_2\text{SH} + \text{CH}_3\text{D}$ <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
$\text{CD}_3\text{SH} + \text{CH}_3 \rightarrow \text{CD}_2\text{SH} + \text{CH}_3\text{D}$ <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
$\text{cy-CH}_2\text{CH}_2\text{S}^* \rightarrow \text{CH}_2=\text{CHSH}$ <i>Thiirane</i> 79 SHE/SAF	1			298	5.0(+10)	–	–		
$\text{cy-CH}_2\text{CH}_2\text{S} + \text{O} \rightarrow \text{CH}_2=\text{CH}_2 + \text{SO}$ <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/DAV1	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()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 ₄ <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 Non-linear Arrhenius behavior. Within the given T range, k increasing from 1.9×10 ¹² at 257K to 3.2×10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 495K.	2 2 2			300 304–421 257–495	1.7(+12) 5.8(+12) 1.9(+12)	— 0 —	— -391±18 —	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
CH ₃ CH ₂ SH + CH ₃ → products <i>Ethanethiol + 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. 80 LEE/TAN1	2 2 2			268-424 300 252-493	8.6(+12) 3.8(+13) 3.8(+13)	0 — —	-366±16 — —	0.9 1.1 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 1.2 0.8 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 1.1 0.6 1.4 0.8 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	
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{CH}_3 \rightarrow \text{cy-CH}_2\text{CH}(\text{CH}_3)\text{S} + \text{CH}_4$ <i>Thietane + Methyl free radical</i> 76 KER/PAR Tentative k.	2			300-450	3.2(+11)	0	4630±750		
$\text{cy-(CH}_3\text{)CHCH}_2\text{S} + \text{S} \rightarrow \text{CH}_3\text{CH=CH}_2 + \text{S}_2$ <i>Thiirane, methyl-, + Sulfur atom</i> 71 STR/O'C $k/k_{\text{ref}}: 8.4\exp(+1057/T)$ $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{S} \rightarrow \text{cy-CH}_2\text{CH}_2\text{S}$ Conventional photolysis method.	2			298-450	-	-	-		
$\text{cy-(CH}_3\text{)CHCH}_2\text{S} + \text{CH}_3 \rightarrow \text{CH}_3\text{CH=CH}_2 + \text{CH}_3\text{S}$ <i>Thiirane, methyl-, + Methyl free radical</i> 72 JAK/AHM Evaluation.	2			339-435	2.1(+11)	0	3750±830	0.1	8.3
$\text{cy-(CH}_3\text{)CHCH}_2\text{S} + \text{CH}_3 \rightarrow \text{cy-[(CH}_3\text{)CHCH}_2\text{)]S} + \text{CH}_4$ <i>Thiirane, methyl-, + Methyl free radical</i> 72 JAK/AHM	2			339-435	1.0(+11)	0	4160±440	0.3	3.0
$\text{CH}_3\text{CH}_2\text{CH}_2\text{SH} + \text{O} \rightarrow \text{products}$ <i>1-Propanethiol + Oxygen atom</i> 78 KIR/VET	2			303-421	8.3(+12)	0	-494±22	0.9	1.1
$(\text{CH}_3)_2\text{CHSH} + \text{CH}_3 \rightarrow \text{products}$ <i>2-Propanethiol + Methyl free radical</i> 76 KER/PAR Tentative k.	2			303	4.1(+7)	-	-		
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{H} \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH}$ <i>Thiophene, tetrahydro-, + Hydrogen atom</i> 78 HOR/NIS At 5 torr.	2			295-576	8.5(+12)	0	1010		
$\text{CH}_3\text{C(S)SCH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{CH}_2$ <i>Ethanedithioic acid ethyl ester</i> 78 ALA/BIG 78 ALA BIG k based on reported ΔH^\ddagger and ΔS^\ddagger .	1			629	1.8(-3)	-	-		
	1			651-716	9.2(+12)	0	22730		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{O} \rightarrow \text{products}$ <i>1-Butanethiol + Oxygen atom</i> 78 KIR/VET	2			306-419	5.8(+12)	0	-321±19	0.9	1.1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 + \text{H}_2\text{S}$ <i>1-Butanethiol + Hydrogen atom</i> 78 HOR/NIS At 5 torr.	2			295-576	1.6(+12)	0	1120		
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} + \text{H} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{H}_2$ <i>1-Butanethiol + Hydrogen atom</i> 78 HOR/NIS At 5 torr.	2			295-576	1.3(+13)	0	1600		
$(\text{CH}_3)_4\text{CSH} \rightarrow (\text{CH}_3)_3\text{C}=\text{CH}_2 + \text{H}_2\text{S}$ <i>2-Propanethiol, 2-methyl-</i> 70 BEN/O'N Critical evaluation.	1			950-1230	2.5(+13)	0	27830		
$(\text{CH}_3)_3\text{CSH} + \text{CH}_3 \rightarrow (\text{CH}_3)_3\text{CS} + \text{CH}_2\text{C}(\text{CH}_3)_2\text{SH} + \text{CH}_4$ <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	
$\text{CH}_2=\text{CHCH}_2\text{SO}_2\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_3\text{SO}_2$ <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 1			629 490-550	1.0(-4) 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 1			629 490-550	7.8(-7) 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-Pentonethiol + 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 1			629 440-480	4.6(-5) 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 1			629 547-584	9.4(-3) 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 1			629 479-502	4.2(-1) 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 1			629 370-420	1.2(-3) 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 1			629 651-716	3.3(-3) 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 1			629 584-639	7.4(-2) 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 BIG 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

3. Bibliography

1970

- 70 BEN/O'N Benson, S. W., and O'Neal, H. E., "Kinetic Data on Gas Phase Unimolecular Reactions," NSRDS-NBS 21 (1970). (Supt. Doc., U.S. Govt. Printing Office, Washington, DC 20402).

1971

- 71 ARM/CUL Armitage, J. W., and Cullis, C. F., "Studies of the Reaction Between Nitrogen Dioxide and Sulfur Dioxide," *Combust. Flame* **16**, 125 (1971).
- 71 BAU/JEF Bauer, S. H., Jeffers, P., Lifshitz, A., and Yadava, B. P., "Reaction Between CO and SO₂ at Elevated Temperatures: A Shock-Tube Investigation," *Symp. (Int.) Combust., (Proc.)* **13**, 1970 (Publ. 1971) 417.
- 71 CON/VAN Connor, J., Van Roodselaar, A., Fair, R. W., and Strausz, O. P., "The Addition of Group Via Atoms to Tetramethylthylene. An Addition Reaction with a Negative Activation Energy," *J. Am. Chem. Soc.* **93**, 560 (1971).
- 71 CUP/GLA Cupitt, L. T., and Glass, G. P., "Calculation of Absolute Concentrations of SH and SO from the E. S. R. Spectra," *Trans. Faraday Soc.* **67**, 1 (1971).
- 71 FAI/VAN Fair, R. W., Van Roodselaar, A., and Strausz, O. P., "The Reaction of S(¹P) Atoms with Molecular Oxygen," *Can. J. Chem.* **49**, 1659 (1971).
- 71 FIF/MOR Fifer, R., Moreau, R., and Bauer, S. H., "The Reactions Between SO₂ and C₂H₂ (and C₂H₄) at Elevated Temperature. A Single-Pulse Shock Tube Investigation," *Int. J. Chem. Kinet.* **3**, 249 (1971).
- 71 HAN/SMI Hancock, G., and Smith, I. W. M., "Infra-red Chemiluminescence from Vibrationally Excited CO. Part I. The Reaction of Atomic Oxygen with Carbon Disulphide," *Trans. Faraday Soc.* **67**, 2586 (1971).
- 71 KRE Krezenski, D. C., "Competitive Reaction of O(¹P) with Ozone and Carbonyl Sulfide," *Diss. Abstr. Int. B* **32**, 2633 (1971).
- 71 KRE/SIM Krezenski, D. C., Simonaitis, R., and Heicklen, J., "The Reactions of O(¹P) with Ozone and Carbonyl Sulfide," *Int. J. Chem. Kinet.* **3**, 467 (1971).
- 71 KUR/PET Kurylo, M. J., Peterson, N. C., and Braun, W., "Absolute Rate of the Reaction H + H₂S," *J. Chem. Phys.* **54**, 943 (1971).
- 71 MER/LEV Merryman, E. L., and Levy, A., "Sulfur Trioxide Flame Chemistry—H₂S and COS Flames," *Symp. (Int.) Combust., (Proc.)* **13**, 1970 (Publ. 1971) 427.
- 71 MIY/TAK1 Miyazaki, S., and Takahashi, S., "On the Reaction of Oxygen Atom with Carbon Disulphide, Part 2," *Mem. Def. Acad. Math. Phys. Chem. Eng. Yokosuka, Jpn.* **11**, 307 (1971).
- 71 MIY/TAK2 Miyazaki, S., and Takahashi, S., "On the Reaction of Oxygen Atom with Carbon Disulphide, Part 3," *Mem. Def. Acad. Math. Phys. Chem. Eng. Yokosuka, Jpn.* **11**, 329 (1971).
- 71 STR/O'C Strausz, O. P., O'Callaghan, W. B., Lown, E. M., and Gunning, H. E., "Reactions of Sulfur Atoms. XII. Arrhenius Parameters for the Addition to Olefins and Acetylenes," *J. Am. Chem. Soc.* **93**, 559 (1971).
- 71 TAK Takahashi, S., "On the Reaction of Oxygen Atom with Carbon-Disulphide, Part 1," *Mem. Def. Acad. Math. Phys. Chem. Eng. Yokosuka, Jpn.* **11**, 191 (1971).

1972

- 72 BRE/WIL Breckenridge, W. H., and Miller, T. A., "Kinetic Study by EPR of the Production and Decay of SO(¹Δ) in the Reaction of O₂(¹Δ_g) with SO(³Σ⁻)," *J. Chem. Phys.* **56**, 465 (1972).

- 72 DAV/KLE1 Davis, D. D., Klemm, R. B., and Pilling, M., "A Flash Photolysis-Resonance Fluorescence Kinetics Study of Ground-State Sulfur Atoms: I. Absolute Rate Parameters for Reaction of S(¹P) with O₂(³Σ⁻)," *Int. J. Chem. Kinet.* **4**, 367 (1972).
- 72 DAV/KLE2 Davis, D. D., Klemm, R. B., Braun, W., and Pilling, M., "A Flash Photolysis-Resonance Fluorescence Kinetics Study of Ground-State Sulfur Atoms. II. Rate Parameters for Reaction of S(¹P) with C₂H₄," *Int. J. Chem. Kinet.* **4**, 383 (1972).
- 72 DON/LIT Donovan, R. J., and Little, D. J., "The Rate of the Reaction S(¹P) + O₂," *Chem. Phys. Lett.* **13**, 488 (1972).
- 72 HAN/RID Hancock, G., Ridley, B. A., and Smith, I. W. M., "Infra-red Chemiluminescence from Vibrationally Excited CO. Part 2. Product Distribution from the Reaction O + CS → CO + S," *J. Chem. Soc. Faraday Trans. II* **68**, 2117 (1972).
- 72 JAC/WIN Jacob, A., and Winkler, C. A., "Kinetics of the Reactions of Oxygen Atoms and Nitrogen Atoms with Sulfur Trioxide," *J. Chem. Soc. Faraday Trans. I* **68**, 2077 (1972).
- 72 JAK/AHW Jakubowski, E., Ahmed, M. G., Lown, E. M., Sandhu, H. S., Gosavi, R. K., and Strausz, O. P., "Sulfur Atom Abstraction from Episulfides and Carbonyl Sulfide by Methyl Radicals," *J. Am. Chem. Soc.* **94**, 4094 (1972).
- 72 KER/PAR Kerr, J. A., and Parsonage, M. J., "Evaluated Kinetic Data on Gas Phase Addition Reactions: Reactions of Atoms and Radicals with Alkenes, Alkynes and Aromatic Compounds," (Butterworths, London, 1972).
- 72 LAN/OLD Langford, R. B., and Oldershaw, G. A., "Flash Photolysis of H₂S," *J. Chem. Soc. Faraday Trans. I* **68**, 1550 (1972).
- 72 LIT/DAL Little, D. J., Dalgleish, A., and Donovan, R. J., "Relative Rate Data for the Reactions of S(¹D₂) using the NS Radical as Spectroscopic Marker," *Faraday Discuss. Chem. Soc.* **53**, 211 (1972).
- 72 NIK/MORI Niki, H., Morris, E. D., Jr., and Breitenbach, L. P., "Reaction of OH with H₂S," *Am. Chem. Soc. 164th Meeting (Abstracts of Papers)* **164**, PHYS-116 (1972).
- 72 ROM/SCH Rommel, H., and Schiff, H. I., "The Reactions of H Atoms with H₂S and COS," *Int. J. Chem. Kinet.* **4**, 547 (1972).
- 72 WOR/COL Worley, S. D., Coltharp, R. N., and Potter, A. E., Jr., "Rates of Interaction of Vibrationally Excited Hydroxyl (v = 9) with Diatomic and Small Polyatomic Molecules," *J. Phys. Chem.* **76**, 511 (1972).

1973

- 73 BRA/TRU Bradley, J. N., Trueman, S. P., Whytock, D. A., and Zaleski, T. A., "Electron Spin Resonance Study of the Reaction of Hydrogen Atoms with Hydrogen Sulphide," *J. Chem. Soc. Faraday Trans. I* **69**, 416 (1973).
- 73 CEH/HEI Gehelnik, E., Heicklen, J., Braslavsky, S., Stockburger, L., and Mathias, E., "Photolysis of SO₂ in the Presence of Foreign Gases IV. Wavelength and Temperature Effects with CO," *J. Photochem.* **2**, 31 (1973).
- 73 DAV/KLE Davis, D. D., and Klemm, R. B., "A Flash Photolysis-Resonance Fluorescence Kinetics Study of the Reactions of Ground-State Sulfur Atoms. V. Rate Parameters for the Reaction of S(¹P) with cis-2-Butene and Tetramethylethylene," *Int. J. Chem. Kinet.* **5**, 841 (1973).
- 73 JAM/KER James, F. C., Kerr, J. A., and Simons, J. P., "Direct Measurement of the Rate of Reaction of the Methyl Radical with Sulphur Dioxide," *J. Chem. Soc. Faraday Trans. I* **69**, 2124 (1973).
- 73 KLE/DAV1 Klemm, R. B., and Davis, D. D., "A Flash Photolysis Resonance Fluorescence Kinetics Study of Ground-State Sulfur Atoms. III. Rate Parameters for Reaction of S(³P) with Ethylene Episulfide," *Int. J. Chem. Kinet.* **5**, 149 (1973).

- 73 KLE/DAV2 Klemm, R. B., and Davis, D. D., "A Flash Photolysis-Resonance Fluorescence Kinetics Study of Ground-State Sulfur Atoms. IV. Rate Parameters for Reaction of $S(^1P)$ with Propene and 1-Butene," *Int. J. Chem. Kinet.* **5**, 375 (1973).
- 73 LAN/OLD Langford, R. B., and Oldershaw, G. A., "Mechanism of Sulfur Formation in the Flash Photolysis of Carbonyl Sulphide," *J. Chem. Soc. Faraday Trans. 1* **69**, 1389 (1973).
- 73 PAY/STI Payne, W. A., Stief, L. J., and Davis, D. D., "A Kinetics Study of the Reaction of HO_2 with SO_2 and NO ," *J. Am. Chem. Soc.* **95**, 7614 (1973).
- 73 SCH Schofield, K., "Evaluated Chemical Kinetic Rate Constants for Various Gas Phase Reactions," *J. Phys. Chem. Ref. Data* **2**, 25 (1973).
- 73 WES/DEB3 Westenberg, A. A., and DeHaas, N., "Rate of the Reaction $OH + H_2S \rightarrow SH + H_2O$ over an Extended Temperature Range," *J. Chem. Phys.* **59**, 6685 (1973).
- 74 ATK/PIT3 Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction of $O(^1P)$ Atoms with $SO_2(M=N_2O)$ Over the Temperature Range 299–392 K," *Chem. Phys. Lett.* **29**, 28 (1974).
- 74 CAD/WIC Cadle, R. D., Wickman, H. H., Hall, C. B., and Eberle, K. M., "The Reaction of Atomic Oxygen with Formaldehyde, Crotonaldehyde, and Dimethyl Sulfide," *Chemosphere* **3**, 115 (1974).
- 74 COX2 Cox, R. A., "The Photolysis of Nitrous Acid in the Presence of Carbon Monoxide and Sulphur Dioxide," *J. Photochem.* **3**, 291 (1974).
- 74 DAV/PRU Davis, D. D., Prusazcyk, J., Dwyer, M., and Kim, P., "A Stop-Flow Time-of-Flight Mass Spectrometry Kinetics Study. Reaction of Ozone with Nitrogen Dioxide and Sulfur Dioxide," *J. Phys. Chem.* **78**, 1775 (1974).
- 74 DEM/CAL Demerjian, K. L., Calvert, J. G., and Thorsell, D. L., "A Kinetic Study of the Chemistry of the $SO_2(^1B_1)$ Reactions with *cis*- and *trans*-2-Butene," *Int. J. Chem. Kinet.* **6**, 829 (1974).
- 74 KAL/BRA Kaldor, A., Braun, W., and Kurylo, M. J., "Infrared Laser Enhanced Reactions: $O_1 + SO$," *J. Chem. Phys.* **61**, 2396 (1974).
- 74 KLE/DAV Klemm, R. B., and Davis, D. D., "A Flash Photolysis-Resonance Fluorescence Kinetics Study of the Reaction $S(^1P) + OCS$," *J. Phys. Chem.* **78**, 1137 (1974).
- 74 KLE/STI Klemm, R. B., and Stief, L. J., "Absolute Rate Parameters for the Reaction of Ground State Atomic Oxygen with Carbonyl Sulfide," *J. Chem. Phys.* **61**, 4900 (1974).
- 74 LLO Lloyd, A. C., "Evaluated and Estimated Kinetic Data for Gas Phase Reactions of the Hydroperoxyl Radical," *Int. J. Chem. Kinet.* **6**, 169–228 (1974).
- 74 SLA/GIL Slagle, I. R., Gilbert, J. R., and Gutman, D., "Kinetics of the Reaction Between Oxygen Atoms and Carbon Disulfide," *J. Chem. Phys.* **61**, 704 (1974).
- 74 STE/ALV Stedman, D. H., Alvord, H., and Baker-Blocker, A., "Chemiluminescent Reactions of Disulfur Monoxide," *J. Phys. Chem.* **78**, 1248 (1974).
- 74 STU Stuhl, F., "Determination of the Rate Constant for the Reaction $OH + H_2S$ by a Pulsed Photolysis-Resonance Fluorescence Method," *Ber. Bunsenges. Phys. Chem.* **78**, 230 (1974).
- 74 TRA Trafton, W. E., Jr., "High Temperature Gas Phase Kinetic Studies of Carbonyl Sulfide, Nitrous Oxide, and Carbon Disulfide in a Shock Tube with Boundary Layer Corrections," *Diss. Abstr. Int. B* **34**, 5935 (1974).
- 75 BEC/INO Becker, K. H., Inocencio, M. A., and Schurath, U., "The Reaction of Ozone with Hydrogen Sulfide and Its Organic Derivatives," *Int. J. Chem. Kinet.* **7** (Symp. 1), 205 (1975).
- 75 BEN/GOL Benson, S. W., Golden, D. M., Lawrence, R. W., Shaw, R., and Woolfolk, R. W., Estimating the Kinetics of Combustion Including Reactions Involving Oxides of Nitrogen and Sulfur," Environmental Protection Agency Report No. EPA-600/2-75-019, August 1975.
- 75 CAS/DAV Castleman, A. W., Jr., Davis, R. E., Munkelwitz, H. R., Tang, I. N., and Wood, W. P., "Kinetics of Association Reactions Pertaining to H_2SO_4 Aerosol Formation," *Int. J. Chem. Kinet.* **7** (Symp. 1), 629 (1975).
- 75 CHU/CAL Chung, K., Calvert, J. G., and Bottenhelm, J. W., "The Photochemistry of Sulfur Dioxide Excited within Its First Allowed Band (3130 Å) and the "Forbidden" Band (3700–4000 Å)," *Int. J. Chem. Kinet.* **7**, 161 (1975).
- 75 CLY/TOW Glyne, M. A. A., and Townsend, L. W., "Rate Constant Measurements for Rapid Reactions of Ground State Sulphur $3p(^1P)$ Atoms," *Int. J. Chem. Kinet.* **7** (Symp. 1), 73 (1975).
- 75 CUP/GLA Cùpitt, L. T., and Glass, G. P., "Reactions of SH with Atomic Oxygen and Hydrogen," *Int. J. Chem. Kinet.* **7** (Symp. 1), 39 (1975).
- 75 DAU/CAL Daubendiek, R. L., and Calvert, J. G., "A Study of the N_2O_5 - SO_2 - O_3 Reaction System," *Environ. Lett.* **8**, 103 (1975).
- 75 GAU/SAE Gauthier, M. J. E., and Snelling, D. R., "La Photolyse de L'ozone a 253.7 nm: Desactivation de $O(^1D)$ et de $O_2(^1\Sigma)$ par Les Gas de L'atmosphere," *J. Photochem.* **4**, 27 (1975).
- 75 GLA/TOB1 Glavas, S., and Tohy, S., "The Reaction Between Ozone and Hydrogen Sulfide: Kinetics and Effect of Added Gases," *Am. Chem. Soc. ACS Symp. Ser.* **17**, 122 (1975).
- 75 GLA/TOB2 Glavas, S., and Toby, S., "Reaction Between Ozone and Hydrogen Sulfide," *J. Phys. Chem.* **79**, 779 (1975).
- 75 GOR/MUL1 Gordon, S., and Mulac, W. A., "Reaction of the $OH(X^2II)$ Radical Produced by the Pulse Radiolysis of Water Vapor," *Int. J. Chem. Kinet.* (Symp. 1), 289 (1975).
- 75 HAR/WAY Harris, G. W., and Wayne, R. P., "Reaction of Hydroxyl Radicals with NO , NO_2 and SO_2 ," *J. Chem. Soc. Faraday Trans. 1* **71**, 610 (1975).
- 75 KIE Kiefer, J. H., "Densitometric Measurements of the Rate of Sulfur Dioxide Dissociation in Shock Waves," *J. Chem. Phys.* **62**, 1354 (1975).
- 75 SLA/GRA1 Slagle, I. R., Graham, R. E., Gilbert, J. R., and Gutman, D., "Direct Atoms with Carbon Monosulphide," *Chem. Phys. Lett.* **32**, 184 (1975).
- 75 TSU/YOK Tsunashima, S., Yokota, T., Saferik, I., Gunning, H. E., Strausz, O. P., "Abstraction of Sulfur Atoms from Carbonyl Sulfide by Atomic Hydrogen," *J. Phys. Chem.* **79**, 775 (1975).
- 75 WEI/TIM Wei, C.-N., and Timmons, R. B., "ESR Study of the Kinetics of the Reactions of $O(^1P)$ Atoms with CS_2 and OCS ," *J. Chem. Phys.* **62**, 3240 (1975).
- 75 WES/DEH1 Westenberg, A. A., and DeHaas, N., "Rate of the $O + SO_2$ Reaction," *J. Chem. Phys.* **62**, 725 (1975).
- 75 WES/DEH2 Westenberg, A. A., and DeHaas, N., "Rate of the Reaction $O + SO_2 + M \rightarrow SO_3 + M$," *J. Chem. Phys.* **63**, 5411 (1975).
- 75 YOK/AHM Yokota, T., Ahmed, M. G., Saferik, I., Strausz, O. P., and Gunning, H. E., "Reaction of Hydrogen Atoms with Thiirane," *J. Phys. Chem.* **79**, 1758 (1975).
- 76 ART/LEE Arthur, N. L., and Lee, M.-S., "Reactions of Methyl Radicals. I. Hydrogen Abstraction from Dimethyl Sulphide," *Aust. J. Chem.* **29**, 1483 (1976).

- 76 ATK/PER3 Atkinson, R., Perry, R. A., and Pitts, J. N., Jr., "Rate Constants for the Reactions of the OH Radical with $\text{NO}_2(\text{M}=\text{Ar and N}_2)$ and $\text{SO}_2(\text{M}=\text{Ar})$," *J. Chem. Phys.* **65**, 306 (1976).
- 76 BAL/DRY Baulch, D. L., Drysdale, D. D., and Horne, D. G., "Evaluated Kinetic Data for High Temperature Reactions, Vol. 2: Homogeneous Gas Phase Reactions of the $\text{O}_2\text{-O}_3$ System, the $\text{CO-O}_2\text{-H}_2$ System, and Sulphur-Containing Species," (Butterworths, London, 1976).
- 76 BID/BRE Bida, G. T., Breckenridge, W. H., and Kolin, W. S., "A Kinetic Study of the Very Fast Reaction: $\text{O}(\text{P}) + \text{CS} \rightarrow \text{CO} + \text{S}(\text{P})$," *J. Chem. Phys.* **64**, 3296 (1976).
- 76 DUM Dumas, J. L., "Etude de la Reactivite Chimique de l'oxygene singulet produit en Phase Gazeuse. I. Etudes en Phase Homogene," *Bull. Soc. Chim. France*, 658 (1976).
- 76 HIG/SAI Higashihara, R., Saito, Ko., and Yamamura, H., " S_2 Formation During the Pyrolysis of H_2S in Shock Waves," *Bull. Chem. Soc. Jpn.* **40**, 965 (1976).
- 76 KER/PAR Kerr, J. A., and Parsonage, J. J., "Evaluated Kinetic Data on Gas Phase Hydrogen Transfer Reactions of Methyl Radicals," (Butterworths, London 1976).
- 76 LEE Lee, J. H., "Gas Phase Kinetic Study of Some Simple Atom-Molecule Reactions Using Fast Flow and Flash Photolysis-Resonance Fluorescence Techniques," *Diss. Abstr. Int. B* **36**, 6192 (1976).
- 76 LEE/TIM Lee, J. H., Timmons, R. B., and Stief, L. J., "Absolute Rate Parameters for the Reaction of Ground State Atomic Oxygen with Dimethyl Sulfide and Episulfide," *J. Chem. Phys.* **64**, 300 (1976).
- 76 MAN/BRA Manning, R. G., Braun, W., and Kurylo, M. J., "The Effect of Infrared Laser Excitation on Reaction Dynamics: $\text{O} + \text{C}_2\text{H}_4$ and $\text{O} + \text{OCS}$," *J. Chem. Phys.* **65**, 2609 (1976).
- 76 MAR/BAR Martin, G., and Barroeta, N., "Gas-phase Thermolysis of Sulphur Compounds. Part I. Di-t-butyl Disulphide," *J. Chem. Soc. Perkin Trans.* **2**, 1421 (1976).
- 76 PER/ATK1 Perry, R. A., Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction $\text{OH} + \text{H}_2\text{S} \rightarrow \text{H}_2\text{O} + \text{SH}$ and $\text{OH} + \text{NH}_3 \rightarrow \text{H}_2\text{O} + \text{NH}_2$ Over the Temperature Range 297-427°K," *J. Chem. Phys.* **64**, 3237 (1976).
- 76 SLA/GRA Slagle, I. R., Graham, R. E., and Gutman, D., "Direct Identification of Reactive Routes and Measurement of Rate Constants in the Reactions of Oxygen Atoms with Methanethiol, Ethanethiol, and Methylsulfide," *Int. J. Chem. Kinet.* **8**, 451 (1976).
- 76 WAM Wampler, F. B., "Photochemistry of the SO_2 , 2-Pentene System at 3660 Å," *Int. J. Chem. Kinet.* **8**, 935 (1976).
- 76 WHY/TIM Whytock, D. A., Timmons, R. B., Lee, J. H., Michael, J. V., Payne, W. A., and Stief, L. J., "Absolute Rate of the Reaction of $\text{O}(\text{P})$ with Hydrogen Sulfide Over the Temperature Range 263 to 495 K," *J. Chem. Phys.* **65**, 2052 (1976).
- 1977
- 77 BOW/DOD Bowman, C. T., and Dodge, L. G., "Kinetics of the Thermal Decomposition of Hydrogen Sulfide Behind Shock Waves," *Symp. (Int.) Combust. (Proc.)* **16**, 1976 (Publ. 1977) 971.
- 77 CAS/TAN Castleman, A. W., Jr., and Tang, I. N., "Kinetics of the Association Reaction of SO_2 with the Hydroxyl Radical," *J. Photochem.* **6**, 349 (1977).
- 77 FRE/PAL Freund, H., and Palmer, H. B., "Shock-Tube Studies of the Reactions of NO_2 with NO_2 , SO_2 , and CO ," *Int. J. Chem. Kinet.* **9**, 887 (1977).
- 77 GRA/GUT Graham, R. E., and Gutman, D., "Temperature Dependence of Rate Constants and Branching Ratios for the Reaction of Oxygen Atoms with Carbon Disulfide," *J. Phys. Chem.* **81**, 207 (1977).
- 77 LEE/STI Lee, J. H., Stief, L. J., and Timmons, R. B., "Absolute Rate Parameters for the Reaction of Atomic Hydrogen with Carbonyl Sulfide and Ethylene Episulfide," *J. Chem. Phys.* **67**, 1705 (1977).
- 77 LIL/RIC Lilienfeld, H. V., and Richardson, R. J., "Temperature Dependence of the Rate Constant for the Reaction Between Carbon Monosulfide and Atomic Oxygen," *J. Chem. Phys.* **67**, 3991 (1977).
- 1978
- 78 ALA/BIG Al-Awadi, N., Bigley, D. B., and Gabbott, R. E., "The Gas-phase Pyrolysis of Dithioacetates: A Remarkable Constancy of Substituent Effects," *J. Chem. Soc. Perkin Trans. II*, 1223 (1978).
- 78 AST/GLA Astholz, D. C., Glaenger, K., and Troe, J., "UV Absorption Study of the Thermal Decomposition of SO , SO_2 , and SO_3 ," *Shock Tube Wave Res., Proc. Int. Symp.* **11**, 1977 (Publ. 1978) 232.
- 78 ATK/PER1 Atkinson, R., Perry, R. A., and Pitts, J. N., Jr., "Rate Constants for the Reaction of OH Radicals with COS , CS_2 and CH_3SCH_3 Over the Temperature Range 299-430 K," *Chem. Phys. Lett.* **54**, 14 (1978).
- 78 ATK/PIT4 Atkinson, R., and Pitts, J. N., Jr., "Kinetics of the Reaction $\text{O}(\text{P}) + \text{SO}_2 + \text{M} \rightarrow \text{SO}_3 + \text{M}$ Over the Temperature Range of 299-440°K," *Int. J. Chem. Kinet.* **10**, 1081 (1978).
- 78 HOR/VIS Horie, O., Nishino, J., and Amano, A., "The Reaction of Hydrogen Atoms with 1-Butanethiol and Thiolane: The Role of Chemically Activated 1-Butanethiol," *Int. J. Chem. Kinet.* **10**, 1043 (1978).
- 78 IWA/PRE Iwamoto, K., Presser, N., and Ross, J., "Kinetics of Aerosol Formation in Irradiated Gaseous $\text{NO}_2\text{-SO}_2$ Mixtures," *J. Chem. Phys.* **68**, 663 (1978).
- 78 JUS/RIU Just, T., and Rimpel, G., "The Thermal Decomposition of SO_2 Between 2500 and 3400°K," *Shock Tube Wave Res., Proc. Int. Symp.* **11**, 1977 (Publ. 1978) 226.
- 78 KIR/VET Kirchner, K., Vettermann, R., and Indruch, H., "Kinetics of the Reactions of Mercaptans with $\text{O}(\text{P})$ Under Consideration of the Influence of Molecular Oxygen," *Ber. Bunsenges. Phys. Chem.* **82**, 1223 (1978).
- 78 KOL Kollin, W. S., "Gas Phase Reactions of Carbon Monosulfide Studied by the Fast Flow Technique," *Diss. Abstr. Int. B* **39**, 771 (1978).
- 78 KUR1 Kurylo, M. J., "Flash Photolysis Resonance Fluorescence Investigation of the Reaction of OH Radicals with Dimethyl Sulfide," *Chem. Phys. Lett.* **58**, 233 (1978).
- 78 KUR2 Kurylo, M. J., "Flash Photolysis Resonance Fluorescence Investigation of the Reactions of OH Radicals with OCS and CS_2 ," *Chem. Phys. Lett.* **58**, 238 (1978).
- 78 MAR/HER Martinez, R. I., and Herron, J. T., "Stopped-Flow Study of the Gas-Phase Reaction of Ozone with Organic Sulfide: Dimethyl Sulfide," *Int. J. Chem. Kinet.* **10**, 433 (1978).
- 78 MAR/REI Marvin, D. C., and Reiss, H., "Cloud Chamber Study of the Gas Phase Photooxidation of Sulfur Dioxide," *J. Chem. Phys.* **69**, 1897 (1978).
- 78 PAR/HEI Partymiller, K., and Heicklen, J., "The Photolysis of Sulfur Dioxide in the Presence of Foreign Gases XII: Photolysis of SO_2 at 313.0 nm in the Presence of Both Allene and Oxygen," *J. Photochem.* **8**, 167 (1978).
- 78 SLA/BAL Slagle, I. R., Balocchi, F., and Gutman, D., "Study of the Reactions of Oxygen Atoms with Hydrogen Sulfide, Methanethiol, Ethanethiol, and Methyl Sulfide," *J. Phys. Chem.* **82**, 1333 (1978).
- 78 SU/CAL Su, F., and Calvert, J. G., "The Mechanism of the Photochemical Reactions of SO_2 with Isobutane Excited," *Int. J. Chem. Kinet.* **10**, 557 (1978).
- 78 VAN/OBI Van Roodselaar, A., Obi, K., and Strausz, O. P., "The Reaction of $\text{S}(\text{P})$ Atoms with Nitric Oxide," *Int. J. Chem. Kinet.* **10**, 31 (1978).

- 78 VAN/SAF Van Roodselaar, A., Safarik, I., Strausz, O. P., and Gunning, H. E., "The Reactions of Sulfur Atoms. 15. Absolute Rate Parameters for the $S(^3P_{2,1,0}) + \text{Alkyne Reactions}$," *J. Am. Chem. Soc.* **100**, 4068 (1978).
- 78 WHY/TIM Whytock, D. A., and Timmons, R. B., "Absolute Rate of the Reaction of $O(^1P)$ with Hydrogen Sulphide," *Nat. Bur. Stand. Spec. Pub.* 526, 339 (1978).
- 78 YOS/SAI Yoshida, N., and Saito, S., "Application of Microwave Spectroscopy to Kinetic Study of Carbonyl Sulfide with Atomic Oxygen," *Bull. Chem. Soc. Jpn.* **51**, 1635 (1978).
- 1979
- 79 ADD/BYR Addison, M. C., Byrne, C. D., and Donovan, R. J., "Direct Observation of $S(^3D_2)$ and Determination of the Absolute Rate of Reaction with OCS ," *Chem. Phys. Lett.* **64**, 57 (1979).
- 79 ADD/LEI Addison, M. C., Leitch, A. J., Fotakis, C., and Donovan, R. J., "Reactions of $CH(X^2\Sigma^+)$ with OCS and Formation of SCN ," *J. Photochem.* **10**, 273 (1979).
- 79 ALA/BIG Al-Awadi, N., and Bigley, D. B., "Carbonate Pyrolysis. Part 5. The Gas-Phase Pyrolysis of Some Unsymmetrical Monothioicarbonates and a Rationalisation of the Rates of Some Related Reactions," *J. Chem. Soc. Perkin Trans. II*, 497, (1979).
- 79 AST/GLA Astholz, D. C., Glanzer, K., and Troe, J., "The Spin-Forbidden Dissociation-Recombination Reaction $SO_2 \rightleftharpoons SO_2 + O$," *J. Chem. Phys.* **70**, 2409 (1979).
- 79 BUR/CLI Burrows, J. P., Cliff, D. I., Harris, G. W., Thrush, B. A., and Wilkinson, J. P. T., "Atmospheric Reactions of the HO_2 Radical Studied by Laser Magnetic Resonance Spectroscopy," *Proc. R. Soc. London A* **368**, 463 (1979).
- 79 CLY/WHI Clyne, M. A., and Whitefield, P. D., "Atomic Resonance Fluorescence for Rate Constants of Rapid Bimolecular Reactions," *J. Chem. Soc. Faraday Trans. II* **75**, 1327 (1979).
- 79 DAV/RAV Davis, D. D., Ravishankara, A. R., and Fischer, S., " SO_2 Oxidation via the Hydroxyl Radical: Atmospheric Fate of HSO_2 Radicals," *Geophys. Res. Lett.* **6**, 113 (1979).
- 79 GRA/WIN Graham, R. A., Winer, A. M., Atkinson, R., and Pitts, J. N., Jr., "Rate Constants for the Reaction of HO_2 with HO_2 , SO_2 , CO , N_2O , trans-2-Butene, and 2,3-Dimethyl-2-Butene at 300 K," *J. Phys. Chem.* **83**, 1563 (1979).
- 79 GRI/REE Grillo, A., Reed, E., and Slack, M. W., "Infrared Measurements of Sulfur Dioxide Thermal Decomposition Rate in Shock Waves," *J. Chem. Phys.* **70**, 1634 (1979).
- 79 HSU/SHA Hsu, D. S. Y., Shaub, W. M., Burks, T. L., and Lin, M. C., "Dynamics of Reactions of $O(^1P)$ Atoms with CS , CS_2 and OCS ," *Chem. Phys.* **44**, 143 (1979).
- 79 JOU/LEB Jourdain, J. L., Le Bras, G., and Combourieu, J., "Kinetic Study of Some Elementary Reactions of Sulfur Compounds Including Reactions of S and SO with OH Radicals," *Int. J. Chem. Kinet.* **11**, 569 (1979).
- 79 KAN/MCQ Kan, C. S., McQuigg, R. D., Whitbeck, M. R., and Calvert, J. G., "Kinetic Flash Spectroscopic Study of the $CH_3O_2-CH_3O_2$ and $CH_3O_2-SO_2$ Reactions," *Int. J. Chem. Kinet.* **11**, 921 (1979).
- 79 MER/LEV Merryman, E. L., and Levy, A., "Enhanced SO_2 Emissions from Staged Combustion," *Symp. (Int.) Combust. (Proc.)*, **17**, (Publ. 1979) 727.
- 79 NIC/AMO Nicholas, J. E., Amodio, C. A., and Baker, M. J., "Kinetics and Mechanism of the Decomposition of H_2S , CH_3SH and $(CH_3)_2S$ in a Radio-Frequency Pulse Discharge," *J. Chem. Soc. Faraday Trans. I* **75**, 1868 (1979).
- 79 SAN/SIM Sanhueza, E., Simonaitis, R., and Heicklen, J., "The Reaction of CH_3O_2 with SO_2 ," *Int. J. Chem. Kinet.* **11**, 907 (1979).
- 79 SHE/SAF Sherwood, A. G., Safarik, I., Verkoczy, B., Almadi, G., Wiehe, H. A., and Strausz, O. P., "Unimolecular Isomerization of Chemically Activated Thiirane to Vinylthiol," *J. Am. Chem. Soc.* **101**, 3000 (1979).
- 79 SIM/HEI Simonaitis, R., and Heicklen, J., "The Mechanism of SO_2 Oxidation by CH_3O_2 Radicals. Rate Coefficients for the Reactions of CH_3O_2 with SO_2 and NO ," *Chem. Phys. Lett.* **65**, 361 (1979).
- 79 SIN/IRW Singleton, D. L., Irwin, R. S., Nip, W. S., and Cvetanovic, R. J., "Kinetics and Mechanism of the Reaction of Oxygen Atoms with Hydrogen Sulfide," *J. Phys. Chem.* **83**, 2195 (1979).
- 79 YOK/STR Yokota, T., and Strausz, O. P., "Reaction of Hydrogen Atoms with Dimethyl Sulfide," *J. Phys. Chem.* **83**, 3196 (1979).
- 1980
- 80 ADD/DON Addison, M. C., Donovan, R. J., and Fotakis, C., "Resonance Fluorescence Study of Electronically Excited Sulfur Atoms: Reactions of $S(^3D_2)$," *Chem. Phys. Lett.* **74**, 58 (1980).
- 80 BAU/COX Baulch, D. L., Cox, R. A., Hampson, R. F., Jr., Kerr, J. A., Troe, J., and Watson, R. T., "Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry," *J. Phys. Chem. Ref. Data* **9**, 295 (1980).
- 80 CLY/MAC Clyne, M. A. A., and Macrobert, A. J., "Kinetic Studies of Free Radical Reactions by Mass Spectrometry. I. The Reactions of $SO + NO_2$ and $ClO + NO$," *Int. J. Chem. Kinet.* **12**, 79 (1980).
- 80 COX/SHE Cox, R. A., and Sheppard, D., "Reactions of OH Radicals with Gaseous Sulphur Compounds," *Nature (London)* **284**, 330 (1980).
- 80 EKW/JOD Ekwenki, M. M., Jodhan, A., and Strausz, O. P., "Reaction of Hydrogen Atoms with Dimethyldisulfide," *Int. J. Chem. Kinet.* **12**, 431 (1980).
- 80 GRI/REE Grillo, A., Reed, R., and Slack, M. W., "Thermal Decomposition of SO_2 Monitored by IR Emission," *Shock Tubes Waves, Proc. Int. Symp.*, 12th, 1979 (Publ. 1980) 486.
- 80 HAR/ATK Harris, G. W., Atkinson, R., and Pitts, J. N., Jr., "Temperature Dependence of the Reaction $OH + SO_2 + M = HSO_2 + M = Ar$ and SF_6 ," *Chem. Phys. Lett.* **69**, 378 (1980).
- 80 HER/HUI Herron, J. T., and Huie, R. E., "Rate Constants at 298 K for the Reactions $SO + SO + M \rightarrow (SO)_2 + M$ and $SO + (SO)_2 \rightarrow SO_2 + S_2O$," *Chem. Phys. Lett.* **76**, 322 (1980).
- 80 HIG/SAI Higashihara, T., Saito, K., and Murakami, I., "The Dissociation Rate of S_2 Produced from COS Pyrolysis," *Bull. Chem. Soc. Jpn.* **53**, 15 (1980).
- 80 HUS/SLA Husain, D., and Slater, N. K. H., "Kinetic Study of the Reactions of Hydrogen and Deuterium Atoms with Hydrogen Bromide and Deuterium Bromide by Time-Resolved Resonance Fluorescence," *J. Chem. Soc. Faraday Trans. 2* **76**, 276 (1980).
- 80 IYE/ROW Iyer, R. W., and Rowland, F. S., "A Significant Upper Limit for the Rate of Formation and OCS from the Reaction of OH with CS_2 ," *Geophys. Res. Lett.* **7**, 797 (1980).
- 80 LEE/TANI Lee, J. H., Tang, I. N., and Klemm, R. B., "Absolute Rate Constant for the Reaction of $O(^1P)$ with CH_3SCH_3 from 272 to 472 K," *J. Chem. Phys.* **72**, 1793 (1980).
- 80 LEE/TAN2 Lee, J. H., and Tang, I. N., "Absolute Rate Constant for the Reaction of $O(^1P)$ with CH_3SSCH_3 from 270 to 329 K," *J. Chem. Phys.* **72**, 5718 (1980).
- 80 MAR/BAR Martin, G., and Barroeta, N., "Gas Phase Thermolysis of Sulfur Compounds. II. Diteriary Butyl Sulfide," *Int. J. Chem. Kinet.* **12**, 699 (1980).
- 80 MAR/HER Martinez, R. L., and Herron, J. T., "Stopped-Flow Study of the Gas-Phase Reactions of Ozone with Organic Sulfides: Thiirane," *Chem. Phys. Lett.* **72**, 74 (1980).

- 80 ROB/SMI Robertshaw, J. H., and Smith, I. W. M., "Rate Data for $O + OCS \rightarrow SO + CO$ and $SO + O_2 \rightarrow SO_2 + O_2$ by a New Time Resolved Technique," *Int. J. Chem. Kinet.* **12**, 729 (1980).
- 80 SAI/TOR Saito, K., Toriyama, Y., Yokubo, T., Higashihara, R., and Murakami, I., "A Measurement of the Thermal Decomposition of CS_2 Behind Reflected Shock Waves," *Bull. Chem. Soc. Jpn.* **53**, 1437 (1980).
- 80 SAI/YOK Saito, K., Yokubo, T., and Murakami, I., "On the Thermal Decomposition of SO_2 Diluted in Ar Behind Reflected Shock Waves," *J. Chem. Phys.* **73**, 3017 (1980).
- 80 SLA/GRI Slack, M., and Grillo, A., "Rate Coefficient Measurements for $SO_2 + O = SO + O_2$," *J. Chem. Phys.* **73**, 967 (1980).
- 80 TYA/BAB Tyaga Raju, M., Babu, S. V., and Subba Rao, V., "Dissociation Rate Measurements in $SO_2 + Ar$ Mixtures Behind Incident Shock Waves," *Chem. Phys.* **43**, 411 (1980).
- 80 WIN/SHA Wine, P. H., Shah, R. C., and Ravishankara, A. R., "Rate of Reaction of OH with CS_2 ," *J. Phys. Chem.* **84**, 2499 (1980).
- 80 YOK/STR Yokota, T., and Strausz, O. P., "Reaction of Hydrogen Atoms with Dimethyl Sulfide," *J. Phys. Chem.* **83**, 3196 (1980).

Appendix: Conversion Tables

Equivalent second order rate constants

A \ B	$\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$\text{m}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$(\text{mm Hg})^{-1} \text{ s}^{-1}$	$\text{atm}^{-1} \text{ s}^{-1}$	$\text{ppm}^{-1} \text{ min}^{-1}$	$\text{m}^2 \text{ kN}^{-1} \text{ s}^{-1}$
$1 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1} =$	1	10^{-3}	10^{-6}	1.66×10^{-24}	$1.604 \times 10^{-5} T^{-1}$	$1.219 \times 10^{-2} T^{-1}$	2.453×10^{-9}	$1.203 \times 10^{-4} T^{-1}$
$1 \text{ dm}^3 \text{ mol}^{-1} \text{ s}^{-1} =$	10^3	1	10^{-3}	1.66×10^{-21}	$1.604 \times 10^{-2} T^{-1}$	$12.19 T^{-1}$	2.453×10^{-6}	$1.203 \times 10^{-1} T^{-1}$
$1 \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1} =$	10^6	10^3	1	1.66×10^{-18}	$16.04 T^{-1}$	$1.219 \times 10^4 T^{-1}$	2.453×10^{-3}	$120.3 T^{-1}$
$1 \text{ cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} =$	6.023×10^{23}	6.023×10^{20}	6.023×10^{17}	1	$9.658 \times 10^{18} T^{-1}$	$7.34 \times 10^{21} T^{-1}$	1.478×10^{15}	$7.244 \times 10^{19} T^{-1}$
$1 (\text{mm Hg})^{-1} \text{ s}^{-1} =$	$6.236 \times 10^4 T$	$62.36 T$	$6.236 \times 10^{-2} T$	$1.035 \times 10^{-19} T$	1	760	4.56×10^{-2}	7.500
$1 \text{ atm}^{-1} \text{ s}^{-1} =$	$82.06 T$	$8.206 \times 10^{-2} T$	$8.206 \times 10^{-5} T$	$1.362 \times 10^{-22} T$	1.316×10^{-3}	1	6×10^{-5}	9.869×10^{-3}
$1 \text{ ppm}^{-1} \text{ min}^{-1} =$ 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
$1 \text{ m}^2 \text{ kN}^{-1} \text{ s}^{-1} =$	$8314 T$	$8.314 T$	$8.314 \times 10^{-3} T$	$1.38 \times 10^{-20} T$	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 $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to $\text{m}^3 \text{ mol}^{-1} \text{ s}^{-1}$ multiply by 6.023×10^{17} .

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

Equivalent third order rate constants

A \ B	$\text{cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$	$\text{dm}^6 \text{ mol}^{-2} \text{ s}^{-1}$	$\text{m}^6 \text{ mol}^{-2} \text{ s}^{-1}$	$\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$	$(\text{mm Hg})^{-2} \text{ s}^{-1}$	$\text{atm}^{-2} \text{ s}^{-1}$	$\text{ppm}^{-2} \text{ min}^{-1}$	$\text{m}^4 \text{ kN}^{-2} \text{ s}^{-1}$
$1 \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1} =$	1	10^{-6}	10^{-12}	2.76×10^{-46}	$2.57 \times 10^{-10} T^{-2}$	$1.48 \times 10^{-4} T^{-2}$	1.003×10^{-19}	$1.447 \times 10^{-6} T^{-2}$
$1 \text{ dm}^6 \text{ mol}^{-2} \text{ s}^{-1} =$	10^6	1	10^{-6}	2.76×10^{-42}	$2.57 \times 10^{-4} T^{-2}$	$148 T^{-2}$	1.003×10^{-13}	$1.447 \times 10^{-2} T^{-2}$
$1 \text{ m}^6 \text{ mol}^{-2} \text{ s}^{-1} =$	10^{12}	10^6	1	2.76×10^{-36}	$257 T^{-2}$	$1.48 \times 10^8 T^{-2}$	1.003×10^{-7}	$1.447 \times 10^4 T^{-2}$
$1 \text{ cm}^6 \text{ molecule}^{-2} \text{ s}^{-1} =$	3.628×10^{47}	3.628×10^{41}	3.628×10^{35}	1	$9.328 \times 10^{37} T^{-2}$	$5.388 \times 10^{43} T^{-2}$	3.64×10^{26}	$5.248 \times 10^{39} T^{-2}$
$1 (\text{mm Hg})^{-2} \text{ s}^{-1} =$	$3.89 \times 10^9 T^2$	$3.89 \times 10^3 T^2$	$3.89 \times 10^{-3} T^2$	$1.07 \times 10^{-38} T^2$	1	5.776×10^5	3.46×10^{-5}	56.25
$1 \text{ atm}^{-2} \text{ s}^{-1} =$	$6.733 \times 10^3 T^2$	$6.733 \times 10^{-3} T^2$	$6.733 \times 10^{-9} T^2$	$1.86 \times 10^{-44} T^2$	1.73×10^{-6}	1	6×10^{-11}	9.74×10^{-5}
$1 \text{ ppm}^{-2} \text{ min}^{-1} =$ 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
$1 \text{ m}^4 \text{ kN}^{-2} \text{ s}^{-1} =$	$6.91 \times 10^7 T^2$	$69.1 T^2$	$6.91 \times 10^{-5} T^2$	$1.904 \times 10^{-40} T^2$	0.0178	1.027×10^4	6.16×10^{-7}	1

See note to table for second order rate constants.

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions)	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 (If joint or other than NBS, see instructions) 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 (Street, City, State, ZIP) Morgantown Energy Technology Center and Office of Standard Reference Data Department of Energy National Bureau of Standards Morgantown, WV 26505 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 (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here) A table of 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 (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons) Arrhenius parameters; chemical kinetics; combustion; decomposition; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur			
13. AVAILABILITY <input checked="" type="checkbox"/> Unlimited <input type="checkbox"/> For Official Distribution. Do Not Release to NTIS <input type="checkbox"/> Order From Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. <input checked="" type="checkbox"/> Order From National Technical Information Service (NTIS), Springfield, VA. 22161			14. NO. OF PRINTED PAGES 42 15. Price

**Announcement of New Publications in
National Standard Reference Data Series**

Superintendent of Documents,
Government Printing Office,
Washington, D.C. 20402

Please add my name to the announcement list of new publications to be issued
in the series: National Standard Reference Data Series—National Bureau of
Standards.

Name_____

Company_____

Address_____

City_____State_____Zip Code_____

(Notification Key N-519)

NBS TECHNICAL PUBLICATIONS

PERIODICALS

JOURNAL OF RESEARCH—The Journal of Research of the National Bureau of Standards reports NBS research and development in those disciplines of the physical and engineering sciences in which the Bureau is active. These include physics, chemistry, engineering, mathematics, and computer sciences. Papers cover a broad range of subjects, with major emphasis on measurement methodology and the basic technology underlying standardization. Also included from time to time are survey articles on topics closely related to the Bureau's technical and scientific programs. As a special service to subscribers each issue contains complete citations to all recent Bureau publications in both NBS and non-NBS media. Issued six times a year. Annual subscription: domestic \$18; foreign \$22.50. Single copy, \$4.25 domestic; \$5.35 foreign.

NONPERIODICALS

Monographs—Major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

Handbooks—Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

Special Publications—Include proceedings of conferences sponsored by NBS, NBS annual reports, and other special publications appropriate to this grouping such as wall charts, pocket cards, and bibliographies.

Applied Mathematics Series—Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers, and others engaged in scientific and technical work.

National Standard Reference Data Series—Provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a worldwide program coordinated by NBS under the authority of the National Standard Data Act (Public Law 90-396).

NOTE: The principal publication outlet for the foregoing data is the Journal of Physical and Chemical Reference Data (JPCRD) published quarterly for NBS by the American Chemical Society (ACS) and the American Institute of Physics (AIP). Subscriptions, reprints, and supplements available from ACS, 1155 Sixteenth St., NW, Washington, DC 20056.

Building Science Series—Disseminates technical information developed at the Bureau on building materials, components, systems, and whole structures. The series presents research results, test methods, and performance criteria related to the structural and environmental functions and the durability and safety characteristics of building elements and systems.

Technical Notes—Studies or reports which are complete in themselves but restrictive in their treatment of a subject. Analogous to monographs but not so comprehensive in scope or definitive in treatment of the subject area. Often serve as a vehicle for final reports of work performed at NBS under the sponsorship of other government agencies.

Voluntary Product Standards—Developed under procedures published by the Department of Commerce in Part 10, Title 15, of the Code of Federal Regulations. The standards establish nationally recognized requirements for products, and provide all concerned interests with a basis for common understanding of the characteristics of the products. NBS administers this program as a supplement to the activities of the private sector standardizing organizations.

Consumer Information Series—Practical information, based on NBS research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

Order the above NBS publications from: Superintendent of Documents, Government Printing Office, Washington, DC 20402.

Order the following NBS publications—FIPS and NBSIR's—from the National Technical Information Services, Springfield, VA 22161.

Federal Information Processing Standards Publications (FIPS PUB)—Publications in this series collectively constitute the Federal Information Processing Standards Register. The Register serves as the official source of information in the Federal Government regarding standards issued by NBS pursuant to the Federal Property and Administrative Services Act of 1949 as amended, Public Law 89-306 (79 Stat. 1127), and as implemented by Executive Order 11717 (38 FR 12315, dated May 11, 1973) and Part 6 of Title 15 CFR (Code of Federal Regulations).

NBS Interagency Reports (NBSIR)—A special series of interim or final reports on work performed by NBS for outside sponsors (both government and non-government). In general, initial distribution is handled by the sponsor; public distribution is by the National Technical Information Services, Springfield, VA 22161, in paper copy or microfiche form.

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
Washington, DC 20234

POSTAGE AND FEES PAID
U.S. DEPARTMENT OF COMMERCE
COM-215



OFFICIAL BUSINESS

Penalty for Private Use, \$300

THIRD CLASS
