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SOLUBILITY DATA SERIES

Volume 12

SULFUR DIOXIDE, CHLORINE, FLUORINE AND CHLORINE OXIDES

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES



Volume 12

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SULFUR DIOXIDE, CHLORINE, FLUORINE AND CHLORINE OXIDES

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FOREWORD

If the knowledge is undigested or simply wrong, more is not better.

How to communicate and disseminate numerical data effectively in chemical science and technology has been a problem of serious and growing concern to IUPAC, the International Union of Pure and Applied Chemistry, for the last two decades. The steadily expanding volume of numerical information, the formulation of new interdisciplinary areas in which chemistry is a partner, and the links between these and existing traditional subdisciplines in chemistry, along with an increasing number of users, have been considered as urgent aspects of the information problem in general, and of the numerical data problem in particular.

Among the several numerical data projects initiated and operated by various IUPAC commissions, the Solubility Data Project is probably one of the most ambitious ones. It is concerned with preparing a comprehensive critical compilation of data on solubilities in all physical systems, of gases, liquids and solids. Both the basic and applied branches of almost all scientific disciplines require a knowledge of solubilities as a function of solvent, temperature and pressure. Solubility data are basic to the fundamental understanding of processes relevant to agronomy, biology, chemistry, geology and oceanography, medicine and pharmacology, and metallurgy and materials science. Knowledge of solubility is very frequently of great importance to such diverse practical applications as drug dosage and drug solubility in biological fluids, anesthesiology, corrosion by dissolution of metals, properties of glasses, ceramics, concretes and coatings, phase relations in the formation of minerals and alloys, the deposits of minerals and radioactive fission products from ocean waters, the composition of ground waters, and the requirements of oxygen and other gases in life support systems.

The widespread relevance of solubility data to many branches and disciplines of science, medicine, technology and engineering, and the difficulty of recovering solubility data from the literature, lead to the proliferation of published data in an ever increasing number of scientific and technical primary sources. The sheer volume of data has overcome the capacity of the classical secondary and tertiary services to respond effectively.

While the proportion of secondary services of the review article type is generally increasing due to the rapid growth of all forms of primary literature, the review articles become more limited in scope, more specialized. The disturbing phenomenon is that in some disciplines, certainly in chemistry, authors are reluctant to treat even those limited-in-scope reviews exhaustively. There is a trend to preselect the literature, sometimes under the pretext of reducing it to manageable size. The crucial problem with such preselection - as far as numerical data are concerned - is that there is no indication as to whether the material was excluded by design or by a less than thorough literature search. We are equally concerned that most current secondary sources, critical in character as they may be, give scant attention to numerical data.

On the other hand, tertiary sources - handbooks, reference books, and other tabulated and graphical compilations - as they exist today, are comprehensive but, as a rule, uncritical. They usually attempt to cover whole disciplines, thus obviously are superficial in treatment. Since they command a wide market, we believe that their service to advancement of science is at least questionable. Additionally, the change which is taking place in the generation of new and diversified numerical data, and the rate at which this is done, is not reflected in an increased third-level service. The emergence of new tertiary literature sources does not parallel the shift that has occurred in the primary literature.

With the status of current secondary and tertiary services being as briefly stated above, the innovative approach of the Solubility Data Project is that its compilation and critical evaluation work involve consolidation and reprocessing services when both activities are based on intellectual and scholarly reworking of information from primary sources.

It comprises compact compilation, rationalization and simplification, and the fitting of isolated numerical data into a critically evaluated general framework.

The Solubility Data Project has developed a mechanism which involves a number of innovations in exploiting the literature fully, and which contains new elements of a more imaginative approach for transfer of reliable information from primary to secondary/tertiary sources. The fundamental trend of the Solubility Data Project is toward integration of secondary and tertiary services with the objective of producing in-depth critical analysis and evaluation which are characteristic to secondary services, in a scope as broad as conventional tertiary services.

Fundamental to the philosophy of the project is the recognition that the basic element of strength is the active participation of career scientists in it. Consolidating primary data, producing a truly critically-evaluated set of numerical data, and synthesizing data in a meaningful relationship are demands considered worthy of the efforts of top Career scientists, who themselves contribute to science by scientists. their involvement in active scientific research, are the backbone of the The scholarly work is commissioned to recognized authorities, project. involving a process of careful selection in the best tradition of IUPAC. This selection in turn is the key to the quality of the output. These top experts are expected to view their specific topics dispassionately, paying equal attention to their own contributions and to those of their peers. They digest literature data into a coherent story by weeding out what is wrong from what is believed to be right. To fulfill this task, the evaluator must cover all relevant open literature. No reference is excluded by design and every effort is made to detect every bit of relevant primary source. Poor quality or wrong data are mentioned and explicitly disqualified as such. In fact, it is only when the reliable data are presented alongside the unreliable data that proper justice can The user is bound to have incomparably more confidence in a succinct evaluative commentary and a comprehensive review with a complete bibliography to both good and poor data.

It is the standard practice that any given solute-solvent system consists of two essential parts: I. Critical Evaluation and Recommended Values, and II. Compiled Data Sheets.

The Critical Evaluation part gives the following information:

- (i) a verbal text of evaluation which discusses the numerical solubility information appearing in the primary sources located in the literature. The evaluation text concerns primarily the quality of data after consideration of the purity of the materials and their characterization, the experimental method employed and the uncertainties in control of physical parameters, the reproducibility of the data, the agreement of the worker's results on accepted test systems with standard values, and finally the fitting of data, with suitable statistical tests, to mathematical functions;
- (ii) a set of recommended numerical data. Whenever possible, the set of recommended data includes weighted average and standard deviations, and a set of smoothing equations derived from the experimental data endorsed by the evaluator;
 - (iii) a graphical plot of recommended data.

The compilation part consists of data sheets of the best experimental data in the primary literature. Generally speaking, such independent data sheets are given only to the best and endorsed data covering the known range of experimental parameters. Data sheets based on primary sources where the data are of a lower precision are given only when no better data are available. Experimental data with a precision poorer than considered acceptable are reproduced in the form of data sheets when they are the only known data for a particular system. Such data are considered to be still suitable for some applications, and their presence in the compilation should alert researchers to areas that need more work.

The typical data sheet carries the following information:

(i) components - definition of the system - their names, formulas and Chemical Abstracts registry numbers; Foreword ix

(ii) reference to the primary source where the numerical information is reported. In cases when the primary source is a less common periodical or a report document, published though of limited availability, abstract references are also given;

- (iii) experimental variables;
- (iv) identification of the compiler;
- (v) experimental values as they appear in the primary source. Whenever available, the data may be given both in tabular and graphical form. If auxiliary information is available, the experimental data are converted also to SI units by the compiler.

Under the general heading of Auxiliary Information, the essential experimental details are summarized:

- (vi) experimental method used for the generation of data;
- (vii) type of apparatus and procedure employed;
- (viii) source and purity of materials;
- (ix) estimated error;
- (x) references relevant to the generation of experimental data as cited in the primary source.

This new approach to numerical data presentation, developed during our four years of existence, has been strongly influenced by the diversity of background of those whom we are supposed to serve. We thus deemed it right to preface the evaluation/compilation sheets in each volume with a detailed discussion of the principles of the accurate determination of relevant solubility data and related thermodynamic information.

Finally, the role of education is more than corollary to the efforts we are seeking. The scientific standards advocated here are necessary to strengthen science and technology, and should be regarded as a major effort in the training and formation of the next generation of scientists and engineers. Specifically, we believe that there is going to be an impact of our project on scientific-communication practices. of consolidation adopted by this program offers down-to-earth guidelines, concrete examples which are bound to make primary publication services more responsive than ever before to the needs of users. The selfregulatory message to scientists of 15 years ago to refrain from unnecessary publication has not achieved much. The literature is still, in 1982, cluttered with poor-quality articles. The Weinberg report (in "Reader in Science Information", Eds. J. Sherrof and A. Hodina, Microcard Editions Books, Indian Head, Ins., 1973, p.292) states that "admonition to authors to restrain themselves from premature, unnecessary publication can have little effect unless the climate of the entire technical and scholarly community encourages restraint..." We think that projects of this kind translate the climate into operational terms by exerting presentations. We think that projects of sure on authors to avoid submitting low-grade material. The type of our output, we hope, will encourage attention to quality as authors will increasingly realize that their work will not be suited for permanent retrievability unless it meets the standards adopted in this project. should help to dispel confusion in the minds of many authors of what represents a permanently useful bit of information of an archival value, and what does not.

If we succeed in that aim, even partially, we have then done our share in protecting the scientific community from unwanted and irrelevant, wrong numerical information.

A. S. Kertes

PREFACE

This volume is concerned with the solubility of sulfur dioxide, chlorine, fluorine and the oxides of chlorine in pureliquids, liquid mixtures, aqueous solutions and miscellaneous fluids and fluid mixtures. The solubility in molten salts, slags, glasses, metals, alloys and polymeric material have been specifically excluded from this volume. There is always a problem in attempting to distinguish between gas solubilities and vapor-liquid equilibria and this problem is particularly troublesome in the case of sulfur dioxide solubilities. There is no absolute distinction between gas solubility and vapor-liquid equilibria. We have been fairly liberal in making the distinction and have included systems which some might classify as vapor-liquid equilibrium. The literature has been searched up until the middle of 1981. The editor or Professor H. L. Clever, Director, Solubility Data Center, Department of Chemistry, Emory University, Atlanta, Georgia USA would appreciate being notified of any omissions or more recent data.

Unlike most of the previous volumes in this series concerned with the solubility of gases in liquids, this volume deals with gases which react with the solvent in several cases. We have not attempted to evaluate equilibrium constants for reactions which take place in solution because the available data are not of sufficient quality or quantity to make a meaningful evaluation of such constants. Despite the industrial importance of both sulfur dioxide and chlorine, the solubility of these gases in most solvents is not known to better than a few per cent. Much of the data were obtained several decades ago and much of the data in this volume is barely accurate enough for modern applications.

In many cases meaningful evaluation of the solubility data has not been possible due to a lack of comparable data. Furthermore, in many cases it is not clear how the quoted solubilities have been calculated from the experimental results. Earlier in this series, Hayduk, in the preface to the ethane volume, made a plea for inclusion of all pertinent data used in the calculation of gas solubility in all future (original) publications and stated that in some instances compilers and evaluators have had to guess which data were used by the authors in their calculation of solubility. A similar plea and statement are relevant to this volume.

In several tables compilers have calculated solubilities not given in the original paper. In most cases the source of additional data needed for such calculations is given in the compiled table. The tables given by Riddick and Bunger in *Technique of Chemistry*, ed. Weissberger, A. Vol. II, Wiley-Interscience, New York, 1970, 3rd Ed. have been used but not specifically referenced in compiled tables.

The Editor acknowledges the advice and helpful suggestions of the members of the IUPAC Commission V8 on Solubility Data. Acknowledgement is also made to the University of Melbourne for travel support under the travel for research and special studies program. Finally, the Editor acknowledges the help of Lesley Flanagan who typed the major part of this volume.

Colin Young

Melbourne, December 1982.

THE SOLUBILITY OF GASES AND LIQUIDS

Introductory Information

C. L. Young, R. Battino, and H. L. Clever

INTRODUCTION

The Solubility Data Project aims to make a comprehensive search of the literature for data on the solubility of gases, liquids and solids in liquids. Data of suitable accuracy are compiled into data sheets set out in a uniform format. The data for each system are evaluated and where data of sufficient accuracy are available values are recommended and in some cases a smoothing equation is given to represent the variation of solubility with pressure and/or temperature. A text giving an evaluation and recommended values and the compiled data sheets are published on consecutive pages. The following paper by E. Wilhelm gives a rigorous thermodynamic treatment on the solubility of gases in liquids.

DEFINITION OF GAS SOLUBILITY

The distinction between vapor-liquid equilibria and the solubility of gases in liquids is arbitrary. It is generally accepted that the equilibrium set up at 300K between a typical gas such as argon and a liquid such as water is gas-liquid solubility whereas the equilibrium set up between hexane and cyclohexane at 350K is an example of vapor-liquid equilibrium. However, the distinction between gas-liquid solubility and vapor-liquid equilibrium is often not so clear. The equilibria set up between methane and propane above the critical temperature of methane and below the critical temperature of propane may be classed as vapor-liquid equilibrium or as gas-liquid solubility depending on the particular range of pressure considered and the particular worker concerned.

The difficulty partly stems from our inability to rigorously distinguish between a gas, a vapor, and a liquid; a subject which has been discussed in numerous textbooks. We have taken a fairly liberal view in these volumes and have included systems which may be regarded, by some workers, as vapor-liquid equilibria.

UNITS AND QUANTITIES

The solubility of gases in liquids is of interest to a wide range of scientific and technological disciplines and not solely to chemistry. Therefore a variety of ways for reporting gas solubility have been used in the primary literature. Sometimes, because of insufficient available information, it has been necessary to use several quantities in the compiled tables. Where possible, the gas solubility has been quoted as a mole fraction of the gaseous component in the liquid phase. The units of pressure used are bar, pascal, millimeters of mercury, and atmosphere. Temperatures are reported in Kelvins.

EVALUATION AND COMPILATION

The solubility of comparatively few systems is known with sufficient accuracy to enable a set of recommended values to be presented. This is true both of the measurements near atmospheric pressure and at high pressures. Although a considerable number of systems have been studied by at least two workers, the range of pressures and/or temperatures is often sufficiently different to make meaningful comparison impossible.

Occasionally, it is not clear why two groups of workers obtained very different sets of results at the same temperature and pressure, although both sets of results were obtained by reliable methods and are internally consistent. In such cases, sometimes an incorrect assessment has been given. There are several examples where two or more sets of data have been classified as tentative although the sets are mutually inconsistent.

Many high pressure solubility data have been published in a smoothed form. Such data are particularly difficult to evaluate, and unless specifically discussed by the authors, the estimated error on such values can only be regarded as an "informed guess".

Many of the high pressure solubility data have been obtained in a more general study of high pressure vapor-liquid equilibrium. In such cases a note is included to indicate that additional vapor-liquid equilibrium data are given in the source. Since the evaluation is for the compiled data, it is possible that the solubility data are given a classification which is better than that which would be given for the complete vapor-liquid data (or vice versa). For example, it is difficult to determine coexisting liquid and vapor compositions near the critical point of a mixture using some widely used experimental techniques which yield accurate high pressure solubility data. As another example, conventional methods of analysis may give results with an expected error which would be regarded as sufficiently small for vapor-liquid equilibrium data but an order of magnitude too large for acceptable high pressure qas-liquid solubility.

It is occasionally possible to evaluate data on mixtures of a given substance with a member of a homologous series by considering all the available data for the given substance with other members of the homologous series. In this study the use of such a technique has been limited.

The estimated error is often omitted in the original article and sometimes the errors quoted do not cover all the variables. In order to increase the usefulness of the compiled tables estimated errors have been included even when absent from the original article. If the error on any variable has been inserted by the compiler, this has been noted.

PURITY OF MATERIALS

The purity of materials has been quoted in the compiled tables where given in the original publication. The solubility is usually more sensitive to impurities in the gaseous component than to liquid impurities in the liquid component. However, the most important impurities are traces of a gas dissolved in the liquid. Inadequate degassing of the absorbing liquid is probably the most often overlooked serious source of error in gas solubility measurements.

APPARATUS AND PROCEDURES

In the compiled tables brief mention is made of the apparatus and procedure. There are several reviews on experimental methods of determining gas solubilities and these are given in References 1-7.

METHODS OF EXPRESSING GAS SOLUBILITIES

Because gas solubilities are important for many different scientific and engineering problems, they have been expressed in a great many ways:

The Mole Fraction, x(g)

The mole fraction solubility for a binary system is given by:

$$x(g) = \underbrace{n(g)}_{n(g) + n(1)}$$

$$= \frac{W(g)/M(g)}{\{W(g)/M(g)\} + \{W(1)/M(1)\}}$$

here n is the number of moles of a substance (an <code>amount</code> of substance), W is the mass of a substance, and M is the molecular mass. To be unambiguous, the partial pressure of the gas (or the total pressure) and the temperature of measurement must be specified.

The Weight Per Cent Solubility, wt%

For a binary system this is given by

$$wt% = 100 W(g)/{W(g) + W(1)}$$

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where W is the weight of substance. As in the case of mole fraction, the pressure (partial or total) and the temperature must be specified. The weight per cent solubility is related to the mole fraction solubility by

$$x(g) = \frac{\{wt\%/M(g)\}}{\{wt\%/M(g)\} + \{(100 - wt\%)/M(1)\}}$$

The Weight Solubility, $\mathbf{C}_{\mathbf{W}}$

The weight solubility is the number of moles of dissolved gas per gram of solvent when the partial pressure of gas is 1 atmosphere. The weight solubility is related to the mole fraction solubility at one atmosphere partial pressure by $C_{M(1)}$

$$x(g)$$
 (partial pressure 1 atm) = $\frac{w}{1 + C_{t,M}(1)}$

where M(1) is the molecular weight of the solvent.

The Moles Per Unit Volume Solubility, n

Often for multicomponent systems the density of the liquid mixture is not known and the solubility is quoted as moles of gas per unit volume of liquid mixture. This is related to the mole fraction solubility by

$$x(g) = \frac{n v^{O}(1)}{1 + n v^{O}(1)}$$

where vo(1) is the molar volume of the liquid component.

The Bunsen Coefficient, a

The Bunsen coefficient is defined as the volume of gas reduced to 273.15K and 1 atmosphere pressure which is absorbed by unit volume of solvent (at the temperature of measurement) under a partial pressure of 1 atmosphere. If ideal gas behavior and Henry's law are assumed to be obeyed, then

$$\alpha = \frac{V(g)}{V(1)} \quad \frac{273.15}{T}$$

where V(g) is the volume of gas absorbed and V(l) is the original (starting) volume of absorbing solvent. The mole fraction solubility x is related to the Bunsen coefficient by

$$x(g, 1 \text{ atm}) = \frac{\alpha}{\alpha + \frac{273.15}{T} \frac{v^{O}(g)}{v^{O}(1)}}$$

where $v^{O}(g)$ and $v^{O}(l)$ are the molar volumes of gas and solvent at a pressure of one atmosphere. If the gas is ideal,

$$x(g) = \frac{\alpha}{\alpha + \frac{273.15R}{v^{0}(1)}}$$

Real gases do not follow the ideal gas law and it is important to establish the real gas law used for calculating α in the original publication and to make the necessary adjustments when calculating the mole fraction solubility.

The Kuenen Coefficient, S

This is the volume of gas, reduced to 273.15K and 1 atmosphere pressure, dissolved at a partial pressure of gas of 1 atmosphere by 1 gram of solvent.

The Ostwald Coefficient, L

The Ostwald coefficient, L, is defined as the ratio of the volume of gas absorbed to the volume of the absorbing liquid, all measured at the same temperature:

$$L = \frac{V(g)}{V(1)}$$

If the gas is ideal and Henry's Law is applicable, the Ostwald coefficient is independent of the partial pressure of the gas. It is necessary, in practice, to state the temperature and total pressure for which the Ostwald coefficient is measured. The mole fraction solubility, x(g), is related to the Ostwald coefficient by

$$x(g) = \begin{bmatrix} \frac{RT}{P(g) L v^{O}(1)} + 1 \end{bmatrix}^{-1}$$

where P is the partial pressure of gas. The mole fraction solubility will be at a partial pressure of P(g). (See the following paper by E. Wilhelm for a more igorous definition of the Ostwald coefficient.)

The Absorption Coefficient, B

There are several "absorption coefficients", the most commonly used one being defined as the volume of gas, reduced to 273.15K and 1 atmosphere, absorbed per unit volume of liquid when the total pressure is 1 atmosphere. β is related to the Bunsen coefficient by

$$\beta = \alpha(1 - P(1))$$

where P(1) is the partial pressure of the liquid in atmospheres.

The Henry's Law Constant

A generally used formulation of Henry's Law may be expressed as

$$P(g) = K_{H}x(g)$$

where $K_{\mbox{\scriptsize H}}$ is the Henry's Law constant and x(g) the mole fraction solubility. Other formulations are

$$P(g) = K_2C(1)$$
 or $C(g) = K_2C(1)$

where K_2 and K_c are constants, C the concentration, and (1) and (g) refer to the liquid and gas phases. Unfortunately, K_H , K_2 and K_c are all sometimes referred to as Henry's Law constants. Henry's Law is a *limiting law* but can sometimes be used for converting solubility data from the experimental pressure to a partial gas pressure of 1 atmosphere, provided the mole fraction of the gas in the liquid is small, and that the difference in pressures is small. Great caution must be exercised in using Henry's Law.

The Mole Ratio, N

The mole ratio, N, is defined by

$$N = n(g)/n(1)$$

Table 1 contains a presentation of the most commonly used inter-conversions not already discussed.

For gas solubilities greater than about 0.01 mole fraciton at a partial pressure of 1 atmosphere there are several additional factors which must be taken into account to unambiguously report gas solubilities. Solution densities or the partial molar volume of gases must be known. Corrections should be made for the possible non-ideality of the gas or the non-applicability of Henry's Law.

Introduction

TABLE 1 Interconversion of parameters used for reporting solubility

L =
$$\alpha(T/273.15)$$

 $C_W = \alpha/v_0\rho$
 $K_H = \frac{17.033 \times 10^6 \rho(soln)}{\alpha M(1)} + 760$
L = $C_W v_{t,gas}^{\rho}$

where v_o is the molal volume of the gas in cm 3 mol $^{-1}$ at 0°C, ρ the density of the solvent at the temperature of the measurement, ρ_{soln} the density of the solution at the temperature of the measurement, and $v_{t,gas}$ the molal volume of the gas (cm 3 mol $^{-1}$) at the temperature of the measurement.

SALT EFFECTS

Salt effect studies have been carried out for many years. The results are often reported as Sechenov (Setchenow) salt effect parameters. There appears to be no common agreement on the units of either the gas solubility, or the electrolyte concentration.

Many of the older papers report the salt effect parameter in a form equivalent to

$$k_{SCC}/mol \ dm^{-3} = (1/(c_2/mol \ dm^{-3})) \log ((c_1^o/mol \ dm^{-3})/(c_1/mol \ dm^{-3}))$$

where the molar gas solubility ratio, c_1°/c_1 , is identical to the Bunsen coefficient ratio, α°/α , or the Ostwald coefficient ratio, L°/L . One can designate the salt effect parameters calculated from the three gas solubility ratios as k_{SCC} , $k_{\text{SC}\alpha}$, k_{SCL} , respectively, but they are identical, and $k_{\text{SCC}}/\text{dm}^3$ mol⁻¹ describes all of them. The superzero refers to the solubility in the pure solvent.

Recent statistical mechanical theories favor a molal measure of the electrolyte and gas solubility. Some of the more recent salt effects are reported in the form

$$k_{smm}/kg \text{ mol}^{-1} = (1/(m_2/mol kg^{-1}) log ((m_1/mol kg^{-1})/(m_1/mol kg^{-1}))$$

In this equation the m_1°/m_1 ratio is identical to the Kuenen coefficient ratio, $\delta_1^{\circ}/\delta_1$, or the solvomolality ratio referenced to water, $A_{\delta m}^{\circ}/A_{\delta m}$. Thus the salt effect parameters $k_{\rm smm}$, $k_{\rm sms}$, and $k_{\rm sm}$ are well represented by the $k_{\rm smm}/k_{\rm g}$ mol⁻¹.

Some experimentalists and theoreticians prefer the gas solubility ratio as a mole fraction ratio, x_1^ρ/x_1 . It appears that most calculate the mole fraction on the basis of the total number of ions. The salt effect parameters

$$k_{SCX}/dm^3 \text{ mol}^{-1} = (1/(c_2/\text{mol dm}^{-3})) \log (x_1^o/x_1)$$

and

$$k_{smx}/kg \text{ mol}^{-1} = (1/(m_2/\text{mol kg}^{-1})) \log (x_1^0/x_1)$$

are both in the literature, but $k_{\scriptsize \texttt{SCX}}$ appears to be the more common.

The following conversions were worked out among the various forms of the salt effect parameter from standard definitions of molarity, molality, and mole fraction assuming the gas solubilities are small.

$$\begin{aligned} & k_{\text{SMC}} = (c_2/m_2) \ k_{\text{SCC}} = (c_2/m_2) \ k_{\text{SCM}} + F_{1m} \\ & k_{\text{SCM}} = k_{\text{SCC}} - F_{1c} = (m_2/c_2) \ k_{\text{SMC}} - F_{1c} = (m_2/c_2) \ \kappa_{\text{SMM}} \\ & k_{\text{SCX}} = (m_2/c_2) \ k_{\text{SMX}} = (m_2/c_2) \ k_{\text{SMM}} + F_{2c} \\ & k_{\text{SMM}} = k_{\text{SMX}} - F_{2m} = (c_2/m_2) \ k_{\text{SCX}} - F_{2m} \\ & k_{\text{SMX}} = (c_2/m_2) \ k_{\text{SCX}} = (c_2/m_2) \ k_{\text{SCC}} + F_{3m} \\ & k_{\text{SCC}} = k_{\text{SCX}} - F_{3c} = (m_2/c_2) \ k_{\text{SMX}} - F_{3c} \end{aligned}$$

$$\end{aligned}$$

$$F_{1m} = (1/m_2) \log [(\rho^{\circ}/\rho) (1000 + m_2M_2)/1000]$$

$$F_{1c} = (m_2/c_2) F_{1m}$$

$$F_{gm} = (1/m_2) \log [(1000 + vm_3 M_3)/1000]$$

$$F_{2c} = (m_2/c_2) F_{2m}$$

$$F_{3m} = (1/m_2) \log [(1000p + (vM_3-M_2) c_2)/1000p^\circ)$$

$$F_{3c} = (m_2/c_2) F_{3m}$$

The factors F_{1m} , F_{1c} , F_{2m} , F_{2c} , F_{3m} , and F_{3c} can easily be calculated from aqueous electrolyte data such as weight per cent and density as found in Volume III of the International Critical Tables. The values are small and change nearly linearly with both temperature and molality. The factors normally amount to no more than 10 to 20 per cent of the value of the salt effect parameter.

The symbols in the equations above are defined below:

Component	Molar Concentration c/mol dm ⁻³	Molal Concentration m/mol kg ⁻¹	Mole Fraction x	Molecular Weight M/g mol ⁻¹
Nonelectrol	yte c ₁ , c ₁	m ₁ , m ₁	x_1°, x_1	м ₁
Electrolyte	c ₂	^m 2	× ₂	M ₂
Solvent	c ₃	^m 3	x 3	М3

The superscript "°" refers to the nonelectrolyte solubility in the pure solvent. The pure solvent and solution densities are $\rho\,^\circ/g$ cm and ρ/g cm , respectively. They should be the densities of gas saturated solvent (water) and salt solution, but the gas free densities will differ negligibly in the $\rho\,^\circ/\rho$ ratio. The number of ions per formula of electrolyte is symbolized by ν .

The following table gives estimated errors in $k_{\rm SCC}$ for various salt concentrations and a range of random errors in the gas solubility measurement $\frac{1}{2} (2m^3 + 1)^{-1}$

nol dm ⁻³	Random	Error in	gas solub	ility Measu	rement
nol dm	±2	±1%	±0.5%	±0.1%	±0.05%
1	±18%	±9%	±5%	±1.5%	±] %
0.1	±175%	±87 ዬ	±43%	±9 ቄ	±4%
0.05	±350%	±174%	±87%	±17%	±9 %
0.01	±1750%	±870%	±435%	±87%	±43%

 $^{^{\}mathrm{a}}$ Based on a $\mathrm{k}_{\mathtt{scc}}$ value of 0.100.

AQUAMOLAL OR SOLVOMOLAL, Asm or m(s)

The term aquamolal was suggested by R. E. Kerwin (9). The unit was first used in connection with $\rm D_2O$ and $\rm H_2O$ + $\rm D_2O$ mixtures. It has since been extended in use to other solvents. The unit represents the numbers of moles of solute per 55.51 moles of solvent. It is represented by

 $m_{i}^{\{\delta\}}/\text{mol kg}^{-1} = (n_{1}M_{2}/w_{2})(w_{2}/M_{o}) = m_{i}(M_{2}/M_{o})$ where an amount of n_{i} of solute i is dissolved in a mass w_{2} of solvent of molar mass M_{2} ; M_{o} is the molar mass of a reference solvent and $m_{i}/\text{mol kg}^{-1}$ is the conventional molality in the reference solvent. The reference solvent is normally water.

TEMPERATURE DEPENDENCE OF GAS SOLUBILITY

In a few cases it has been found possible to fit the mole fraction solubility at various temperatures using an equation of the form

$$\ln x = A + B / (T/100K) + C \ln (T/100K) + DT/100K$$

It is then possible to write the thermodynamic functions $\Delta \overline{G}_1^{\circ}$, $\Delta \overline{H}_1^{\circ}$, $\Delta \overline{S}_1^{\circ}$ and $\Delta \overline{C}_p$ for the transfer of the gas from the vapor phase at 1

101,325 Pa partial pressure to the (hypothetical) solution phase of unit mole fraction as:

$$\Delta \overline{G}_1^{\circ} = -RAT - 100 RB - RCT ln (T/100) - RDT^2/100$$

$$\Delta \overline{S}_{1}^{\circ} = RA + RC \ln (T/100) + RC + 2 RDT/100$$

$$\Delta \overline{H}_{1}^{o} = -100 \text{ RB} + \text{RCT} + \text{RDT}^{2}/100$$

$$\Delta \overline{C}_{p_1}^{\circ} = RC + 2 RDT/100$$

In cases where there are solubilities at only a few temperatures it is convenient to use the simpler equations

$$\Delta \overline{G}_1^{\circ} = -RT \ln x = A + BT$$

in which case $A = \Delta \overline{H}_1^{\circ}$ and $-B = \Delta \overline{S}_1^{\circ}$

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Revised: April 1982 (R.B., H.L.C.)

- Sulfur dioxide; SO₂; [7446-09-5]
- Miscellaneous compounds of similar volatility to sulfur dioxide.

EVALUATOR:

March 1982

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

EVALUATION:

In general measurements generally referred to as vapor-liquid equilibrium determinations are not considered in the Solubility Data Series since it is necessary to limit the scope of the mixtures considered. Many studies of mixtures containing sulfur dioxide, which has a boiling point of 263 K are usually classified as vapor-liquid equilibrium determinations rather than gas solubility measurements.

Below is a list of systems which have been excluded from the compilation on the grounds that

- (a) the experimental method was such that it was only suitable if both components were of similar volatility;
- (b) the data were presented only in graphical form;
- (c) the vapor pressure of the two pure components did not vary by a factor greater than three at the temperature of the measurements.

The list, which includes vapor-liquid equilibrium determinations, is given so that the user of this volume can refer to the original article if further information is required.

Solvent			Reference
1,2,3-Trichloropropane 1,2-Dichloropropane Tetrachloromethane Trichloromethane Trichloromethane Trichloromethane Tetrachloroethene 1,1,2-Trichloroethene 1,1-Dichloroethene 1,1-Dichloroethene 1,1,2-Trichloroethane 1,1,2-Trichloroethane 1,1,2-Trichloroethane 1,1,1-Trichloroethane 1,1-Dichloroethane 1,2-Dichloroethane 1-Chloropentane 1-Chloropentane 1-Chlorohexane	C3H5Cl3 C3H6Cl2 CCCl4 CCCl4 CCCl4 C2HCl3 C2HC2Cl2 C2HC2 C3HC2 C	[156-59-2]	l 1 1,2 1,6 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
Hydrogen fluoride Benzenamine (Aniline)	HF C ₆ H ₇ N	[7664-39-3] [62-53-3]	7 8

(cont.)

- Sulfur dioxide; SO₂; [7446-09-5]
- Miscellaneous compounds of similar volatility to sulfur dioxide.

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia. March 1982

In addition to the above systems the work of Komissarov et al. (9) have not been compiled. These workers studied the system sulfur dioxide + oxygen + tetradecane. It is, however, not clear as to what conditions the reported numerical data refer.

References

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Water

3

COMPONENTS:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]

EVALUATOR:

Rubin Battino, Department of Chemistry, Wright State University, Dayton, Ohio 45435, U.S.A. July 1981

CRITICAL EVALUATION:

For this critical evaluation of the solubility of sulfur dioxide in water at around atmospheric pressure, we examined the literature from 1855 until the present. Surprisingly, the earliest work (1) (that of Schönfeld as reported by Bunsen in several papers) is very close to the best modern values — in the middle of the temperature range studied (273-313 K). These early results are within 2-4 per cent of the values to be recommended in this section.

Reactive gases like sulfur dioxide pose a special problem with respect to gas solubilities. $SO_2(g)$ is in equilibrium (at saturation) with $SO_2(aq)$, but the $SO_2(aq)$ is also in equilibrium with other species in solution. The solubilities reported here as mole fractions at 101.325 kPa partial pressure of gas are <u>bulk</u> solubilities, i.e., they are taken as if all of the SO_2 -containing species in solution were simply $SO_2(aq)$. There are many papers dealing with the remaining ionization and equilibrium constants.

Many of the measurements made on sulfur dioxide solubilities were carried out at different partial pressures. Due to the high solubilities (mole fractions at 101.325 kPa partial pressure of gas of 0.003 to 0.06) exhibited by this system and the chemical interactions involved, the system does not obey Henry's law even over relatively small extrapolations. We limited our interpolations to within about 13 kPa either side of 101.325 kPa.

Of the more modern determinations we judged the work of four workers to be sufficiently reliable to use for smoothing via least squares analysis. Individual data points which were more than about two standard deviations from the smoothed values were rejected. Thus, 24 points were used for the final smoothing and were obtained as follows (reference — number of data points used from that reference): 2-10, 3-8, 4-1, 5-5. The best fit for the 24 points is

 $\ln x_1 = -25.26286 + 45.75521/(T/100K) + 5.685450 \ln (T/100K)$

where x_1 is the mole fraction solubility at 101.325 kPa partial pressure of gas. The standard deviation in x_1 was 1.7 × 10⁻⁴ or about ±1.8 per cent at the mid-range of 283 to 380 K. The following table gives the recommended smoothed values of the mole fraction and the Ostwald coefficient at 5 K intervals calculated from the above equation. (Thermodynamic properties are not presented – due to the complexity of the aqueous solution. They would be meaningless.)

T/K	x_1^a	r_p	T/K	$10^2 x_1^a$	$^{\mathtt{L}^{\mathtt{b}}}$
278.15	0.0499	66.6	333.15	9.22	13.9
283.15	0.0413	55.6	338.15	8.19	12.5
288.15	0.0345	46.9	343.15	7.31	11.3
293.15	0.0290	39.8	348.15	6.55	10.2
298.15	0.0246	34.1	353.15	5.90	9.27
303.15	0.0210	29.5	358.15	5.33	8.47
308.15	0.0180	25.6	363.15	4.84	7.76
313.15	0.0156	22.4	368.15	4.41	7.14
318.15	0.0136	19.7	373.15	4.03	6.59
323.15	0.0119	19.7	378.15	3.70	6.10
328.15	0.0104	15.5	383.15	3.40	5.66

^a Mole fraction solubility at 101.325 kPa partial pressure of gas.

b Ostwald coefficient. (cont.)

- 1. Sulfur dioxide; SO₂;
 [7446-09-5]
- 2. Water; H₂O; [7732-18-5]

EVALUATOR:

Rubin Battino, Department of Chemistry, Wright State University, Dayton, Ohio 45435, U.S.A. July 1981

CRITICAL EVALUATION:

The results of several workers were not used in the smoothing process. Bunsen/Schönfeld's early measurements (1) were surprisingly good at the middle of their temperature range of 273 to 313 K but differed strongly at the extremes. Sims' early work (6) ranged 4-5 per cent high and low. Fox's two values (7) were high and very high. Lindner's values (8) were all at lower pressures. Baume and Tykociner's values at three temperatures (9) were very high when interpolated to 101.325 kPa. Smith and Parkhurst's results (10) were erratically low and high. Öman's results (11) were very low at all temperatures he investigated (313-368 K). The interpolated Maass and Maass results (12) were over 10 per cent low. The interpolated Morgan and Maass (13) results were also quite low (4-7 per cent). The extrapolared value for Conrad and Beuschlein (14) from data over a pressure range of 41 to 97 kPa at 298 K was low. Johnstone and Leppla's results (15) were at too low pressures to be reasonably Johnstone extrapolated. Otuka's results (16) were mostly at pressures above atmospheric and not readily extrapolated. Parkinson's determinations (17) were at rather low partial pressures of sulfur dioxide (0.08-3.5 kPa). The Bodor $et\ al.$ (18) results were quite low (7-14 per cent) after extrapolation and interpolation to 101.325 kPa. Tokunaga's measurements (19) were of reasonable precision but systematically higher than the recommended values. Douabul and Riley's results (20) were 6 to 14 per cent higher than the recommended values. Byerley $et\ al$.'s two values (21) were 8 and 12 per cent low. Vosolsobe $e\bar{t}$ al.'s results (22) were at too low pressure to be extrapolated. Sano and Nakamoto's value agrees with the value in the table. This system awaits a definitive study.

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- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]

EVALUATOR:

Rubin Battino, Department of Chemistry, Wright State University, Dayton, Ohio 45435, U.S.A. July 1981

CRITICAL EVALUATION:

- 22. Vosolsobe, J.; Simecek, S.; Michalek, J.; Kadler, B. Chem. Prumys1. <u>1965</u>, 15, 401.
- 23. Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 Sulfur dioxide; SO₂; [7446-09-5] Water; H₂O; [7732-18-5] 	Bunsen, R. Ann. <u>1855</u> , 93, 1-50. (Schönfeld, M. Ann. <u>1855</u> , 93, 26).		
VARIABLES: T/K = 273-313	PREPARED BY: R. Battino		
EXPERIMENTAL VALUES: $\alpha^{\text{C}}/\text{cm}^3$ (STP)	α ^C /cm³ (STP)		

FYPERIM	ENTAL VALU	FC.		1			C -
t/°C	т ^а /к	$x_1^{a,b}$	α^{C}/cm^{3} (STP) cm^{-3} atm ⁻¹	t/°C	т ^а /К	x_1^a,b	α^{C}/cm^{3} (STP) cm^{-3} atm ⁻¹
0	273	0.0525	68.861	21	294	0.0274	34.989
1 2	274	0.0511	67.003	22	295	0.0266	33.910
2	275	0.0498	65.169	23	296	0.0258	32.847
3	276	0.0485	63.360	24	297	0.0250	31.800
4	277	0.0472	61.576	25	298	0.0242	30.766
5	278	0.0459	59.816	26	299	0.0234	29.748
6	279	0.0446	58.080	27	300	0.0227	28.744
7	280	0.0434	56.369	28	301	0.0219	27.754
8	281	0.0421	54.683	29	302	0.0212	26.780
9	282	0.0409	53.021	30	303	0.0204	25.819
10	283	0.0397	51.383	31	304	0.0197	24.873
11	284	0.0385	49.770	32	305	0.0190	23.942
12	285	0.0373	48.182	33	306	0.0183	23.025
13	286	0.0361	46.618	34	307	0.0176	22,122
14	287	0.0350	45.079	35	308	0.0169	21.234
15	288	0.0339	43.564	36	309	0.0162	20.361
16	289	0.0327	42.073	37	310	0.0155	19.502
17	290	0.0316	40.608	38	311	0.0149	18.658
18	291	0.0306	39.165	39	312	0.0142	17.827
19	292	0.0295	37.749	40	313	0.0136	17.013
20	293	0.0283	36.216	- •			
ł							

a Calculated by compiler.

METHOD/APPARATUS/PROCEDURE:

AUXILIARY	INFORMATION	

Analysed chemically. This is really Schönfeld's data (1) as

cited by Bunsen. Data were smoothed by Schönfeld.

No details given.

SOURCE AND PURITY OF MATERIALS:

ESTIMATED ERROR:

 $\delta\alpha/\alpha = \pm 0.03$ (compiler's estimate).

REFERENCES:

1. Schönfeld, M.

Ann.

1855, 93, 26.

 $^{^{\}mathrm{b}}$ Mole fraction solubility at 101.325 kPa partial pressure of gas.

Bunsen coefficient.

- 1. Sulfur dioxide; SO₂;
 [7746-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sims, T. H.

J. Chem. Soc.

1862, 14, 1-22.

VARIABLES:

T/K = 281-323

PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

t ^a /°C	т ^b /к	x_1 b,c	Solubility ^d (volume)	Solubility ^e (weight)
8	281.2	0.0451	58.7	0.168
10	283.2	0.0415	53.9	0.154
12	285.2	0.0384	49.6	0.142
14	287.2	0.0353	45.6	0.130
16	289.2	0.0329	42.2	0.121
18	291.2	0.0305	39.3	0.112
20	293.2	0.0284	36.4	0.104
22	295.2	0.0268	34.2	0.098
24	297.2	0.0252	32.3	0.092
26	299.2	0.0239	30.5	0.087
28	301.2	0.0228	28.9	0.083
30	303.2	0.0215	27.3	0.078
32	305.2	0.0201	25.7	0.073
34	307.2	0.0190	24.3	0.069
36	309.2	0.0180	22.8	0.065
38	311.2	0.0171	21.6	0.062
40	313.2	0.0160	20.4	0.058
42	315.2	0.0152	19.3	0.055
44	317.2	0.0147	18.4	0.053
]				

(cont.)

AUXILIARY INFORMATION .

METHOD/APPARATUS/PROCEDURE:

The experimental method is similar to that of Roscoe (1).

Accurate analysis was used to determine the quantity of gas absorbed by a known weight of water under known conditions of temperature and pressure. The analysis was iodimetric. Details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

- Evolved from sulfuric acid and copper and washed with water before freezing into a container.
- 2. No details given.

ESTIMATED ERROR:

Solubility/Solubility = 0.03 (compiler's estimate).

REFERENCES:

- 1. Roscoe, H. E. J. Chem. Soc.
 - 1855, 8, 14.

 Sulfur dioxide; SO₂; [7746-09-5]

2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sims, J. H.

J. Chem. Soc.

1862, 14, 1-22.

EXPERIMENTAL VALUES:

t ^a /°C	т ^b /к	x_1 b,c	Solubility ^d (volume)	Solubility ^e (weight)
46	319.2	0.0139	17.4	0.050
48	321.2	0.0130	16.4	0.047
50	323.2	0.0125	15.6	0.045

- These are smoothed values presented by Sims at 2 K intervals. The smoothed values are based on extensive pressure-dependent measurements at 7, 20, 39.8, and 50 °C. They were calculated for an $\rm SO_2$ partial pressure of 760 mmHg. The pressure range at each temperature ranged from about 27 to 2000 mmHg, so the smoothed values at 760 mmHg are interpolations.
- b Calculated by compiler.
- Mole fraction solubility at 101.325 kPa partial pressure of gas.
- d Solubility in cm³ SO₂/g H₂O. Effectively an Ostwald coefficient.
- e Solubility in g SO₂/g H₂O. Mole fraction solubilities were calculated from the values in this column.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Fox, C.J.J.
2. Water; H ₂ O; [7732-18-5]	Z. Phys. Chem. 1902, 41, 458-482.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES: Partial pressure	= 0.101325 MPa
T/K Ostwald coeffi L	cient, Mole fraction of sulfur dioxide, c
298.2 32.76 a 308.2 22.43 b	0.0257 0.0178
a average of 6 values.	
b average of 5 values.	
<pre>c calculated by compiler a molar volume for sulfur</pre>	ssuming ideal gas dioxide.
	1 2
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Sulfur dioxide was passed through the water until saturated at the barometric pressure. After saturation	1. Purity 99.8 mole per cent major impurity water.
a sample of solution was analysed, the amount of sulfur dioxide being determined by iodine-thiosulfate titration.	2. Conductivity grade.
	ESTIMATED ERROR: $\delta x_{SO_2} = \pm 3\%$
	REFERENCES:

0			de Solubilities
COMPONENTS:			ORIGINAL MEASUREMENTS:
	r dioxide; SO:	2;	Lindner, J.
	5-09-5]		Monatsh.
2. Water	:; H ₂ O; [7732-	-18-5]	<u>1912</u> , 33, 613-672.
VARIABLES:			PREPARED BY:
	Temperature,	pressure	C. L. Young
EXPERIMENTA	L VALUES:		
т/к	p/mmHg	p/kPa	Solubility /(g(SO ₂) /10 ² cm ³ (sat.soln.)
273.2	0.4	0.05	0.0537
	3.5 29.4	0.47 3.92	0.237 1.227
293.2	109.4 1.4	14.59 0.19	3.804 0.0534
293.2	11.75	1.57	0.234
	87.9 313	11.72 41.7	1.212 3.750
323.2	4.9	0.65	0.0525 0.2276
	30.5 204.5	4.07 27.26	1.181
	696	92.8	3.628
		AUXILIARY	INFORMATION
METHOD/APPA	RATUS/PROCEDURE:	***	SOURCE AND PURITY OF MATERIALS:
		- 4 1	
	ric method. Fated method, of	airly historical	No purity data given.
COMPTIC			no parto, accordance

Manometric method. Fairly complicated method, of historical interest only. ESTIMATED ERROR: REFERENCES:

	vva	ater	
COMPONENTS:		ORIGINAL MEASUREMEN	VTS:
1. Sulfur die	oxide; SO ₂ ; [7446-09-5]	Smith, W.T.; P	Parkhurst, R.B.
2. Water; H ₂	0; [7732-18-5]	J. Am. Chem. S	Soc. <u>1922</u> ,44, 1918-192
/ARIABLES: Temperatu	re, pressure	PREPARED BY:	L. Young
EXPERIMENTAL VALU	EC.		
T/K	Partial pressure of sulfur dioxide p/mmHg p/kPa	Wt. of SO ₂ per 100 cm ³ water /g	Mole fraction of sulfur dioxide, x _{SO2}
278.2 293.2	474.8 63.30 198.6 26.48 224.4 29.92 366.6 48.88 1107.8 147.69	11.55 2.97 3.34 5.22 15.01	0.0315 0.00828 0.00931 0.0145 0.0405
313.2 333.2	306.4 40.85 373.8 49.84 175.7 23.42	2.21 2.68 0.84	0.00618 0.00748 0.00236
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/	PROCEDURE:	SOURCE AND PURITY	OF MATERIALS:
saturated with stated pressur- saturated solu	in which water was h sulfur dioxide at re. Samples of utions analysed by lfate titration.	1. Virginia S 2. Degassed.	Smelting Co. sample.
			1; $\delta x_{\text{SO}_2} = \pm 5\%$ d by compiler)
		REFERENCES:	

COMPONENTS: 1. Sulfur dioxide; SO₂; [7746-09-5] 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hudson, J. C.

J. Chem. Soc.

1925, 1332-1347.

VARIABLES:

Temperature

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Total pressure P/mmHg	Part pres p/mmHg		Solub S1	ility $s_{m{\circ}}^{\#}$	Mole fraction of sulfur dioxide, "SO ₂ at a partial pressure of 101.3 kPa
283.15	777.3	764.2	101.9	15.53	15.44	0.04162
	776.3	767.1	102.3	15.50	15.36	0.04141
	776.3	767.0	102.3	15.58	15.44	0.04162
	775.4	766.2	102.2	15.48	15.36	0.04141
288.15	766.2	757.0	100.9	15.28	15.32	0.04131
	769.5	757.6	101.0	12.72	12.76	0.03464
	772.5	760.6	101.4	12.75	12.74	0.03459
	769.5	757.6	101.0	12.64	12.68	0.03443
293.15	787.7	771.3	102.8	10.79	10.63	0.02903
	773.3	765.9	102.1	10.61	10.66	0.02911
	778.6	762.2	101.6	10.68	10.64	0.02905
	779.1	762.7	101.7	10.65	10.61	0.02898
	773.9	757.5	101.0	10.64	10.68	0.02916
303.05	798.5	768.5	102.5	7.640	7.554	0.02080
	789.4	759.4	101.2	7.600	7.607	0.02095
	791.0	761.0	101.5	7.610	7.600	0.02093
	800.9	770.9	102.8	7.674	7.565	0.02083
313.15	800.9	747.3	99.63	5.428	5.520	0.01529
	801.4	747.8	99.70	5.441	5.529	0.01531
	798.1	744.5	99.26	5.406	5.516	0.01528
						(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled through water in a thermostatted tube.

Mercury manometer used to measure total pressure at sautration. After saturation, tube weighed and sulfur dioxide content determined by oxidation with hydrogen peroxide in sodium hydroxide solution and the gravimetric estimation of sulfate as barium sulfate. The partial pressure of sulfur dioxide was calculated assuming partial pressure of water could be calculated from Raoult's Law.

SOURCE AND PURITY OF MATERIALS:

- Obtained from a cylinder; the purity was stated to be high, the major impurity being water, less than 0.4%.
- 2. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta p/mmHg = \pm 0.2$; $\delta x_{SO_2} = \pm 0.001$ (estimated by compiler).

REFERENCES:

- Sulfur dioxide; SO₂; [7746-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hudson, J. C.

J. Chem. Soc.

1925, 1332-1347.

EXPERIMENTAL VALUES:

T/K	Total pressure P/mmHg	Part. press p/mmHg		Solu s_1^\star	sility $s^{\#}_{ullet}$	Mole fraction of sulfur dioxide, **SO at a partial pressure of 101.3 kPa
313.15	816.7 815.7	763.1 762.1	101.7	5.593 5.585	5.569 5.555	0.01542 0.01538
321.30	815.7	762.1	101.6	5.581	5.550	0.01537
	799.0	717.0	95.59	4.147	4.395	0.01221
	801.5	719.5	95.93	4.132	4.365	0.01213
	794.3	712.3	94.97	4.108	4.382	0.01217
333.15	840.9	758.9	101.2	4.409	4.415	0.01226
	881.5	735	98.0	3.151	3.257	0.009077
	894.5	748	99.7	3.192	3.244	0.009041
343.15	894.5	748	99.7	3.215	3.268	0.009107
	886.5	740	98.7	3.142	3.220	0.008975
	897	666.5	88.86	2.278	2.598	0.007254
353.15	892.5	662	88.3	2.277	2.614	0.007298
	893	662.5	88.33	2.300	2.637	0.007362
	892	661.5	88.19	2.251	2.585	0.007218
	883	531.5	70.86	1.496	2.139	0.005980
	883	531.5	70.86	1.490	2.131	0.005958
	958	606.5	80.86	1.704	2.130	0.005955
	967	616	82.1	1.714	2.114	0.005910
363.15	893	378	50.4	0.901	1.801	0.005040
	954.3	439.5	58.60	1.037	1.785	0.004995
	960	439	58.5	1.056	1.829	0.005118

 $^{^{\}mbox{\scriptsize *}}$ g of \mbox{SO}_{2} per 100 g of water at stated pressure.

 $^{^{\}sharp}$ g of SO₂ per 100 g of water at pressure of 101.3 kPa.

4	Sullur Dioxide Solubliities					
COMPONENTS:				ORIGI	NAL MEASUREMENTS:	
1. Sulfur	r dioxide; SO ₂ ; [7446-09-5]			Maa	ass, C.E.; Maass, O.	
2. Water;	; H ₂ O; [773	2-18-5]	!	J. Am. Chem. Soc. 1928, 50, 1352-1368.		
VARIABLES:				PREP	ARED BY:	
	emperature,	pressure			C.L. Young	
EXPERIMENTAL	VALUES:			L		
T/K	Total P P/cmHg	ressure p/10 ⁴ Pa		s % SO₂		
283.2	24.3 45.2 67.4 87.4 124.5 128.8	3.24 6.03 8.99 11.65 16.60	4. 8. 11. 14. 18.	19 64 75 91 86	0.0133 0.0245 0.0357 0.0464 0.0615 0.0652	
289.7	154.3 31.0 57.2 84.4 111.4 151.9 156.0	20.57 4.13 7.63 11.25 14.85 20.25 20.80	23. 4. 8. 11. 14. 18.	48 03 42 31 57	0.0779 0.0130 0.0240 0.0350 0.0449 0.0603 0.0637	
295.2	188.4 37.8 69.3 102.2 132.6 178.3 186.1	25.12 5.04 9.24 13.63 17.68 23.77 24.81	22. 4. 7. 11. 14. 18.	40 88 17 04 22	0.0763 0.0128 0.0235 0.0342 0.0439 0.0590 0.0624	**
298.2	222.2 66.2	29.62 8.83	22. 6.	9	0.0748 0.0204	
300.2	246.9 44.8 81.0	32.92 5.97 10.80	22. 4. 7.	32	0.0751 0.0125 0.0230	
		AUA	KILIARY	TNFO	RMATION	
METHOD/APPAR	ATUS/PROCEDUR				CE AND PURITY OF MATERIALS:	
The vapor	pressure o	f solutions mount of su		1.		
				2.	Degassed.	
				ESTI	MATED ERROR:	
					$\delta T/K = \pm 0.1$; $\delta x_{SO_2} = \pm 2\%$ (estimated by compiler)	
				REFE	CRENCES:	-

- 1. Sulfur dioxide; SO₂; [7746-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Maass, C.E.; Maass, O.

J. Am. Chem. Soc. 1928, 50, 1352-1368.

EXPERIMENTAL VALUES:

т/к	Total Pr p/cmHg	p/10 ⁴ Pa	Mass % of SO ₂	Mole fraction of sulfur dioxide, $x_{\rm SO_2}$
00.2	118.3	15.77	10.95	0.0334
	152.8	20.37	13.74	0.0429
	206.9	27.58	17.85	0.0576
	255.6	34.08	21.86	0.0729

T/K	^x SO ₂	
283.2 290.0 295.2 298.2 300.2	0.03838 0.03053 0.02518 0.02157 0.02141	

 $^{^{\}rm a}$ Calculated by compiler for a partial pressure of sulfur dioxide of 101.3 kPa.

		Garrar Blox	ac oolabilities			
COMPONENTS:			ORIGINAL MEASU	JREMENTS:		
l. Sulfur	dioxide; SO	2;	Morgan,	0. M.; Maas	s, O.	
[7746-	-09-5]		Can. J. Res.			
2 Water	. 11 0. [7722	10 61				
2. Water; H ₂ O; [7732-18-5]			1931,	5, 162-99.		
VARIABLES:			PREPARED BY:			
	T/K = 273-298			R. Battino		
EXPERIMENTAL	VALUES.					
	P ^a /kPa	8 SO2 b	P/cm Ha	P ^a ∕kPa	% so₂b	
			-,			
•	C = 0 T/K		•	C = 18 T/K		
0.17	0.23 0.84	0.1369 0.3374	0.32 1.10	0.43 1.47	0.0816 0.2605	
0.63 1.97	2 (2	U.33/4 n 0000	J 60	3.57	0.2605	
1.97 6.05	2.63 8.07	0.8888 2.284	2.68 5.92	7.89	1.103	
11.55	15.40	2.404 3.978	14.83	19.77	2.458	
17.30	15.40 22.06	3.978 5.597	14.83 26.66	35.54	4.150	
29.21	38.94	8.630 11.52	39.01	52.01		
41.63	38.94 55.50	11.52	51.44	52.01 68.58	7.340	
	73.35	14.23	63.69	84.91	8.831	
			76.04	101.38	10.30	
t/°(C = 10 T/K	= 283	$t/^{\circ}C = 25$ $T/K = 298$			
0.35	0.47 1.33	0.1267	0.79	1.05	0.1735	
1.00	1.33	0.3414	3.42	4.56	0.5448	
2.12	2.83	0.6360	7.37	9.83	1.056	
4.71	6.28	0.6360 1.261	13.61	18.15	1.809	
10.98	14.64		25.28	33.70 53.33	3.116	
19.52	20.02	2.593 4.256	40.00	53.33	4.672	
28.37	37.82 62.15	5.872 8.937	55.00	73.33 93.17	6.184	
46.62				93.17	7.640	
64.18	85.57	11.68	81.17	108.22	8.756	
73.58	98.10	13.03			(cont.)	
		AJIVILIADV	INFORMATION			
METHOD/APPARA	ATUS/PROCEDURE:			RITY OF MATERIAL	c.	
mb			1. From Ansul Chemical Co.,			
The amoun	nt of sulfur d	ıoxıde	Marinette, Wisconsin.			
dissolved	l was determin	ed via	Distill	ed three time	s.	
conductiv	vity measureme	nts.	2. "Conductivity water".			
			2. "Conque	ctivity water	•	
			ESTIMATED ERR	OR.		
			1	$60_2 = \pm 0.05$		
)			
			(compiler	s estimate).		
l Í			REFERENCES:			
			1			

- Sulfur dioxide; SO₂;
 [7746-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Morgan, O. M.; Maass, O.

Can. J. Res.

1931, 5, 162-99.

EXPERIMENTAL VALUES:

a Calculated by compiler.

 $^{\rm b}$ Presumably a weight per cent of the total amount of sulfur dioxide as ${\rm SO}_2$ in the water.

T/K	н ^а	x ₁ ^D
283	0.01080	0.0386
291	0.00870	0.0295
298	0.00758	0.0235

^a Henry's law constant calculated by authors from [SO₂] = Hp where [SO₂] is in mol dm⁻³ and p is in cm Hg. These are smoothed and averaged values.

Mole fraction solubility at 101.325 kPa partial pressure of gas calculated by compiler from data around 101.325 kPa given in the paper. Mole fractions calculated from the Henry's law constants given by the authors are quite different since for this system H (as calculated) is concentration-dependent.

COMPONENTS:			ORIGINAL MEASUREME	NTS:		
[7446-0	Hioxide; SO 9-5] H ₂ O; [7732		J. Am. Chem. S	Conrad, F. H.; Beuschlein, W. L. J. Am. Chem. Soc. 1934, 56, 2554-2562.		
VARIABLES:	*************************************		PREPARED BY:			
	Pressure			C. L. Young		
EXPERIMENTAL V	ALUES:					
т/к		dioxide	Solubility, S /(gSO ₂ /100gH ₂ O)	Mole fraction of sulfur dioxide in solution, x_{SO_2}		
298.2	308 299 593 640 611 730 760 a	41.1 39.9 79.1 85.3 81.5 97.3	3.72 3.63 6.89 7.28 6.99 8.37	0.0104 0.0101 0.0190 0.0201 0.0193 0.0230 0.0237 ^a		

a Extrapolated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was passed into a measuring pipet and then into a flask containing water. The flask was shaken until a constant total pressure was achieved. The pressure was measured using a mercury manometer. The solution was analysed by titration using the iodine-thiosulfate procedure.

SOURCE AND PURITY OF MATERIALS:

- Refrigeration grade from Virginia Smelting Co. No trace of sulfur trioxide detected.
- 2. Distilled and freshly boiled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$; $\delta x_{SO_2} = \pm 4\%$ (estimated by compiler).

REFERENCES:

Pressure

1. Sulfur dioxide; SO₂; [7446-09-5]

2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Johnstone, H.F.; Leppla, P.W.

J. Am. Chem. Soc. 1934, 56, 2233-2238.

VARIABLES:

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

Т/К	Partial pr of sulfur 10 ³ p/atm		Moles of SO ₂ per 1000g water	Mole fraction of sulfur dioxide 10 ³ x SO ₂
298.2	0.27 1.20 2.29 2.67 6.71 9.11	0.027 0.122 0.232 0.271 0.680 0.923	0.002484 0.006203 0.009546 0.01084 0.02059 0.02561	0.0448 0.1117 0.1720 0.1953 0.3708 0.4612
308.2	13.50 1.03 2.49 4.12 5.80 9.55	1.368 0.104 0.252 0.417 0.588 0.968	0.03328 0.00419 0.00745 0.00999 0.01356	0.5992 0.0755 0.1342 0.1799 0.2442 0.3579
323.2	2.30 3.83 5.38 8.79	0.233 0.388 0.545 0.891	0.01987 0.00467 0.00637 0.00838 0.01057	0.0841 0.1147 0.1510 0.1904

AUXILIARY INFORMATION ~

METHOD/APPARATUS/PROCEDURE:

The low partial pressure of sulfur dioxide was obtained by using a mixture of nitrogen and sulfur dioxide. This mixture was bubbled through water in a "Pyrex saturator" (Bichowsky and Starch, ref (1)) until equilibrium was reached. Samples of solution were analysed by adding excess iodate and titrating with thiosulfate solution.

SOURCE AND PURITY OF MATERIALS:

- 1. Stated to be of high purity.
- 2. Conductivity water, degassed.

ESTIMATED ERROR:

REFERENCES:

- 1. Bichowsky, F.R.; Starch, H.
 - J. Am. Chem. Soc. 1915, 37, 2695.

20			Sulfur Diox	ide Solubilities	
COMPO	ONENTS: Sulfur o	dioxide; SO ₂ ;	[7746-09-5]	ORIGINAL MEASUREMENTS: Otuka, Y.	
2.	Water; I	H ₂ O; [7732-18-	5]	J. Soc. Chem. Ind 1939, 42, 205B-20	
VARI	ABLES:			PREPARED BY:	
	Tempera	ture, pressure		W. Ge	rrard
EXPE	RIMENTAL V	ALUES: 760 mm	Hg = 1 atm =	101.325 kPa	
	T/K	P _{Total} /atm		Mole SO ₂ /dm³soln	H
	373	1.72	0.73	0.1763	0.242 0.257
	378	1.94 2.01	0.95 0.83	0.2443 0.1728	0.208
ļ		2.26	1.08	0.2401	0.222
	383	2.29	0.89	0.1708	0.192 0.190
	388	2.63 2.70	1.24 1.05	0.2352 0.1656	0.158
	500	3.03	1.38	0.2311	0.168
	393	3.12	1.18	0.1616	0.137
	200	3.50	1.56	0.2259	0.145
	398	3.58 4.00	1.31 1.74	0.1578 0.2210	0.120 0.127
	403	4.10	1.45	0.1535	0.106
		4.55	1.91	0.2164	0.113
İ	408	4.63	1.57	0.1502	0.096
	412	5.12	2.07	0.2123	0.103
ļ	413	5.24 5.73	1.71 2.21	0.1464 0.2087	0.086 0.094
	418	5.91	1.85	0.1428	0.077
		6.41	2.36	0.2050	0.087
	423	6.60	1.96	0.1400	0.071
		7.08	2.46	0.2028	0.082
ŀ	The a	uthor defined	the "solubili	ty" as $H = (H_2SO_3)/$	p _{SO2} , the
	press	ure being in a	tm. (H ₂ SO ₃)	evidently means mol	e SO ₂ /dm ³ thor refers
<u> </u>	to "pi	ure sulfurous			
			AUXILIA	RY INFORMATION	
METH	IOD/APPARAT	rus/procedure:		SOURCE AND PURITY OF M	ATERIALS:
The	total p	ressure, p _{Tota}	, was	Not stated.	
		by means of a		inou buducu.	
mano	ermineu : ometer.	It was stated	that the		
		ssures were ap			
from	m the di	mensions of th	e apparatus,		
but	details	were not give	n.		
1					
1					
1				ESTIMATED ERROR:	
1				POITUMIED EKKOK:	
1					
1					
				REFERENCES:	
1					
1					

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7746-09-5] Water; H₂O; [7732-18-5] 	Beuschlein, W. L.; Simenson, L. O. J. Am. Chem. Soc. 1940, 62, 610-2.
VARIABLES: T/K = 296-386 P/kPa = 7-192	PREPARED BY: R. Battino

t/°C	т ^а /к	x_1^a,b	P ^C /mmHg	P ^a /kPa	
	0	.51 g SO ₂ /100 g H ₂ 0)		_
35.6 41.0 47.0 52.0 62.6 71.0 78.6 85.0 92.2 99.0 105.2 111.8 113.0	308.8 314.2 320.2 325.2 335.8 344.2 351.8 358.2 365.4 372.2 378.4 385.0 386.2	0.02227 0.01914 0.01559 0.01364 0.00925 0.00727 0.00590 0.00506 0.004364 0.003822 0.003404 0.003048	49 57 70 80 118 150 185 215.5 250 285.5 320.5 358 367.5	6.53 7.60 9.33 10.67 15.73 20.00 24.66 28.73 33.33 38.06 42.73 47.73 49.00	
	1	.09 g SO ₂ /100 g H ₂ 0)		
26.8 33.6 39.4 44.2 50.6	300.0 306.8 312.6 317.4 323.8	0.03308 0.02429 0.01873 0.01586 0.01310	70.5 96 124.5 147 178	9.40 12.80 16.60 19.60 23.73	
			(coı	nt.)	

AUXILIARY INFORMATION ~

METHOD/APPARATUS/PROCEDURE:

Solutions were prepared by passing sulfur dioxide through freshly boiled, distilled water until saturated and then diluting to the desired concentration. Analysis was by running the sulfur dioxide solution into an excess of iodine and back titrating with sodium thiosulfate. Details and a drawing are in the paper.

SOURCE AND PURITY OF MATERIALS:

- "Refrigeration dry", 99.99 per cent.
- 2. Distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta P/kPa = \pm 0.07$; $\delta x_1/x_1 = \pm 0.03$ (compiler's estimate)

1. Sulfur dioxide; SO₂;
 [7746-09-5]

2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Beuschlein, W. L.; Simenson, L. O.

J. Am. Chem. Soc.

1940, 62, 610-2.

EXPERIMENTAL VALUES:

t/°C	т ^а /к	x ₁ a,b	P ^C /mmHg	P ^a /kPa
	1.	.09 g SO ₂ /100 g H ₂ O		
61.6 67.4 73.4 79.2 86.4 98.4 100.6	334.8 340.6 346.6 352.4 359.6 371.6 373.8 379.8	0.00952 0.00831 0.00712 0.00627 0.005234 0.004572 0.003886 0.003491	245 280.5 327.5 372 445.5 510 600 668	32.66 37.40 43.66 49.60 59.39 67.99 79.99
	4.	.36 g SO ₂ /100 g H ₂ O	1	
23.2 27.2 30.0 33 36 38.2 42.2 45.2 48.2 52 55.3 58.4 61.2 63 67.2 70.8 72.4	296.4 300.4 303.2 306.2 309.2 311.4 315.4 318.4 321.4 325.2 328.5 331.6 334.4 336.2 340.4 344.0 345.6	0.02809 0.02501 0.02221 0.02004 0.01818 0.01691 0.01507 0.01371 0.01259 0.01141 0.01041 0.00961 0.00961 0.00900 0.00859 0.00777 0.00722 0.00705	332 373 420 465.5 513 551.5 619 680.5 741 818 896 970.5 1036.5 1085.5 1290.5	44.26 49.73 56.00 62.06 68.39 73.53 82.53 90.73 98.79 109.06 119.46 129.39 138.19 144.72 160.05 172.25 176.45
	7.	45 g SO ₂ /100 g H ₂ O		
25.2 31.4 34.2 37.4 41 44 47.2 50.4 54.4 55.6	298.4 304.6 307.4 310.6 314.2 317.2 320.4 323.6 327.6 328.8	0.02463 0.02042 0.01902 0.01741 0.01612 0.01491 0.01383 0.01269 0.01146 0.01104	647 780.5 838 915.5 989 1069 1152.5 1255.5 1391.0	86.26 104.06 111.72 122.06 131.86 142.52 153.65 167.39 185.45 192.45

a Calculated by compiler.

b Mole fraction solubility at 101.325 kPa partial pressure of gas. These values are only reasonable at pressures close to 101.325 kPa.

 $^{^{\}rm C}$ Partial pressure of ${\rm SO_2}\,.$

		Water		23
COMPONENTS: 1. Sulfur dioxide; SO: [7446-09-5] 2. Water; H ₂ O; [7732-	l	ORIGINAL MEAS Parkison Tappi 1956, 39	, R. V.	
VARIABLES: T/K = 283-305 P/kPa = 0.08-3	. 6	PREPARED BY:	R. Battino	D
EXPERIMENTAL VALUES: t/°F T ^a /K	P ^b /atm	P ^{a,b} /kPa	Solubility/ (1b moles/ ft³)	a,c Solubility/ (mol dm ⁻³)

EXPERIMENTA	L VALUES:				
t/°F	т ^а /к	P ^b /atm	P ^{a,b} ∕kPa	Solubility/ (1b moles/ ft3)	a,c Solubility/ (mol dm ⁻³)
50	283	0.000809 0.00193 0.00292 0.00440 0.00480 0.00537 0.00668 0.00916 0.00987 0.0174 0.0185 0.0261 0.0281 0.0332	0.0820 0.196 0.296 0.446 0.486 0.544 0.677 0.928 1.00 1.76 1.88 2.64 2.85 3.36	0.000511 0.000912 0.00119 0.00144 0.00164 0.00167 0.00212 0.00265 0.00279 0.00441 0.00446 0.00599 0.00622 0.00712	0.00819 0.0146 0.0191 0.0231 0.0263 0.0268 0.0340 0.0425 0.0447 0.0707 0.0715 0.0960 0.0997
60	289	0.0350 0.00659 0.00910	3.55 0.668 0.922	0.00745 0.00168 0.00214	0.119 0.0269 0.0343
70	294	0.00979 0.00102 0.00201 0.00209 0.00465 0.00507	0.992 0.103 0.204 0.212 0.472 0.514	0.00225 0.000326 0.000568 0.000642 0.00109 0.00116	0.0361 0.00523 0.00911 0.0103 0.0175 0.0186
				(co:	nt.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A nitrogen/sulfur dioxide mixture of varying composition was bubbled through water. The analysis of the gas and liquid phase was done by a modified Palmrose technique (1,2) via a chemical titration. Details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Triple distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$.

- Palmrose, G. V. Paper Trade J. 1935, 100, 38-9.
- 2. White, C. K.; Vivian, J. E.; Whitney, R. P. Paper Trade J. 1948, 126, 26-8.

ORIGINAL MEASUREMENTS:

COMPONENTS:

1. Sulfur dioxide; SO2; Parkison, R. V. [7446-09-5] Tappi 2. Water; H₂O; [7732-18-5] 1956, 39, 517-9. **EXPERIMENTAL VALUES:** a,c Solubility/ Solubility/ P^b/atm Pa,b/kPa т^а/к t/°F (1b moles/ $(mol dm^{-3})$ ft3) 294 70 0.00660 0.669 0.00141 0.0226 0.0213 0.00734 0.744 0.00133 0.00913 0.925 0.00176 0.0282 0.00983 0.996 0.00188 0.0301 0.0172 1.74 0.00288 0.0462 0.0280 2.84 0.00417 0.0668 3.54 0.0349 0.00498 0.0798 80 263 0.00150 0.153 0.000320 0.00513 0.000580 0.00362 0.367 0.00930 0.00469 0.475 0.000722 0.0116 0.000921 0.0148 0.00633 0.641 0.00641 0.649 0.000918 0.0147 0.00812 0.823 0.00111 0.0178 0.00885 0.897 0.00120 0.0192 0.00952 0.965 0.00126 0.0202 0.0110 1.11 0.00138 0.0221 1.80 0.0178 0.00204 0.0327 0.0251 2.54 0.00265 0.0425 0.00334 0.0336 3.40 0.0535

a Calculated by compiler.

b Partial pressure of SO₂.

 $^{^{\}mbox{\scriptsize C}}$ Molar solubility calculated by multiplying previous column by 16.03.

- Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rabe, A. E.; Harris, J. F. J. Chem. Engng. Data 1963, 8, 333-336.

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMEN'	TAL VALUES:		Conc.	Mole fraction * of
T/K	p_{SO_2} /mmHg	P _{SO₂} /kPa	g _{SO₂} /100 g H ₂ O	sulfur dioxide
303.15	443.5	59.13	4.46	0.01238
	443.9	59.18	4.46	0.01238
	442.4	58.98	4.46	0.01238
	444.5	59.26	4.48	0.01245
	451.6	60.21	4.48	0.01245
	308.6	41.14	3.21	0.00894
	304.9	40.65	3.21	0.00894
	308.4	41.12	3.21	0.00894
	309.0	41.20	3.21	0.00894
	312.0	41.60	3.21	0.00894
	172.2	22.96	1.92	0.00537
	181.0	24.13	1.92	0.00537
	177.0	23.60	1.92	0.00537
212	39.2	5.23	0.59	0.00166
	42.7	5.69	0.59	0.00166
313.15	624.4	83.25	4.48	0.01245
	638.8	85.17	4.48	0.01245
	418.0	55.73	3.21	0.00894
	420.0	56.00	3.21	0.00894
	242.0	32.26	1.92	0.00537

^{*} calculated by compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Partial vapor pressure of sulfur dioxide above solution containing known masses of sulfur dioxide determined by estimating amount of sulfur dioxide vapor in known volume. Sulfur dioxide estimated by dissolving gas sample up in dilute aqueous acetaldehyde soln. and titrating α -hydroxy sulfonic acid against sodium hydroxide potentiometrically. Details in source.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.02 \text{ or less; } \delta p/p = 0.0044 \text{ (std. dev.).}$

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Rabe, A. E.; Harris, J. F. J. Chem. Engng. Data 1963, 8, 333-336.

EXPERIMENTAL VALUES:

T/K	^p SO₂/mmHg	^p SO₂ ^{/kPa}	Conc. g _{SO2} /100 g H ₂ O	Mole fraction [*] of sulfur dioxide
313.15	249.0	33.20	1.92	0.00537
	57.8	7.71	0.59	0.00166
	60.6	8.08	0.59	0.00166
323.15	583.3	77.77	3.20	0.00892
	592.9	79.05	3.20	0.00892
	608.4	81.11	3.20	0.00892
	583.3	77.77	3.21	0.00894
	585.7	78.09	3.21	0.00894
	324.6	43.28	1.92	0.00537
	328.5	43.80	1.92	0.00537
	330.9	44.12	1.92	0.00537
	335.1	44.68	1.92	0.00537
	85.8	11.44	0.59	0.00166
	86.7	11.56	0.59	0.00166
333.15	742.0	98.93	3.21	0.00894
	756.0	100.8	3.21	0.00894
	447.5	59.66	1.92	0.00537
	437.1	58.28	1.92	0.00537
	114.0	15.20	0.59	0.00166
	116.0	15.47	0.59	0.00166
343.15	151.0	20.13	0.59	0.00166
	153.0	20.40	0.59	0.00166
353.15	189.0	25.20	0.59	0.00166

^{*} calculated by compiler

T/K	^x SO ₂ a
313.15	0.01498
323.15	0.01149
333.15	0.00907

a Interpolated mole fraction solubility at a partial pressure of sulfur dioxide of 101.325 kPa; calculated by compiler.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Vosolsobe, J.; Simecek, S.; Michalek, J.; Kadler, B. 2. Water; H₂O; [7732-18-5] Chem. Prumysl. 1965, 15, 401-404. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: T/K 103x_{SO2} g SO₂ p_{SO2/mmHq} (T/°C) p/kPa 100 q H₂O 293.2 1.97 0.33 0.927 14.8 1.60 (20) 0.57 29.7 3.96 44.5 5.93 0.78 2.19 2.86 59.4 7.92 1.02 74.2 9.89 1.26 3.53 89.1 11.88 1.48 4.15 16.80 5.70 2.04 126 303.2 0.703 14.6 1.95 0.25 1.26 1.71 (30) 29.1 3.88 0.45 43.7 5.83 0.61 7.76 0.77 2.16 58.2 72.8 9.71 0.92 2.58 2.97 1.06 11.65 87.4 16.51 1.45 4.06 123.8 313.2 0.534 1.88 0.19 14.1 (40)0.899 28.2 3.76 0.32 0.46 1.29 5.77 43.3 7.65 57.4 0.54 1.52 0.67 1.88 70.5 9.40 84.6 11.28 0.78 2.19 1.08 3.03 15.97 119.8 (cont.) AUXILIARY INFORMATION " METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Flow system apparatus in which a sulfur dioxide plus nitrogen gas mixture was bubbled through water. No details given. The partial pressure of sulfur dioxide could be varied by changing the composition of the gas mixture. Samples of water saturated with sulfur dioxide were analysed by ESTIMATED ERROR: iosometry. $\delta x_{SO_2} = \pm 3\%$ $\delta T/K = \pm 0.1;$ (estimated by compiler). REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Vosolsobe, J.; Simecek, S.; Michalek, J.; Kadler, B.

Chem. Prumysl.

1965, 15, 401-404.

EXPERIMENTAL VALUES:

m / m	_		g SO₂	
T/K (T/°C)	^P SO₂/mmHg	p/kPa	100 g H ₂ O	10 ³ x _{SO₂}
323.2	13.3	1.77	0.16	0.450
(50)	26.7	3.56	0.26	0.731
	40.0	5.33	0.34	0.955
	53.4	7.12	0.42	1.18
	66.7	8.89	0.50	1.40
Į	80.1	10.68	0.60	1.68
	113.5	15.13	0.80	2.24
333.2	12.2	1.63	0.11	0.309
(60)	24.4	3.25	0.20	0.562
	36.6	4.88	0.24	0.674
	48.8	6.51	0.33	0.927
	61.1	8.15	0.36	1.01
	73.3	9.77	0.42	1.18
	103.8	13.84	0.58	1.63

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] Water; H₂O; [7732-18-5] 	Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369-373.
VARIABLES:	PREPARED BY: C. L. Young

 $T/^{\circ}C = 30$ T/K = 303 Vapor pressure of water = 0.040 atm

Absorption coefficient, sa,b	Bunsen b coefficient, b	Bunsen coefficient, c	_l c,d	Mole ratio	Mole fraction ^e
29.8	28.3	25.6	24.5	0.023	0.022

- a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.
- b Determined by static absorption method.
- C Determined by flow method.
- d $\alpha = l(1 p_s^o)$ where p_s^o is the vapor pressure of solvent.
- e Calculated by compiler.

AUXILIARY INFORMATION -

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

COMPONENTS:		ORIGINAL MEASU	REMENTS:	
 Sulfur dioxide [7446-09-5] Water; H₂O; 		Tokunaga, J. J. Chem. Engng. Data 1974, 19, 162-165.		
VARIABLES:		PREPARED BY:	C. L. Young	
EXPERIMENTAL VALUES:				
T/K	Solubility ^{#*}	Ostwald coefficient	Mole fraction * of sulfur dioxide, x SO $_2$	
283.15 293.15 303.15 313.15	0.1566 0.1090 0.0777 0.0576	56.8 40.9 30.0 22.9	0.0422 0.0297 0.0214 0.0159	

 $^{^{\#}}$ (g of SO₂/g H₂O).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide bubbled through water. Saturated solution analysed by iodometric titration. Details in source.

The apparatus employed was similar to that of Hudson, ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. High purity sample with purity of 99.96 mole per cent.
- 2. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta x_{SO_2} = \pm 1\%$ (estimated by compiler).

REFERENCES:

Hudson, J. C.
 J. Chem. Soc.
 1925, 1332.

^{*} at partial pressure of 101.3 kPa.

- Sulfur dioxide; SO₂; [7746-09-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Lavrova, E. M.; Tudorovskaya, L. L. Zhur. Prikl. Khim.

1977, 50, 1146-51.

VARIABLES:

T/K = 299-363

PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

t/°C	т ^а /К	$x_1^{\mathbf{b}}$	wt-% ^C	
26	299.2	0.02387	8.00	
40	313.2	0.01534	5.25	
60	333.2	0.009063	3.15	
80	353.2	0.0059	2.08	
90	363.2	0.00504	1.77	

- a Calculated by compiler.
- b Mole fraction solubility at 101.325 kPa partial pressure of gas.
- $^{\mathrm{C}}$ Presumably at 101.325 kPa partial pressure of gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was saturated with SO_2 . The liquid phase was analyzed acidimetrically after oxidation of the dissolved SO_2 to SO_3 by hydrogen peroxide. The paper also reports on SO_2 solubilities in aqueous HCl solutions.

- SOURCE AND PURITY OF MATERIALS:
 - Obtained by the action of cp H₂SO₄ on analytical grade sodium sulfite.
 - 2. No details given.

ESTIMATED ERROR:

 $T/K = \pm 0.2$; $\delta x_1/x_1 = \pm 0.05$

32 Sullui Dioxi	ide Soldbillilles
COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Douabul, A.; Riley, J.
2. Water; H ₂ O; [7732-18-5]	J. Chem. Engng. Data, <u>1979</u> ,24, 274-276.
VARIABLES:	PREPARED BY:
VARIABBES.	
Temperature	C.L. Young.
EXPERIMENTAL VALUES:	
T/K Solubility ⁺ /π	mol dm ⁻³ Mole fraction of sulfur dioxide, $^{\infty}$ SO ₂
278.97 2.959 283.12 2.482 288.10 2.065 292.98 1.697 298.15 1.419	0.05685 0.04693 0.03876 0.03168 0.02644
303.25	0.02644
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Sulfur dioxide bubbled through water for 21 hours with gentle stirring. Pressure measured with mercury manometer. Samples of about 60 cm³ were withdrawn and mixed with 150 cm³ of hydrogen peroxide solution. Solution then titrated with carbonate free sodium hydroxide solution.	 Refrigeration grade obtained from BDH. Mass spectrometric analysis showed its purity was better than 99.9 mole per cent. Distilled.
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.01; \ \delta x_{SO_2} = \pm 0.1$ %
	REFERENCES:

	'	/vater	33
COMPONENTS: 1. Sulfur dioxide; SO: [7746-09-5] 2. Water; H ₂ O; [7732-		ORIGINAL MEASUR Byerley, J. Le, V. T. J. Chem. En 1980, 25, 5	J.; Rempel, G. L.;
VARIABLES: T/K = 298-323	3	PREPARED BY:	R. Battino
EXPERIMENTAL VALUES:			
t/°C	T ^a /K	w ₁ a,b	g SO ₂ ^C /100 g H ₂ O
25 50	298.15 323.15	0.02265 0.01049	8.24 3.77

a Calculated by compiler.

AUXILIARY INFORMATION

Sulfur dioxide was bubbled through water and the amount dissolved was determined by titrating excess iodine with standard thiosulfate solution. (The authors also studied the solubility of SO_2 in water-acetonitrile solutions.)

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

- Anhydrous from Union Carbide Canada Ltd.
- 2. Distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta x_1/x_1 = \pm 0.02$ (compiler's estimate).

b Mole fraction solubility at 101.325 kPa partial pressure of gas.

^C At 101.325 kPa partial pressure of gas.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Seawater

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia

December 1981

CRITICAL EVALUATION:

This system has been investigated by Douabul and Riley (1) in some Although their data are self-consistent there is some doubt as to detail. absolute accuracy of the measurements since data on the solubility of sulfur dioxide in pure water given in the same appear appear to be at least several per cent in error. (See sulfur dioxide + water evaluation.) The only other measurements on this system are those of Abdulsattar (2) whose data are very limited in scope and are of questionable accuracy, Abdulsattar's data are therefore rejected. ±15% at the best. solubility of sulfur dioxide in seawater has been calculated by Abdulsattar $et\ al.$ (3) based on a simplified chemical model. However, such calculated data are for a lower partial pressure of sulfur dioxide than used in the experimental work of Douabul and Riley (1). Under these conditions a relatively large proportion of the sulfur dioxide is accounted for in neutralizing the natural alkalinity of the sea water. It should also be pointed out that the data of Douabul and Riley (1) should not be extra-polated to low partial pressures assuming Henry's Law to be obeyed. Such an assumption is not valid in the present context.

References

- Douabul, A.; Riley, J.
 J. Chem. Eng. Data 1979, 24, 274.
- Abdulsattar, A. H. M.Sc. Thesis, University of California, Berkeley, 1971.
- 3. Abdulsattar, A. H.; Sridhar, S.; Bromley, L. A.

 Am. Inst. Chem. Engnrs. J. 1977, 23, 62.

- Sulfur dioxide; SO₂; [7446-09-5]
- 2. Seawater

ORIGINAL MEASUREMENTS:

Douabul, A.; Riley, J.

J. Chem. Engng. Data. <u>1979</u>, 24, 274-276.

VARIABLES:

PREPARED BY:

Temperature, salinity.

C.L. Young

EXPERIMENTAL VALUES:

т/к	Salinity /gkg-1	Specific gravity of soln.	Solubilit exptl.	ty ⁺ /mol dm ⁻³ smoothed	
278.97	0.0	1.074	2.959	2.959	
	10.065 20.034	1.080 1.087	2.956 2.954	2.956 2.954	
	30.074	1.095	2.954	2.953	
	40.005	1.103	2.953	2.953	
283.12	0.0	1.067	2.482	2.491	
203.12	10.065	1.075	2.479	2.488	
	20.034	1.082	2.477	2.487	
	30.074	1.088	2.477	2.486	
	40.005	1.094	2.476	2.485	
288.10	0.0	1.055	2.065	2.047	
	10.065	1.063	2.062	2.044	
	20.034	1.071	2.061	2.042	
	30.074	1.078	2.060	2.042	
	40.005	1.085	2.059	2.041	
292.98	0.0	1.045	1.697	1.706	
	10.065	1.052	1.694	1.704	
	20.034	1.059	1.693	1.703	
	30.074	1.066	1.692	1.701	
200 1 =	40.005	1.074	1.691	1.700 1.421	
298.15	0.0	1.032 1.042	1.419 1.417	1.421	
	10.065	1.042	1.417	1.420	
	20.034 30.074	1.058	1.414	1.417	
	30.074	1.000	T.474		

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Sulfur dioxide bubbled through seawater for 21 hours with gentle stirring. Pressure measured with mercury manometer. Samples of about 60 cm³ were withdrawn and mixed with 150 cm³ of hydrogen peroxide solution. Solution then titrated with carbonate free sodium hydroxide solution. Allowance made for acid originally in sample.

SOURCE AND PURITY OF MATERIALS:

- Refrigeration grade obtained from BDH. Mass spectrometric analysis showed its purity to be better than 99.9 mole per cent.
- 2. Surface water from Irish sea filtered and samples of salinities ranging from 10-40% prepared by evaporation or dilution with distilled water, acidified to pH 2.8 with sulfuric acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01; \delta x_{SO_2} = \pm 0.1$ %

- 1. Sulfur dioxide; SO; [7446-09-5]
- 2. Seawater

ORIGINAL MEASUREMENTS:

Douabul, A.; Riley, J.

J. Chem. Engng. Data. 1979,24, 274-276.

EXPERIMENTAL	WATTEC.
EXPERIMENTAL	VALUES:

T/K	Salinity, /gkg ⁻¹	Specific gravity of soln.	Solubilite exptl.	ty ⁺ /mol dm ⁻³ smoothed
298.15	40.005	1.064	1.414	1.416
303.25	0.0	1.028	1.201	1.199
	10.065	1.034	1.200	1.198
	20.034	1.040	1.198	1.196
	30.074	1.048	1.197	1.195
	40.005	1.056	1.196	1.194

+ Partial pressure of SO₂ = 1 atm = 101.3 kPa.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Metallic salts

EVALUATOR:

C. L. Young, *
School of Chemistry,
University of Melbourne,
Parkville, Victoria 3052,
Australia.

August 1980

CRITICAL EVALUATION:

The evaluation of the data for aqueous solutions of 19 salts reported by Fox (1) is uncertain, because of unsatisfactory presentation. Fox expressed the concentration of the salt as "normality," using one half of the molecular weight in the examples of the sulfates of sodium, potassium and ammonium, and of the halides and sulfate of cadmium. "solubility" was expressed as the Ostwald coefficient, L; but it is not absolutely clear if the volume used was that of the original liquid (initial solution of salt) or that of the solution saturated with sulfur Densities were not recorded, and therefore mole fractions cannot be accurately estimated. The weights of sulfur dioxide absorbed by a given volume or weight of solution were not reported, although these data were determined. The particular weight was converted into a volume of gas by the use of 22.4 dm3 as the molar volume of sulfur dioxide at 273.15 K and 1 atm; whereas the real volume is 21.87 dm^3 . This means that the L values as given are about 2% too large.

In Seidell and Linke (2) the data were given (p.1413) as the "Ostwald Solubility Expression ml SO₂ at t°, l atm per ml solvent". Bancroft and Gould (3) gave a table of Bunsen absorption coefficients for sulfur dioxide and aqueous solutions of sodium and potassium salts restricted to "0.5 molar." These data are based entirely on the Fox data, although this source was not acknowledged. The coefficients for the sulfates, given as for "0.5 molar" are based on Fox's L values for 0.5 normal, i.e., 0.25 molar. In Seidell and Linke (p.1414) the Bancroft and Gould list is given as if these were original data.

Hudson's (4) data were presented in the rudimentary form of g SO₂/ 100 g water content for each concentration of salt (only potassium chloride and sodium sulfate were studied) as g salt/100 g of water content. main uncertainty in the Hudson values lies in the allowance for the vapor pressure of water over the final solution. Data on the lowering of the vapor pressure of water over the aqueous solution of potassium chloride were taken from the work of Tammann (5), and could be as much as 75 mmHg The lowering due to dissolved sulfur dioxide was calculated on at 363 K. the basis of Raoult's law, and was estimated as about 0.1% at 283 K and The author believed the corrections to be only approxi-1.25% at 363 K. mate, "as there are grounds for believing that sulphur dioxide combines both with the water and with the added salts." Hudson assumed the application of Henry's law (mole ratio form) in the adjustment of the g SO₂/100 g H₂O value from the estimated p_{SO_2} to 1 atm. As presented, the data for sodium sulfate solutions did not show the breakdown into p_{Total}

based on a more detailed evaluation in terms of the R-line approach (11) by W. Gerrard.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Metallic salts

EVALUATOR:

C. L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

August 1980

CRITICAL EVALUATION:

and p_{SO_2} because it was concluded that the estimated p_{SO_2} values were within 10 mmHg of 1 atm. Again the adjustment to 1 atm was based on Henry's law (mole ratio form). Attempts to correlate the Hudson data and the Fox data are frustrated by the lack of density data in the Fox work. Hudson stated that the densities of the salt solutions themselves are insufficient, for "considerable expansion of the solutions occurs when sulphur dioxide dissolves."

The evaluation of the data of Conrad and Beuschlein (6) on the CaO-water-SO₂ system, and of Conrad and Brice (7) on the MgO-water-SO₂ system requires cognition of the purpose of the measurements, and the definition of "total", "combined", and "free" sulfur dioxide, and that a solid phase was present. The amount of sulfur dioxide in the liquid phase at equilibrium was expressed as g SO₂/100 g water. done in connection with the use of the "Sulfite Process" in the manu-These authors used the following definition decided facture of wood pulp. upon by the Technical Association of Pulp and Paper Institute: SO2 is the actual free SO2 plus half of the SO2 in the bisulfite of calcium (or magnesium), and is more properly called the available SO2 as it indicates the SO2 in excess of the amount necessary to form monosulfite." The authors defined the term "combined sulfur dioxide" as that required to form the monosulfite.

Data by White, Vivian and Whitney (8) are for the calcium sulfite system in which there was no solid phase, and the solution may be deemed as unsaturated with respect to the calcium sulfite. These workers stated the partial pressure, p_{SO_2} , and they reported data for water itself to show the reliability of their data for the salt solutions.

The data of Domansky and Rendos (9) for dilute solutions of "ammonium bisulfite" are deemed acceptable (see compilation sheets).

The earlier data of Smith and Parkhurst (10), determined in relation to the paper-pulp industry, were based on a combined sulfur dioxide (C) fixed by the "normality" of $Ca(SO_3H)_2$ or $Mg(SO_3H)_2$, and not on $CaSO_3$ as in the later TAPPI definition. In the former definition, the free SO_2 is the total (T) SO_2 minus the SO_2 combined as $Ca(SO_3H)_2$ or $Mg(SO_3H)_2$, and is therefore less than that based on the second definition for the same value of SO_2 (T).

References:

- 1. Fox, C. J. J. Z. Phys. Chem. 1902, 41, 458.
- 2. Seidell, A.; Linke, W. F. Solubilities of Inorganic and Organic Compounds, 1958, 1865.

(cont.)

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Metallic salts

EVALUATOR:

C. L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

August 1980

CRITICAL EVALUATION:

References (cont.)

- 3. Bancroft, W. D.; Gould, L. P. J. Phys. Chem. 1934, 38, 197.
- 4. Hudson, J. C. J. Chem. Soc. 1925, 127, 1332.
- 5. Tammann, G. Ann. Phys. Chem. 1885, [2], 24, 523.
- 6. Conrad, F. H.; Beuschlein, W. L. J. Am. Chem. Soc. 1934, 56, 2554.
- 7. Conrad, F. H.; Brice, D. B. J. Am. Chem. Soc. 1948, 70, 2179.
- 8. White, C. K.; Vivian, J. E.; Whitney, R. P. Paper Trade J. <u>194</u>8, 126, 46.
- 9. Domansky, R.; Rendos, F. Chem. Zvesti 1957, 11, 453-460.
- 10. Smith, W. T.; Parkhurst, R. B. J. Am. Chem. Soc. 1922, 44, 1918.
- 11. Gerrard, W. Solubility of Gases and Liquids, 1976, Plenum Press, New York.

40 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Lavrova, E. M.; Tudorovskaya, G. L. 2. Water; H₂O; [7732-18-5] Zh. Prikl. Khim. 1977, 50, 1146-3. Hydrogen chloride; HCl; 1151: J. Appl. Chem. USSR 1977, 50, 1102-[7647-01-0] 1106. VARIABLES: PREPARED BY: C. L. Young Temperature, liquid composition EXPERIMENTAL VALUES: Conc. of HCl in Solubility of Mole fraction of sulfur dioxide sulfur dioxide absorbing soln. T/K /wt-% /wt-8 ^xso₂ 299.2 8.00 0 0.02387 313.2 0.01534 5.25 333.2 0.009063 3.15 353.2 0.0059 2.08 0.00504 363.2 1.77 299.2 2.2 0.02407 8.00 313.2 0.01603 5.42 333.2 3.40 0.0099 353.2 2.75 0.00798 363.2 2.24 0.00647 4.30 299.2 7.76 0.02354 313.2 5.25 0.01569 333.2 2.89 0.0084 353.2 2.47 0.00723 363.2 2.24 0.00654 299.2 11.0 8.40 0.02671 313.2 5.35 0.01660 0.009353 333.2 3.25 353.2 2.50 0.00769 363.2 2.00 0.00607 299.2 15.0 8.40 0.02891 313.2 5.50 0.01750 333.2 3.48 0.01089 (cont.) AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide bubbled into 1. Prepared by action of "cp" hydrochloric acid solution. sulfuric acid on analytical Solubility determined by acidimetric grade sodium sulfite. Dried. analysis of liquid phase after 2. No details given. oxidation of dissolved sulfur 3. "cp" grade.

dioxide to sulfuric acid using hydrogen peroxide.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \quad \delta x_{SO_2} = \pm 5\%.$

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Hydrogen chloride; HCl; [7647-01-0]

ORIGINAL MEASUREMENTS:

Lavrova, E. M.; Tudorovskaya, G. L. Zh. Prikl. Khim. 1977, 50, 1146-1151;

J. Appl. Chem. USSR 1977, 50, 1102-

EXPERIMENTAL VALUES:

T/K	Conc. of HCl in absorbing soln. /wt-%	Solubility of sulfur dioxide /wt-%	Mole fraction of sulfur dioxide \$\pi_{SO_2}\$
353.2	15.0	2.67	0.00830
363.2		2.06	0.00637
299.2	20.0	13.65	0.0470
313.2		6.28	0.02113
333.2		4.00	0.0130
353.2		3.60	0.01160
363.2		2.67	0.00854
299.2	21.5	13.65	0.00484
313.2		6.47	0.02199
333.2		3.72	0.01267
353.2		3.01	0.00975
363.2		2.73	0.00880
299.2	24.8	18.8	0.07154
313.2		6.14	0.02081
333.2		3.15	0.01040
353.2		2.90	0.00956
363.2		0.909	0.00295
299.2	28.0	13.7	0.05034

Smoothing equations of the form $\log x_{SO_2} = -A + B/(T/K)$

were given.

Conc. of HCl/wt-%	A	В
0	5.47	1.41
2.2	4.77	0.937
4.3	4.85	0.953
11.0	5.1	1.050
15.0	5.1	1.051
22.0	5.19	1.128
21.5	5.43	1.20
24.8	7.8	1.96

42 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Miles, F.D.; Fenton, J. J. Chem. Soc. 1920, 117, 59-61. Water; H₂O; [7732-18-5] Sulfuric acid; H2SO4; [7664-93-9] VARIABLES: PREPARED BY: Concentration of acid. W. Gerrard. EXPERIMENTAL VALUES: T/K Sulfuric acid SO₂dissolved *Moles SO₂ *Moles SO₂/ total by 100 g of acid / g /100 g acid number of moles, per cent $H_2SO_4 + H_2O$ in 100 q of acid. 0.0802 0.0262 293 55.1 5.13 0.0269 59.6 4.90 0.0766 0.0273 61.6 4.82 0.0753 0.0267 68.9 4.16 0.0650 74.1 3.63 0.0567 0.0258 78.3 3.23 0.0505 0.0252 80.2 3.12 0.0488 0.0254 82.5 2.99 0.0467 0.0258 84.2 2.88 0.0450 0.0259 85.3 2.83 0.0442 0.0261 85.8 2.80 0.0438 0.0263 86.5 2.82 0.0441 0.0270 0.0290 88.1 2.9 0.0453 90.8 0.0484 0.0337 3.10 0.0372 92.8 0.0502 3.21 3.27 93.7 0.0511 0.0391 94.0 3.31 0.0517 0.0400 94.6 0.0432 3.50 0.0547 95.5 0.0577 0.0471 3.69 95.6 0.0589 3.77 0.0483 96.5 3.83 0.0598 0.0508 98.0 3.98 0.0622 0.0560 98.5 4.03 0.0630 0.0579 "Sulfuric acid per cent" probably means by weight. The term NOTE: "acid" refers to the aqueous solution of sulfuric acid. Calculated by compiler. AUXILLIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide was passed into the No information given. acid (15-20 g), mechanically stirred in a test-tube held in a thermostat. Samples of the saturated solution were withdrawn into small weighed glass bulbs that were sealed, weighed, and opened under (1) N-sodium hydroxide, (2) N/10-ESTIMATED ERROR: iodine for chemical titrations. $\delta T/K = \pm 0.1$ "A correction was applied when the barometer diverged appreciably from 760 mm." REFERENCES:

- Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Sulfuric acid; H₂SO₄; [7664-93-9]

ORIGINAL MEASUREMENTS:

Cupr, V.

Rec. Trav. Chim. 1928, 47, 55-72.

VARIABLES:

PREPARED BY:

Temperature, concentration of acid.

W. Gerrard.

EXPERIMENTAL VALUES:

The values were stated to be for a total pressure of 760 mmHg, i.e., for 1 atm = 101.325 kPa.

T/K 314.15

T/K 335.15

.5		1/1/ 22	2.12		
Wt. of SO ₂ /100 g solution of H ₂ SO ₄ /g	L	in 100 g	/100 g	L	
4.88	16.9	0.00	2.16	7.42	
4.75	16.5	0.00	2.13	7.32	
3.65	13.3	10.02	1.71	6.28	
3.35	12.8	30.26	1.26	5.25	
3.29	12.8	30.52	1.20	5.00	
2.57	11.9	54.06	1.20	5.90	
1.68	9.47	79.07	1.19	6.95	
1.54	9.18	84.34	1.15	6.95	
1.36	8.40	84.82	1.17	7.08	
1.45	8.96	90.73	1.19	7.36	
1.47	9.09	91.20	1.17	7.28	
1.81	11.5	93.68	1.16	7.26	
2.06	13.1	96.10	1.16	7.29	
2.15	13.6				
	Wt. of SO ₂ /100 g solution of H ₂ SO ₄ /g 4.88 4.75 3.65 3.35 3.29 2.57 1.68 1.54 1.36 1.45 1.47 1.81 2.06	Wt. of SO ₂ /100 g solution of H ₂ SO ₄ /g 4.88 4.75 16.5 3.65 13.3 3.35 12.8 3.29 12.8 2.57 11.9 1.68 9.47 1.54 9.18 1.36 8.40 1.45 8.96 1.47 9.09 1.81 11.5 2.06 13.1	Wt. of SO ₂ /100 g solution of H ₂ SO ₄ /g in 100 g solution / g 4.88 16.9 0.00 4.75 16.5 0.00 3.65 13.3 10.02 3.35 12.8 30.26 3.29 12.8 30.52 2.57 11.9 54.06 1.68 9.47 79.07 1.54 9.18 84.34 1.36 8.40 84.82 1.45 8.96 90.73 1.47 9.09 91.20 1.81 11.5 93.68 2.06 13.1 96.10	Wt. of SO2 Weight of H2SO4 Wt. of SO2 /100 g L in 100 g /100 g solution of H2SO4/g solution / g solution of H2SO4/g 4.88 16.9 0.00 2.16 4.75 16.5 0.00 2.13 3.65 13.3 10.02 1.71 3.35 12.8 30.26 1.26 3.29 12.8 30.52 1.20 2.57 11.9 54.06 1.20 1.68 9.47 79.07 1.19 1.54 9.18 84.34 1.15 1.36 8.40 84.82 1.17 1.45 8.96 90.73 1.19 1.47 9.09 91.20 1.17 1.81 11.5 93.68 1.16 2.06 13.1 96.10 1.16	Wt. of SO2 /100 g solution of H2SO4/g Weight of H2SO4 solution of H2SO4/g Wt. of SO2 /100 g solution of H2SO4/g L solution / g solution of H2SO4/g 4.88 16.9 0.00 2.16 7.42 4.75 16.5 0.00 2.13 7.32 3.65 13.3 10.02 1.71 6.28 3.35 12.8 30.26 1.26 5.25 3.29 12.8 30.52 1.20 5.00 2.57 11.9 54.06 1.20 5.90 1.68 9.47 79.07 1.19 6.95 1.54 9.18 84.34 1.15 6.95 1.36 8.40 84.82 1.17 7.08 1.36 8.40 84.82 1.17 7.08 1.45 8.96 90.73 1.19 7.36 1.47 9.09 91.20 1.17 7.28 1.81 11.5 93.68 1.16 7.26 2.06 13.1 96.10 1.16 7.29

The symbol L indicates the "absorption coefficient" which appears to be the volume in cm³ (adjusted to 273 K) of SO_2 absorbed to give one cm³ of solution saturated with SO_2 at 760 mmHg and at the temperature recorded in the table. These were calculated from the weight values and the published densities of aqueous solutions of sulfuric acid. See evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was passed into the aqueous solution in an "absorption apparatus." A sample was withdrawn into a weighed flask for the determination of sulfur dioxide by a chemical titration, using the iodine-thiosulfate technique.

The "absorption coefficient, L" was determined by calculation from the weight data. The molar volume of 22400 cm³ appears to have been used to convert weight of SO_2 into volume

SOURCE AND PURITY OF MATERIALS:

- (1) Sulfur dioxide was obtained from Merck quality sodium sulfite and concentrated sulfuric acid, and passed through the acid.
- (2) Water may be taken as of satisfactory purity.
- (3) Sulfuric acid was of satisfactory purity. The solutions were attested volumetrically.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Lopatto, E.K.; Savinaev, A.M. Sulfur dioxide; SO_2 ; [7446-09-5] J. Applied Chem. (USSR) 1934, 7, 2. Water; H₂O; [7732-18-5] Sulfuric acid; H₂SO₄; [7664-93-9] 881-886. VARIABLES: PREPARED BY: Concentration of acid, partial W. Gerrard. pressure of gas. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaWeight % of % SO_2 in aqueous solution of acid at T/K *% SO2 in H₂SO₄ in aqueous mixture of 323 333 313 solution air + SO₂ 293 303 (initial). 61.59 9 0.345 0.262 0.194 0.153 0.250 12 -0.587 0.449 0.314 1.990 1.495 1.00 1.730 24 66.71 7.2 0.304 0.221 0.167 0.253 0.342 11.2 17.6 0.809 0.560 0.401 0.569 0.486 19.2 1.172 23.8 0.734 0.891 0.726 27.9 1.920 34.2 1.317 1.043 2.058 37.6 0.255 0.137 0.104 0.175 70.74 9 0.199 0.270 12 0.362 0.162 0.420 0.344 0.271 18 0.522 0.418 0.355 24 0.744 0.542 0.249 73.64 9 0.415 0.327 0.169 12 0.523 0.395 0.270 0.210 0.474 24 0.854 0.609 0.371 78.04 9 0.380 0.262 0.209 0.146 0.353 0.252 12 0.455 0.194 0.439 0.340 18 0.586 0.263 24 0.779 0.542 0.452 0.364 * By volume + Typographical error in original. Should be 0.730. This error was copied without comment in "Solubilities of Inorganic and Organic Compounds", Seidell, A.; Linke, W.F. 1958-1965. METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A mixture of air and sulfur dioxide May be taken as satisfactory. was passed into the bottom of an absorption tube via a porous plate above which the aqueous solution was held. A thermometer reaching below the liquid was fitted into the tube. The tube was immersed in a thermostat. ESTIMATED ERROR: REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Johnstone, H.F.; Leppla, P.W. 2. Water; H₂O; [7732-18-5] J. Am. Chem. Soc. 1934, 56, 2233-2238 З. Sulfuric acid; H2SO4; [7664-93-9] VARIABLES: PREPARED BY: W. Gerrard. Pressure, concentration of acid EXPERIMENTAL VALUES: T/K = 298.15Conc. of H2SO4, Pressure, Conc. of SO2, Ratio of *Mole fraction $/mol kg^{-1} (H_2O)$ /mol kg^{-1} (H₂O) $p_{\rm SO_2}$ /atm conc. of x_{SO,} $\frac{\text{SO}_2/p_{\text{SO}_2}}{\text{/mol}_1\text{kg}^{-1}}$ referred to H₂O (**) atm-1 0.0879 0.00130 0.00193 1.485 0.0260 0.0879 0.00571 0.01129 1.977 0.0344 0.0879 0.01022 0.01878 1.838 0.0320 0.5174 0.00130 0.00161 1.238 0.0218 0.5174 0.00571 0.00796 1.394 0.0245 0.01022 0.01345 1.316 0.0232 0.5174 0.00131 0.00134 1.023 0.0181 1.103 1.103 0.00573 0.00719 1.255 0.0221 1.103 0.01022 0.01253 1.226 0.0216 * Calculated by the compiler ** Assuming all the liquid is pure water.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The low partial pressures of sulfur dioxide were attained by using a mixture of nitrogen and sulfur dioxide, the latter being measured from a gas buret. The sulfur diox was passed into a "Pyrex saturator (Bichowsky, and Storch) (1)" until The sulfur dioxide 2. Conductivity water. equilibrium was reached, as indicated by concordance of successive analyses Samples were withdrawn for titration With iodine and thiosulfate solutions

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide stated to be of high purity from a tank of the liquid.
- 3. Not stated.

ESTIMATED ERROR:

REFERENCES:

1. Bichowsky, F.R.; Storch, H. J. Am. Chem. Soc. 1915, 37, 2695.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Milbauer, J. Water; H₂O; [7732-18-5] Sulfuric acid; H₂SO₄; 2. Bull. Soc. Chim. 1935, (5), 3, 221-224 3. [7664-93-9] VARIABLES: PREPARED BY: W. Gerrard Temperature EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaWeight of SO₂ T/K Density of the acid solution, /g cm⁻³ absorbed by 100 g of the original acid solution/q 296.15 3.075 1.824 2.270 (90.8% H₂SO₄) 303.15 323.15 1.525 0.436 373.15 0.171 423.15 473.15 0.053 510.15 0.040 298.15 1.53 3.1582 (62% H₂SO₄) 318.15 1.4597 1.0200 333.15 353.15 0.5813 373.15 1.4908 * (Probably meant to be 0.4908) * By compiler. There was no mention of pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide was passed into a Sulfur dioxide was stated to be weighed amount of the aqueous acid "pure," and was dried by sulfuric solution in a bubbler tube fitted with an inlet tap and an outlet tap. acid. The temperature was stated to be 2. Distilled water was mentioned in controlled to within ±0.1°C. the description of the chemical Pressure was not mentioned. The titration. weight of sulfur dioxide absorbed was determined by a chemical titrat-3. Presumably good quality sulfuric ion using iodine-thiosulfate acid was used. solutions. ESTIMATED ERROR: REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Sulfuric acid; H₂SO₄; [7664-93-9]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c, f	_l c,d	Mole ratio	Mole fraction ^e
_S a,b	α	α			
21,2	19.2	19.2	19.2	0.046	0.044

- a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.
- b Determined by static absorption method.
- ^c Determined by flow method.
- d α = l(1 p_s°) where p_s° is the vapor pressure of solvent.
- e Calculated by compiler.
- f Assuming vapor pressure of sulfuric acid is negligible.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Sulfuric acid (fuming); H₂SO₄; [7664-93-9]

ORIGINAL MEASUREMENTS:

Miles, F.D.; Carson, T.

J. Chem. Soc. 1946, 786-790.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:	760 mmHg =	= 1 atm = 101	.325 kPa.	
T/K	SO ₃ , % Total	SO ₂	*Mole SO ₂ / mole SO ₃	
293.15	80.21 80.37 80.64 80.81 81.63 82.07 82.12 82.13 82.17 82.53 82.75 82.8 82.85 82.90 82.90 82.91 83.65 84.57 85.77 85.77 85.77 86.49 86.49 86.65 86.71	3.85 3.81 3.66 3.65 3.88 3.95 3.95 3.96 3.98 4.66 4.18 4.58 4.58 4.58 4.60 4.48 4.28 4.96 5.62 6.18 6.27 6.77 5.99 7.06	0.0600 0.0593 0.0567 0.0565 0.0594 0.0602 0.0586 0.0595 0.0603 0.0605 0.0706 0.0631 0.0691 0.0653 0.0694 0.0675 0.0645 0.0741 0.0831 0.0901 0.0912 0.0979 0.0866 0.0864 0.0864	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The "absorber" was a glass vessel "5 inches by 1.25 inches", closed by a large tap. A gas inlet was attached to the side, and had a perforated end. "Acid or oleum" was weighed in the tube. Sulfur dioxide was passed into the liquid, which was shaken; and saturation was deemed to be complete after 1-2 hours. Samples of the final liquid were obtained by means of capillary-bulb tubes and the sulfur dioxide was determined by iodine-thiosulfate titrations.

The weight of sulfur dioxide was stated to be corrected to correspond with "an atmosphere of dioxide at 760 mm pressure by multiplying each of the experimental values by the factor 760/(P-p),"P being the atmospheric pressure recorded during the determination, and p being the vapor pressure of sulfuric trioxide over the oleum at the temperature of saturation .

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was used from a cylinder.
- 2. No information.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Miles, F.D.; Carson, T. 2. Sulfuric acid (fuming); H2SO4; [7664-93-9] J. Chem. Soc. 1946, 786-790. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa*Mole SO2/ T/K SO₃ % SO₂ Total mole SO3 293.15 86.93 7.52 0.1081 87.11 6.47 0.0928 9.06 0.1288 87.90 88.30 9.17 0.1298 9.58 0.1352 88.60 9.41 0.1323 88.90 90.65 11.98 0.1652 12.05 0.1661 90.70 12.17 0.1670 91.10 0.1662 12.14 91.30 18.73 0.2513 93.16 18.93 0.2536 93.30 20.42 0.2736 93.30 0.2716 93.34 20.28 0.3093 94.20 23.31 94.60 22.13 0.2924 95.22 25.78 0.3384 95.02 27.58 0.3628 95.10 28.34 0.3725 95.23 28.16 0.3696 313.15 56.75 1.798 0.0396 1.747 0.0384 56.90 56.90 1.764 0.0387 1.712 0.0375 57.0 57.05 1.702 0.0373 1.602 0.0308 64.99 65.04 1.406 0.0270 0.0275 1.431 65.13 65.87 1.406 0.0267 0.0276 73.64 1.628 0.0277 73.70 1.634 0.0307 78.15 1.920 1.792 0.0286 78.20 78.20 1.928 0.0308 1.981 0.0312 79.38 79.39 2.035 0.0320 79.52 2.050 0.0322 80.80 2.020 0.0313 80.95 2.050 0.0317 82.70 2.468 0.0373 85.0 3.176 0.0467 85.0 3,132 0.0461 333.15 57.75 0.983 0.0213 0.986 57.9 0.0213 57.91 0.988 0.0213 0.855 65.88 0.0162 66.03 0.834 0.0158 0.0160 66.14 0.848 66.23 0.858 0.0162 0.949 0.0161 73.75 0.953 0.0161 73.82 0.990 73.87 0.0168 0.0191 78.22 1.196 1.172 0.0187 78.31 1.346 0.0212 79.50 1.337 0.0210 79.57 79.60 1.359 0.0213 1.371 0.0214 79.90 1.625 0.0241 84.30 1.610 0.0238 84.40 Calculated by compiler (cont'd)

Sulfur dioxide; SO₂; [7446-09-5]
 Sulfuric acid (fuming); H₂SO₄;

1

Miles, F.D.; Carson, T. J. Chem. Soc. <u>1946</u>, 786-790.

ORIGINAL MEASUREMENTS:

[7664-93-9]

EXPERIMENTAL VALUES:

- % Total SO₃ = 100 SO₃/(SO₃ + H₂O);
 - % SO_2 = g of SO_2 dissolved by 100 g of acid or oleum, corrected for a pressure of 760 mm of SO_2 .

The authors stated "to obtain a rough check on the applicability of Henry's law, some measurements of the equilibrium absorption from a gas mixture containing 6% of sulfur dioxide were also made." The gas mixture was stated to contain 94% of air, $p_{\rm SO_2}$ then being taken as 0.06 atm.

e.	T/K	Liquid composition	Solubility at 1 atm S1	Solubility S at 0.06 atm S_2	S ₁ x 0.06
	293	80.2% H ₂ SO ₄ 65.4% total SO ₃	3.10	0.187	0.186
	313 333		1.43 0.85	0.0974 0.0637	0.086 0.051
	293 313 333	96.5% H ₂ SO ₄ 78.6% total SO ₃	3.80, 1.95 1.28	0.222 0.126 0.0863	0.228 0.117 0.0768
	293 313 333	104% H ₂ SO ₄ 17.8% free SO ₃	5.70 2.90 1.74	0.342 0.193 0.120	0.342 0.174 0.105

 S_1 and S_2 are g $SO_2/100$ g acid.

- Sulfur dioxide; SO_2 ; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- З. Sulfuric acid; H₂SO₄; [7664-93-9]

ORIGINAL MEASUREMENTS:

Parkison, R.V.

TAPPI, 1956, 39, (7), 517-519.

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa

T/K	$p_{\mathrm{SO}_2}/\mathrm{atm}$	SO_2 /lb mol ft ⁻³	**SO2	**so2/pso2
283.15 (50°F)	0.00150 0.00505 0.0174 0.0185 0.0261 0.0281 0.0332 0.0350	0.000255 0.000850 0.00307 0.00329 0.00470 0.00498 0.00588	0.0000735 0.000245 0.000885 0.000949 0.001355 0.00144 0.00170 0.00177	0.0467 0.0463 0.0484 0.0488 0.0493 0.0486 0.0486
294.26 (70°F)	0.00153 0.00339 0.00480 0.00662 0.00913 0.00983 0.0182 0.0257 0.0345 0.0349	0.000171 0.000413 0.000503 0.000738 0.00102 0.00115 0.00203 0.00289 0.00380 0.00381	0.0000493 0.000119 0.000145 0.000213 0.000294 0.000332 0.000585 0.000833 0.00110	0.0322 0.0351 0.0302 0.0321 0.0322 0.0337 0.0322 0.0324 0.0318 0.0315
305.37 (90°F)	0.00633 0.00641 0.00812 0.00885 0.00952	0.000466 0.000494 0.000601 0.000600 0.000759	0.000134 0.000142 0.000173 0.000173 0.000219	0.0212 0.0222 0.0213 0.0195 0.0230

AUXILIARY INFORMATION .-

METHOD/APPARATUS/PROCEDURE:

A mixture of sulfur dioxide and nitrogen (of desired "solute" concentration) was passed into the "equilibrium"solubility cell by an inlet tube shaped as a funnel at the end under the liquid. A tapped exit for sampling was attached to a bottom corner of the cell. The gas outlet was at the top of the cell. The cell was placed in a thermostat. The and liquid were analyzed by the The gas Palmrose technique(1), an iodine-thiosulfate type of titration. T The gas mixtures were analyzed by drawing samples into gas weighing balloons of l dm3 capacity.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was of refriger-(1) ant grade.
- (2) Water was "triple-distilled from a Pyrex still."

ESTIMATED ERROR:

REFERENCES:

1. Palmrose, G.V.

Paper Trade J. 1935, 100, No. 3, 38.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Sulfuric acid; H₂SO₄; [7664-93-9]

ORIGINAL MEASUREMENTS:

Parkison, R.V. *TAPPI*, 1956, 39, (7),517-519.

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa.

T/K	p _{SO2} /atm	SO ₂ /lb mol ft ⁻³	* ^x SO ₂	** _{SO2} /p _{SO2}
305.37 (90°F)	0.0110 0.0178 0.0251 0.0336	0.000801 0.00126 0.00205 0.00244	0.000231 0.000363 0.000591 0.0007035	0.0210 0.0204 0.0235 0.0209

* Calculated by compiler

Molality of sulfuric acid was 0.058, i.e., 5.684 g $\rm H_2SO_4$ in 1 kg of water. *The approximate mole fraction, $x_{\rm SO_2}$ was referred to 1 cu.ft. of water, taking 3.468 lb. moles of water per cu.ft.

NOTE:

At these low partial pressures the average value of 64.08 was used by Parkison for computing the partial pressure of sulfur dioxide from the analysis of the dry gas. The vapor pressure of water over the solutions of sulfur dioxide was taken to be the same as for pure water.

Aqueous electrolyte solutions 53 COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Hansen, C.J. 2. Water; H₂O; [7732-18-5] 3. Thiocyanic acid; HCNS; Ber. 1933, 66 447-450 [463-56-9] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: At 277.65 K, 76.9 g (76 cm 3 , density = 1.012 g cm $^{-3}$) of solution containing 5.52 g HCNS (0.0936 mole) and 0.20 g "H₂SO₄" absorbed 16.9 g SO₂(0.264 mole) to give 93.8 g (82.5 cm³, density, 1.14 g cm⁻³). The mole ratio, SO₂/HCNS (not given by the author) is 2.821; mole fraction, $x_{\rm SO_2}$ is 0.738. At 283.15 K, 63.2g (57 cm 3 , density, 1.11 g cm $^{-3}$) of solution containing 23.8 g HCNS, 0.403 (given by the author as 0.402) mole, absorbed 27.1 g SO₂(0.423 mole) to give 90.3 g (72.5 cm 3 , density, 1.247 g cm $^{-3}$) of final solution. The mole ratio, SO₂/HCNS was given as 1.054, the compiler gives 1.050, mole fraction, $x_{SO_2} = 0.512$. The total pressure appeared to be an unspecified barometric pressure. The author gave the concentration of the NOTE: hydrocyanic acid as 46.30% in the second determination; but the concentration should be given as 37.66%. AUXILIARY INFORMATION ... METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. The sulfur dioxide was stated Sulfur dioxide was passed into a known amount of the to be pure. acid solution in a measuring cylinder. The final solut-3. Prepared from barium thiocyanate. ion was weighed, and its volume determined. ESTIMATED ERROR: REFERENCES:

Sulfur Dioxide Solubilities 54 ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. 2. Water; H₂O; [7732-18-5] Z. Phys. Chem. 1902, 41, 458-482 3. Ammonium chloride; NH₄Cl; [12125-02-9] VARIABLES: PREPARED BY: Concentration of salt W. Gerrard. EXPERIMENTAL VALUES: T/K "Normality" 3 2.5 1.5 0.5 Ostwald coefficient, 42.78 41.37 39.76 38.06 36.37 298 34.58 (L for water given as 32.76). The following arithmetic was shown by the original author: $a = cm^3 SO_2$ (273 K, 760 mmHg) in 1 cm³ of "solution" presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm^3 ; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂. 1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO $_2$ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the L values are about 2% too large. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine—thiosulfate titration.

- Sulfur dioxide, 99.8% SO₂, 0.2% water, commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

STIMATED	ERROR:
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COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] l. 2.

Water; H₂O; [7732-18-5]

Ammonium bromide; NH, Br; [12124-97-9]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

PREPARED BY:

Concentration of salt

W. Gerrard.

EXPERIMENTAL VALUES:

T/K "Normality"

2.5

2

1

298

Ostwald coefficient, 52.25 49.17

46.06

42.78 39.46 36.28

0.5

(L for water given as 32.76)

The following arithmetic was shown by the original author:

- $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution", presumably meaning the salt solution before absorption of gas.
- cm3 of iodine solution containing s equivalents per dm3; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂.

1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, $\alpha = (11.2 \text{ sx})/c$ (T/K / 273 K). The coefficient L was taken to be equal to α (760/b). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, $^{2.9266}$ g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO₂ is 21.87 dm 3 and not 22.4 dm3 under these conditions; therefore all the L values are about 2% too large.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus 3. being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet $(0.9181 to 1.436 cm^3)$, and the amount of SO₂ determined by iodine thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO2, 0.2% water, commercial.
- Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallized and analytically attested.

ESTIMATED ERROR:

56 Sulfur Dioxide Solubilities ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Fox, C.J.J. ٦. Water; H₂O; [7732-18-5] 2. Ammonium sulfate; (NH4)2SO4; Z. Phys. Chem. 1902, 41, 458-482. 3. [7783-20-2] VARIABLES: Temperature, concentration of salt. "Normality" 2.5 T/K 35.47 Ostwald coefficient, 35.96 298 L(L for water given as 32.76) Ostwald coefficient, 24.60 24.23 308 (L for water given as 22.43) I₂ taken to be equivalent to 0.001 mole SO₂.

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES: Equivalent taken by the author as 1/2 (NH4) 2SO4

0.5 1.5 34.95 34.34 33.82 33.35 22.91 23.93 23.49 23.14

The following arithmetic was shown by the original author:

- $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole

 $1/2 \ sx = a/22.4$, for one cm³ of the saturated solution. For $c \ cm^3$ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation)

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm^{-3} at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm³ and not 22.4 dm3 under these conditions; therefore all the L values are about 2% too large.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel was fitted with 1. electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus 3. Salt of Kahlbaum grade, rebeing held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodinethiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO2 , 0.2% water, commercial.
- 2. Presumably conductivity grade.
- crystallised and analytically attested.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Otuka, Y. 2. Water; H₂O; [7732-18-5] J. Soc. Chem. Ind., Japan. Suppl. Ammonium bisulfite; NH₄HSO₃; 1939, 42, 205B-20 B [10192-30-0] VARIABLES: PREPARED BY: W. Gerrard Temperature, pressure EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaMole SO₂/dm³ HT/K P_{Total}/atm P_{SO2}/atm solution 373 1.73 0.75 0.1857 0.248 0.2518 0.252 1.00 1.98 0.1819 378 2.03 0.87 0.209 0.2478 0.219 1.13 2.29 0.98 0.1788 0.183 383 2.36 1.28 0.2434 0.190 2.66 1.10 0.1753 0.159 388 2.73 1.40 0.2399 0.171 3.03 0.142 1.21 0.1724 393 3.13 1.56 3.47 0.2354 0.151 1.32 1.72 398 3.56 0.1693 0.128 0.2311 3.95 0.134 403 4.06 1.45 0.1659 0.114 4.48 1.88 0.2269 0.121 408 4.61 1.59 0.1624 0.102 0.110 5.03 2.02 0.2233 1.70 0.1598 0.094 413 5.19 5.61 2.14 0.2203 0.103 5.80 1.80 0.1574 0.087 418 2.23 0.2180 0.098 6.22 0.1562 0.084 423 1.85 6.42 0.096 6.83 2.27 0.2170 "Solution" appears to mean final solution. The author defined the solubility as $H=(H_2SO_3)/p_{SO_2}$, the pressure being in atm. (H_2SO_3) evidently means mole SO_2/dm^3 of solution. The concentration of NH_4HSO_3 was given as 0.3000 mole/dm 3 . NOTE: The author refers to "pure sulfurous acid, H2SO3.' METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The total pressure, P_{Total}, was Not stated. determined by means of a glass spring manometer. It was stated that the partial pressures were approximated from the dimensions of the apparatus, but details were not given. ESTIMATED ERROR: REFERENCES:

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Marriner, D. E.; Whitney, R. P. 2. Water; H₂O; [7732-18-5] Paper Trade J. 1948, 126 (Tappi section), 52-54. [10192-30-0] VARIABLES: Temperature, pressure ORIGINAL MEASUREMENTS: Marriner, D. E.; Whitney, R. P. Paper Trade J. 1948, 126 (Tappi section), 52-54. W. Gerrard

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa.

The liquid concentrations are expressed in g SO_2 per 100 g of water. The Total (T) SO_2 is all the SO_2 absorbed by the original aqueous solution of ammonia. The "Combined" (C) SO_2 was defined as that required to convert all "the lime to $CaSO_3$." This presumably means the amount to convert all the ammonia into $(NH_4)SO_3$. The Free SO_2 (F) is the difference T - C.

T/K	p _{SO₂} /mmHg	SO ₂ (T)	SO ₂ (C)	T/K	p _{SO₂} /mmHg	SO ₂ (T)	SO₂ (C)
277.65	124 367 560 655 119 354 569 162 388 580 686 117 350 548	4.4 10.3 15.2 17.9 5.1 11.3 16.5 7.1 12.6 17.6 20.2 6.8 12.5 17.2	0.51 0.47 0.49 0.50 0.97 0.95 0.99 1.40 1.50 1.40 1.35 1.93 1.93	283.15	123 333 567 696 125 313 507 691 139 355 528 660 129 331	3.7 7.9 12.4 14.7 4.6 8.3 12.3 15.4 5.7 9.9 13.2 15.9 6.6 10.3	0.54 0.60 0.55 0.56 1.01 0.94 1.04 0.95 1.44 1.19 1.33 1.97 1.85 cont.)

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

A mixture of sulfur dioxide and nitrogen was passed into aqueous ammonia in a glass cell until equilibrium was reached. Sulfur dioxide in the liquid and in the exit gas was estimated by a chemical tiration - iodine-thiosulfate, see White et al. (1). Temperature was controlled to within ± 0.5 °C. For water at 283.15 K the SO₂ (T) (p_{SO2}) were: 2.1 (86); 6.9 (320); 13.9 (678 mmHq). Total and combined sulfur dioxide were estimated by a modification of the Palmrose technique (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide: refrigeration grade.
- 2. Water: may be taken as pure.
- Chemically pure ammonia solution was used.

Nitrogen from cylinder was mixed with the sulfur dioxide to obtain mixtures of determined sulfur dioxide content to estimate the $p_{\rm SO_2}$.

ESTIMATED ERROR:

- White, C. K. Jr.; Vivian, J. E.; Whitney, R. P. Ann. Meet. Tech. Ass. Pulp and Paper Industry, Feb. 1948.
- Palmrose, G. V. Paper Trade J. 1935, 100, 38.

ORIGINAL MEASUREMENTS:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Ammonium bisulfite; NH4HSO3;
 [10192-30-0]

Marriner, D. E.; Whitney, R. P. $Paper\ Trade\ J.\ \underline{1948}$, 126, (Tappi section), 52-54.

EXPERIMENTAL VALUES:

T/K	$p_{SO_2}/mmHg$	SO ₂ (T)	SO ₂ (C)	T/K	p _{SO2} /mmHg	SO ₂ (T)	SO ₂ (C)
283.15 291.15	518 663 117 562 736 132 360 551 (?)00 115 364 552 706 175 420 610	13.9 16.8 2.9 9.3 11.6 3.7 6.7 9.8 2.7 4.4 7.7 10.5 12.7 6.2 9.8 13.0	2.00 1.67 0.57 0.56 0.49 1.00 1.35 1.35 1.36 1.38 1.34 1.93 1.93 2.00	298.15	119 329 565 706 116 335 532 696 117 343 544 692 (?)00 116 365 558 710	2.5 4.9 7.3 9.2 3.3 5.7 8.1 9.6 4.1 6.6 8.8 10.5 3.8 5.2 7.9 10.1	0.51 0.52 0.57 0.58 0.90 0.98 1.97 0.90 1.40 1.36 1.42 1.40 1.95 1.96 1.98 2.04
1							

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- Ammonium bisulfite; NH, SO₃H; [7803-63-6]

ORIGINAL MEASUREMENTS:

Domansky, R.; Rendos, F.

Chem. Zvesti

1957, 11, 453-460.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa

The values of SO_2/g (T, total), (C, combined as NH_4SO_3H), (F, free = T - C) were given in the original table (as shown in the table here) were for SO_2 absorbed by 100 g water at $p_{SO_2} = 600$ mmHg. The treatment seems to imply that there is a linear change of the weight of SO_2 absorbed with pressure; therefore it may be taken that weight of SO_2 absorbed for $p_{SO_2} = 1$ atm may be approximately calculated by multiplying the stated value by 1.267.

"Concentration of ammonia	*	0%	0.5% SOn/a	1.0% per 100	1.5% g water	2.0%
T/K 288.15	T C F	10.3 - 10.3	11.20 1.90 9.30	12.80 3.80 9.05	14.65 5.70 8.95	17.90 7.60 10.3
293.15	T	8.50	9.70	11.55	13.20	15.65
	C	-	1.90	3.80	5.70	7.60
	F	8.50	7.80	7.75	7.50	8.05
298.15	T	7.5 [,]	8.5	10.25	11.95	14.40
	C	-	1.90	3.80	5.70	7.60
	F	7.5	6.60	6.45	6.25	6.75
303.15	T	6.1	7.50	8.90	11.05	13.50
	C	-	1.90	3.80	5.70	7.60
	F	6.1	5.60	5.10	5.35	5.90
* appears to be	wt-%.				(c	ont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An absorption vessel was fitted with a stirrer, a manometer, one limb bent to pass just through the vessel cover, and the other limb open to the atmosphere, a tapped inlet tube, and a tapped outlet tube, each just passing through the cover of the vessel, for the passage of SO_2 , and The absorption a thermometer. vessel was immersed in a thermostat. A stoppered sampling tube also passed through the cover and ended well below the surface of the solution in the vessel. The weight of SO2 in a withdrawn sample was determined by an iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

It is probable that the components were of acceptable purity for the purpose of the measurements.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- Ammonium bisulfite; NH₄SO₃H; [7803-63-6]

ORIGINAL MEASUREMENTS:

Domansky, R.; Rendos, F.

Chem. Zvesti

1957, 11, 453-460.

EXPERIMENTAL VALUES:

Four small diagrams were given, each for one of the stated concentrations of ammonia, and each showing plots of $p_{\rm SO_2}$ (mmHg) vs. $\rm SO_2/100$ g of ammonia solution for each of the four temperatures stated. All the lines appear to be linear, and the value of g $\rm SO_2$ for 600 mmHg corresponds closely with the appropriate value of $\rm SO_2/g$ (T) in the table. In each diagram, the four lines terminate on the base line ($p_{\rm SO_2}=0$) at the following values of g $\rm SO_2/100$ g ammonia solution: 1.9 (0.5% ammonia); 3.8 (1.0% NH₃); 5.7 (1.5% NH₃); and 7.6 (2.0% NH₃), and these values are recorded in the table as $\rm SO_2/g$ (C), *i.e.*, combined as NH₄SO₃H.

Sulfur Dioxide Solubilities 62 COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. Water: H₂O; [7732-18-5] Z. Phys. Chem. 1902, 41, 458-482 2. 3. Ammonium nitrate; NH4NO3; [6484-52-2] VARIABLES: PREPARED BY: Temperature, concentration of salt W. Gerrard. EXPERIMENTAL VALUES: T/K "Normality" 3 2.5 1.5 2 1 35.07 Ostwald coefficient, 39.14 38.01 37.27 36.28 298 (L for water given as 32.76) Ostwald coefficient, 24.78 24.23 308 27.43 26.66 25.57 (L for water given as 22.43) The following arithmetic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. cm3 of iodine solution containing s equivalents per dm3; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2. $1/2 \ sx = \alpha/22.4$, for one cm³ of the saturated solution. For $c \ cm³$ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation) NOTE by compiler: based on the published density of sulfur dioxide, about 2% too large.

2.9266 g dm⁻³ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm³ and not 22.4 dm³ under these conditions; therefore all the L values are

AUXILIARY INFORMATION

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus 3. being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet $(0.9181 to 1.436 cm^3)$, and the amount of SO₂ determined by iodinethiosulfate titration.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

Sulfur dioxide, 99.8% SO2, 0.2% water, commercial.

0.5

33.96

23,35

- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ER	RC	R:
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0.5

37.78

Aqueous electrolyte solutions COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] ٦. Fox, C.J.J. Water; H₂O; [7732-18-5] 2. Ammonium thiocyanate; Z. Phys. Chem. 1902, 41,458-482. NH₄CNS; [1762-95-4] VARIABLES: PREPARED BY: Concentration of salt W. Gerrard. EXPERIMENTAL VALUES: 3 2.5 2 1.5 "Normality" T/K 52.26 61.46 57.01 47.26 42.74 298 Ostwald coefficient, (L for water given as 32.76) The following arithm tic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2. 1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation). NOTE: by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO $_2$ is 21.87 dm 3 2.9266 g dm⁻³ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 d and not 22.4 dm³ under these conditions; therefore all the L values are about 2% too large. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD /APPARATUS / PROCEDURE: The absorption vessel was fitted with electrodes for the measurement water, commercial. of conductance, data not herein 2. Presumably conductivity grade. recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus 3.

being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount Of SO₂ determined by iodinethiosulfate titration.

- Sulfur dioxide, 99.8% SO2, 0.2%
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED	ERROR
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Sulfur Dioxide Solubilities 64 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Hansen, C. J. 2. Water: H₂O: [7732-18-5] Ber. 1933, 66B, 447-450. 3. Thiocyanic acid, ammonium salt Ammonium thiocvanate; NH₄CNS; [1762-95-4] VARIABLES: PREPARED BY: W. Gerrard Temperature EXPERIMENTAL VALUES: Wt. of SO₂ Vol. Vol. Wt. Conc. of Wt. of abof of of soln. soln. soln. soln. sorbed T/K q salt/ soln. $/cm^3$ /g /g /g /cm³ q soln.

86.0

91.0

97.9

109.6

The total pressure appears to have been unspecified barometric pressure.

53

53

53

53

60

60

60

60

AUXILIARY INFORMATION

was treated in a measuring cylinder with pure sulfur dioxide. The final solution was weighed, and its volume measured, and the weight of sulfur dioxide absorbed was thereby It appears that the determined.

A known amount of the salt solution

290.15

286.65

281.85

276.15

0.5

0.5

0.5

0.5

METHOD /APPARATUS / PROCEDURE:

first temperature was 17 °C, and then the passage of SO2 was continued to get results for the lower temperatures.

SOURCE AND PURITY OF MATERIALS:

68

70.5

73.5

80.5

1. Pure SO₂ was stated to be used.

Mole

ratio

SO₂/

NH 4 CNS

1.028

1.226

1.499

1.962

26.01

31.0

37.9

49.6

2. and 3. Not specified; but may be taken of satisfactory purity.

ESTIMATED ERROR:

[†] Before adsorption of sulfur dioxide.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Applebey, M.P. Water; H₂O; [7732-18-5] J. Soc. Chem. Ind. (Chem. Ind.) Trans. 1937, 56, 139-146. "Basic aluminium sulfate" (approx. $Al_2(SO_4)_3 + Al_2O_3$) VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaData were presented only as a small diagram showing plots of ($\$SO_2$ by volume in the gas phase") vs ("g SO_2 by 100 ml of absorbent solution"). The compiler has interpreted the $\$SO_2$ by volume as the partial pressure, p_{SO_2} , of SO_2 in atm, and has read the following data from the plots. p_{SO},/atm g SO₂/100 ml No. of solution. T/K 293 1 0.01 4.7 0.02 5.5 0.03 0.04 6.3 6.7 0.05 0.06 7.0 0.07 7.4 0.08 0.09 7.8 0.10 293 0.01 6.1 2 0.02 7.1 0.03 7.7 0.04 8.1 8.4 0.05 0.06 8.8 8.95 0.07 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: None were given. The purpose of the measurements was in None given. connection with the recovery of sulfur from smelter gases. ESTIMATED ERROR: REFERENCES:

- Sulfur dioxide; SO₂; [7446-09-5] Water; H₂O; [7732-18-5] "Basic aluminium sulfate" (approx. $Al_2(SO_4)_3 + Al_2O_3$

ORIGINAL MEASUREMENTS:

Applebey, M.P.

J. Soc. Chem. Ind. (Chem. Ind.) Trans. 1937, 56, 139-146.

EXPERIMENTAL VALUES:

No. of solution	т/к	p _{SO2} /atm	g SO ₂ /100 ml
2	293	0.08 0.09 0.10	9.2 9.4 9 6
2	298	0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09	5.6 6.5 7.05 7.45 7.85 8.05 8.3 8.6 8.8
2	303	0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09	5.0 5.9 6.5 6.9 7.2 7.45 7.7 7.9 8.05
3	293	0.01 0.02 0.03 0.04 0.05 0.06 0.07 0.08 0.09	6.9 8.3 9.05 9.55 9.85 10.1 10.35 10.65 10.8

The solution was described as "basic aluminium sulphate solution," the composition being defined as follows:

Solution No.		"Alumina" g/100 ml				
	Free	Combined	\mathtt{Total}			
1 2	3.44 4.00	6.61	10.05	34.2		
3	4.55	5.82	9.82	40.8		
~	4.33	5.32	9.87	46.1		

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Calcium sulfite; CaSO₃;
 [10257-55-3]

ORIGINAL MEASUREMENTS:

White, C.K., Jr.; Vivian, J.E.; Whitney, R.P.

Paper Trade Journal 1948, 126, (20), 46-48.

VARIABLES:

PREPARED BY:

W. Gerrard.

				
EXPERIMENTAL V	Wt. of SO ₂ (C)	g = 1 atm = 101. Wt. of SO ₂ (T) /g		Mole fraction ***SO ₂
283.15	0	1.98 6.70 7.54 10.53 15.45	75 311 353 510 751	0.0056 0.0185 0.0208 0.0288 0.0416
	0.65	2.10 2.23 3.54 3.81 5.25 7.53 9.05 15.80	50 55 118 126 204 324 405 757	0.00408 0.00442 0.00806 0.00881 0.0128 0.0190 0.0231 0.0409
	1.20	2.69 3.61 4.60 7.35 7.94 12.51 12.85 16.03	19 67 122 276 304 564 583 748	0.00417 0.00673 0.00947 0.0170 0.0186 0.0308 0.0315 0.0400

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of nitrogen and sulfur dioxide was passed into a cell containing water and calcium hydroxide until all the calcium hydroxide had disappeared. The final temperature was controlled to within ±0.05°C. Samples of the solution and effluent gas were taken in evacuated weighing bulbs. Total sulfur dioxide in the liquid was determined by a modified Palmrose technique (1) entailing an iodinethiosulfate titration. From the Weight of the calcium hydroxide added the combined sulfur dioxide could be determined. The pressure of the sulfur dioxide was calculated from the analysis, utilizing the measured total pressure, and correcting for deviations from the perfect gas laws.

SOURCE AND PURITY OF MATERIALS:

- (1) The sulfur dioxide was of refrigeration grade.
- (2) Water was presumably of satisfactory purity.
- (3) C.P. calcium hydroxide was used.

ESTIMATED ERROR:

REFERENCES:

(1) Palmrose, G.V.; Paper Trade J. 1935, 100, No. 3, 38.

See also Whitney, R.P.; Vivian, J.E. Ind. Eng. Chem. 1941, 33, 741.

- Sulfur dioxide; SO₂; [7446-09-5]
 Water; H₂O; [7732-18-5]
- Calcium sulfite; CaSO₃; [10257-55-3]

ORIGINAL MEASUREMENTS:

White, C.K., Jr.; Vivian, J.E.; Whitney, R.P.

Paper Trade Journal, 1948, 126, (20), 46-48.

EXPERIMENTAL VALUES:

DAT DIVITION	TILL VILLOUD.				
т/к	Wt. of SO ₂ (C) /g	Wt. of SO ₂ (T) /g	Partial Pressure P _{SO2} /mmHg	Mole fraction *xSO2	
283.15	2.10	5.80 8.33 12.24 17.10	94 246 479 763	0.0103 0.0169 0.0277 0.0405	
291.15	0	4.03 6.21 11.20	250 403 743	0.0112 0.0172 0.0305	
	0.65	1.74 3.21 7.84 11.79	37 140 477 749	0.00306 0.00714 0.0198 0.0304	
	1.20	2.86 4.39 7.89 12.36	38 153 415 748	0.00465 0.00889 0.0185 0.0304	
	2.10	5.03 5.89 6.87 10.62 13.45	71 146 233 541 759	0.00817 0.0105 0.0132 0.0234 0.0309	
298.15	0	2.26 5.34 8.64	169 444 724	0.00632 0.0148 0.0237	
	0.65	2.06 3.05 5.40 9.32	76 167 385 742	0.00395 0.00670 0.0132 0.0238	
	1.20	2.90 3.82 5.91 10.01	53 144 347 741	0.00476 0.00731 0.0128 0.0242	
	2.10	5.05 5.70 8.35 11.26	98 168 448 739	0.00823 0.0100 0.0173 0.0251	

^{*} Calculated by compiler.

Weights of ${\rm SO_2}$ are for (c) "combined as ${\rm CaSO_3}$ " and (T) total per 100 g of water at $p_{\rm SO_2}$.

[&]quot;Free SO_2 " = (T-C)/g. Mole fraction is for free SO2.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Otuka, Y. Water; H₂O; [7732-18-5] 2. J. Soc. Chem. Ind. Japan. Suppl. 3. Calcium bisulfite; Ca(HSO3)2; 1939, 42, 205B-207B. [13780-03-5] VARIABLES: PREPARED BY: W. Gerrard Temperature, pressure EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa $p_{\mathtt{Total}}/\mathtt{atm}$ p_{SO_2}/atm Mole SO₂/dm³ HT/K solution 0.4192 0.217 373 2.90 1.93 2.30 0.5189 0.226 3.27 0.228 2.67 0.6099 3.63 2.12 0.4130 0.195 3.28 378 0.202 2.53 0.5118 3.68 2.92 0.6023 0.206 4.07 0.4071 0.175 3.69 2.32 383 0.183 0.5048 4.13 2.76 4.54 3.18 0.5949 0.187 4.14 2.52 0.4012 0.159 388 0.166 0.4980 4.61 2.99 5.05 3.44 0.5878 0.171 0.3982 0.152 393 4.52 2.62 0.4916 0.153 5.12 3.22 0.5809 0.157 5.59 3.70 0.3927 0.140 5.03 2.81 398 0.140 3.46 0.4849 5.67 0.145 0.5739 6.17 3.97 AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: The total vapor pressure, p_{Total} , was determined by means of a glass Not stated. spring manometer. It was stated that the partial pressures were approximated from the dimensions of the apparatus, but details were not given. ESTIMATED ERROR: REFERENCES:

- Sulfur dioxide; SO₂; [7446-09-5]
 Water; H₂O; [7732-18-5]
- Calcium bisulfite; Ca(HSO₃)₂; [13780-03-5]

ORIGINAL MEASUREMENTS:

Otuka, Y.

J. Soc. Chem. Ind. Japan. Suppl. 1939, 42, 205B-207B

l				
EXPERIMENTAL	VALUES: 760	mmHg = 1 atm =	= 101.325 kPa	
T/K	p _{Total} /atm	p_{SO_2}/atm	Mole SO ₂ /dm ³ solution	Н
403	5.58	2.99	0.3877	0.130
	6.25	3.67	0.4792	0.130
	6.79	4.22	0.5674	0.134
408	6.16	3.16	0.3831	0.121
	6.86	3.88	0.4735	0.122
	7.45	4.48	0.5607	0.125
413	6.77	3.31	0.3792	0.114
	7.51	4.06	0.4688	0.115
	8.15	4.72	0.5548	0.117
418	7.43	3.46	0.3752	0.108
	8.21	4.26	0.4636	0.109
	8.90	4.94	0.5488	0.110
423	8.13	3.59	0.3720	0.103
	8.96	4.44	0.4592	0.103
	9.69	5.19	0.5438	0.105

"Solution" appears to mean the final solution.

The author defined the "solubility" as $H = (H_2SO_3)/p_{SO_2}$,

 $p_{\rm SO_2}$ in atm. (H₂SO₃) evidently means moles SO₂/dm³ of solution.

The concentration of ${\rm HSO_3}$ was given as 0.1476 mol ${\rm dm^{-3}}$ for the first two values of ${\it H}$ at each temperature and 0.1481 for the third value of H at each temperature.

NOTE: The author refers to "pure sulfurous acid, H2SO3."

- Sulfur dioxide; SO_2 ; [7446-09-5]
- Water; H_2O ; [7732-18-5]
- Calcium bisulfite from CaO + water + SO₂.

ORIGINAL MEASUREMENTS:

Conrad, F.H.; Beuschlein, W.L.

J. Am. Chem. Soc. 1934, 56, 2554-2562.

VARIABLES:

PREPARED BY:

W. Gerrard.

EXPERIMENTAL	VALUES:						
_	Total	g SO	2/100 g wa	ater	r Free SO ₂		
T/K	Pressur /mmHg	e Total	Combined	Free	*Mole ratio	*Mole fraction	
							
288.15	22	1.83	0.89	0.94	0.0026	0.0026	i
	49	3.99	1.85	2.14	0.0060	0.0060	
	115	7.47	3.12	4.35	0.0122	0.0121	
	154	8.72	3.51	5.21	0.0147	0.0144	
ţ	263	11.00	4.23	6.77	0.0190	0.0187	
ļ	408	13.76	4.78	8.98	0.0253	0.0246	
ļ	517	15.92	5.47	10.45	0.0294	0.0285	
,	761	19.25	5.95	13.30	0.0374	0.0361	
298.15	40	1.91	0.91	1.00	0.0028	0.0028	ļ
	52	2.81	1.33	1.48	0.00416	0.00414	-
1	136	5.55	2.43	3.12	0.00877	0.00870	
	254	8.37	3.14	5.23	0.0147	0.0145	
	461	11.52	4.06	7.46	0.0210	0.0205	
	594	13.28	4.59	8.69	0.0244	0.0238	
	756	15.38	5.12	10.26	0.0289	0.0281	
	763	15.16	4.88	10.30	0.0290	0.0282	
308.15	761	12.02	4.03	7.99	0.0225	0.0220	

Calculated by compiler.

NOTE: A solid phase, referred to as calcium oxide was present. liquid phase was looked upon as a saturated solution of calcium (cont'd)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was passed into a measuring pipet, and then into a flask containing "calcium oxide" and water. The flask was shaken until a constant total pressure was achieved. The total pressure was 3. Calcium oxide was obtained by measured by a manometer containing mercury. The system was allowed to settle, and a sample of the clear liquid, above the solid phase, was Withdrawn into a weighed pipet for chemical titration by the iodinethiosulfate procedure. The temperature of the thermostat was regulated to within 0.05°C. The total, free and combined sulfur dioxide were determined by the method of Hohn (see Ref. 2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was of "refrigeration grade." and was passed through concentrated sulfuric acid before absorption.
- 2. Water was freshly distilled.
- the ignition of "C.P. analysed" calcium oxalate monohydrate.

ESTIMATED ERROR:

- Technical Association of Pulp and Paper Institute Standards, "Analysis of Bisulfite Cooking Liquor", T604m, 1931, December, 24.
- Birchard, W.H. Paper Industry, 1926, 8, 793. 2.

- Sulfur dioxide; SO₂; [7446-09-5] Water; H₂O; [7732-18-5]
- water; n₂O, [,,,oz 10 5].
 Calcium bisulfite from CaO + water + SO2.

ORIGINAL MEASUREMENTS:

Conrad, F.H.; Beuschlein, W.L. J. Am. Chem. Soc. 1934, 56, 2554-2562.

EXPERIMENTAL VALUES: (Cont'd)

bisulfite, $Ca(SO_3H)_2$. "Free SO_2 " is defined by the Technical Association of Pulp and Paper Institute (1) "as the actual free SO_2 plus half of the SO_2 in the bisulfite of calcium and is more properly called the 'available SO2' as it indicates SO2 in excess of the amount necessary to form monosulfite". "The combined SO2" is that required to form the monosulfite, CaSO3; the total SO2 is the sum of these. The total, free and combined SO2 were estimated by the method of Hohn, as described by Birchard (2).

- 1. Sulfur dioxide; SO_2 ; [7446-09-5]
- 2. Water; H_2O ; [7732-18-5] 3. Calcium bisulfite; $Ca(HSO_3)_2$; [13780-03-5]
- or Magnesium bisulfite; Mg(HSO3)2; [13774-25-9]

ORIGINAL MEASUREMENTS:

Chodakov, K. V. Bumaznaja

Promyslennost 1937 (No. 9), 33-38.

VARIABLES:

PREPARED BY:

Temperature, pressure, concentration

W. Gerrard

EXPERIMENTAL VALUES:

1 atm = 101.325 kPa

Calculated by compiler: mole fraction, x_{SO_2} , is based on the supposition that the liquid is 100 cm3 of water. The weights are given as g in 100 cm³ of final solution. C SO₂ is combined SO₂ equivalent to Ca(HSO₃)₂: F SO₂ is free SO₂, from Total (T)-C: p_{SO_2} is the pressure in atm, from the % by volume in the gas phase.

T/K	Base /g	p _{SO₂} /atm	SO ₂ ,T	SO ₂ ,F	SO ₂	^x so₂
297.15	CaO 1.40 g	0.089 0.264 0.441 0.616 0.662 0.850	4.26 5.66 7.01 8.48 8.48 10.16	1.06 2.46 3.81 5.29 5.28 6.96	0.0166 0.0384 0.0595 0.0827 0.0825 0.109	0.0030 0.0069 0.0106 0.0147 0.0146 0.0192
297.15	Dolomite equivalent to CaO, 1.40 g	0.063 0.052 0.231 0.278 0.525 0.700 0.820	3.98 4.00 5.31 5.79 7.60 9.02 9.90	0.78 0.80 2.11 2.59 4.40 5.82 6.70	0.0122 0.0125 0.0330 0.0405 0.0688 0.0909 0.105	0.0022 0.0023 0.0059 0.0072 0.0122 0.0161 0.0185

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide in the liquid and in the vapor phase was determined by an iodine titration.

One half of SO2 present as bisulfite was determined by titration with alkali.

SOURCE AND PURITY OF MATERIALS:

May be taken as of satisfactory purity.

ESTIMATED	ERROR:
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- Sulfur dioxide; SO₂; [7446-09-5]
 Water; H₂O; [7732-18-5]
 Calcium bisulfite; Ca(HSO₃)₂; [13780-03-5]

or Magnesium bisulfite; Mg(HSO $_3$) $_2$; [13774-25-9]

ORIGINAL MEASUREMENTS:

Chodakov, K. V. Bumaznaja

Promyslennost 1937 (No. 9), 33-38.

	NTAL VALUES:				~~	*
T/K	Base	p _{SO₂}	SO ₂ ,T	SO ₂ ,F	SO ₂	^x SO₂
	/g 	/atm	/g 	/g 	mole	
297.15	MgO	0.091	4.16	0.85	0.0133	0.0024
	equivalent to CaO	0.092 0.316	4.35 5.98	1.04 2.67	0.0163 0.0417	0.0029 0.0075
	1.45 g	0.451	7.10	3.79	0.0592	0.0106
		0.483 0.645	7.20 8.64	3.89 5.33	0.0608 0.0833	0.0108 0.0148
		0.770	9.38	6.07	0.0948	0.0168
		0.882 0.888	10.47 10.56	7.16 7.25	0.112 0.113	0.0197 0.0200
297.15	Wt. of CaO/q	0.05	1.79	0.65	0.113	0.0200
297.13	0.5	0.14	2.70	1.56		
		0.34	4.32	3.18		
		0.48 0.69	5.60 7.29	4.46 6.15		
		0.87	8.64	7.50		
	1.0	0.07 0.24	3.07 4.64	0.78 2.35		
		0.48	6.40	4.11		
		0.49 0.78	6.62 8.90	4.33 6.61		
		0.84	9.05	6.76		
	1.4	0.06	3.98	0.78		
		0.05 0.23	4.00 5.31	0.80 2.11		
		0.28	5.79	2.59		
		0.53 0.70	7.60 9.03	4.40 5.83		
		0.82	9.90	6.70		
	2.0	0.065 0.17	5.28 6.00	0.71 1.43		
		0.25	6.66	2.09		
		0.47 0.56	8.30 8.99	3.73 4.42		
		0.82	10.90	6.33		
		0.84	11.07	6.50		
313.15	1.0	0.16 0.31	3.50 4.13	1.21 1.84		
		0.38	4.67	2.38		
		0.60 0.62	5.63 5.70	3.34		
		0.87	6.88	3.41 4.59		
333.15	1.0	0.08	3.07	0.78		
		0.19 0.39	3.42	1.13		
		0.39	4.00 5.12	1.71 2.83		
353.15	1.0	0.15	3.07	0.78		
		0.22	3.32	1.03		
		0.29 0.34	3.52 3.68	1.23 1.39		
		0.47	3.84	1.55		
279.15	1.0	0.055	3.71	1.42		
		0.07 0.08	3.90 4.20	1.61 1.91		
		0.17	5.63	3.34		

- Sulfur dioxide; SO₂; [7446-09-5]
 Water; H₂O; [7732-18-5]
 Calcium bisulfite; Ca(HSO₃)₂; [13780-03-5]
- or Magnesium bisulfite; Mg(HSO₃)₂; [13774-25-9]

ORIGINAL MEASUREMENTS:

Chodakov, K. V. Bumaznaja

Promyslennost 1937 (No. 9), 33-38.

EXPERIMENTAL VALUES:

T/K	Base /g	SO ₂ /atm	SO ₂ ,T /g	SO ₂ ,F /g	SO ₂ mole	x _{SO₂}
279.15	Wt. of CaO 1.0	0.39 0.39 0.65 0.62 0.83 0.91	8.64 8.75 11.80 12.00 15.00	6.35 6.46 9.51 9.71 12.71 13.71		
	1.4	0.025 0.02 0.06 0.155 0.27 0.44 0.67 0.72 0.78 0.855	4.44 4.48 5.18 6.56 8.29 10.60 13.44 14.70 15.30 16.20	1.24 1.28 1.98 3.36 5.09 7.40 10.24 11.50 12.10 13.00		
313.15	1.4	0.06 0.25 0.47 0.84 0.88	3.65 4.58 5.65 7.36 7.52	0.45 1.38 2.45 4.16 4.32		
333.15	1.4	0.09 0.29 0.64 0.79	3.78 4.54 5.44 5.92	0.58 1.34 2.24 2.72		
353.15	1.4	0.17 0.11 0.28 0.48	3.84 3.48 4.16 4.48	0.64 0.28 0.96 1.28		

	<u></u>
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>1 Sulfur dioxide; SO₂; [7446-09-5] 2. Water; H₂O; [7732-18-5]</pre>	Hansen, C.J.
 Thiocyanic acid, calcium salt, (Calcium thiocyanate); Ca(CNS)₂; 	Ber, <u>1933</u> , 66B,447-450
[2092-16-2]	
VARIABLES:	PREPARED BY:
	W. Gerrard.
	W. GCITATA.
EXPERIMENTAL VALUES:	
At 280.15 K, 81.65 g of the origing of calcium thiocyanate (volume	inal solution containing 22.07 = 70 cm^3 , density = 1.167 g cm^{-3} ,
moles, as $Ca(CNS)_2 = 0.141$, but	given by the author as 0.2828.
based on one half of Ca(CNS); about to give 102.9 g, and 82.3 cm of	sorbed 21.25 g SO ₂ , 0.332 More, solution (final), density =
1.25 g cm ⁻³ . The mole ratio SO_2 , 0.141 = 2.355, mole fraction, x_{SO}	/Ca(CNS) ₂ is therefore = 0.332/ , = 0.702. The author gave
the mole ratio as 1.175, based or	n one half of the molecular
formula, $Ca(CNS)_2$. The pressure barometric pressure.	was presumably the unspecified
2012 20 F 2022 20 C	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known amount of salt solution was treated in a measuring	1. Sulfur dioxide was stated to be pure.
cylinder with sulfur dioxide.	_
The final solution was weighed and its volume determined.	2. and 3. May be assumed to be of satisfactory purity.
	ESTIMATED ERROR:
	REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- Magnesium bisulfite from MgO + water + SO₂

ORIGINAL MEASUREMENTS:

Conrad, F.H.; Brice, D.B.

J. Am. Chem. Soc. 1948, 70, 2179-2182.

VARIABLES:

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

T/K	Total pressure /mmHg				Free So	
288.15	75.5 87.5 110.7 156.8 162.3 245.5 419.3 448.7 726.8 730.3	30.4 28.05 29.65 32.9 31.4 39.9 46.9 44.8 54.6 53.3	15.7 14.75 15.05 16.9 16.55 21.0 23.55 22.4 27.8 26.75	14.7 13.3 14.6 16.0 14.85 18.9 23.35 22.4 26.8 26.55	0.0413 0.0374 0.0411 0.0450 0.0418 0.0532 0.0657 0.0630 0.0754	0.0397 0.0361 0.0395 0.0431 0.0401 0.0505 0.0616 0.0593 0.0701 0.0695
298.15	130.2 154.4 213.2 264.3 288.0 326.5 410.9 560.7 638.4 726.8 728.4	28.2 28.0 35.6 35.2 37.5 40.7 42.1 50.2 51.6 50.7 52.0	14.2 14.85 18.2 17.9 18.75 20.35 21.3 25.4 26.3 25.85 26.2	14.0 13.15 17.4 17.3 18.75 20.35 20.8 24.9 25.3 24.85 25.8	0.0489 0.0487 0.0527 0.0572 0.0585	0.0379 0.0365 0.0467 0.0464 0.0500 0.0541 0.0553 0.0654 0.0665 0.0653
308.15	728.7	50.1	25.7	25.8 calculat	0.0726 ed by compile:	0.0677

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

As described by Conrad and Beuschlein (1).

NOTE: For definition of "total", "combined" and "free" sulfur dioxide see Ref. (1).

Sulfur dioxide was passed into a suspension of magnesium oxide in water. The solution was deemed to be a saturated solution of sulfur dioxide in a saturated solution of magnesium bisulfite. A solid phase was present, and a sample of the clear liquid phase was removed for chemical titrations.

- (1) Sulfur dioxide was of refrigeration grade, see ref. (1)
- (2) Water was freshly distilled, see ref. (1).
- (3) Magnesium oxide was "C.P. analyzed."

ESTIMATED ERROR:

REFERENCES:

Conrad, F.H.; Beuschlein, W.L.
 J. Am. Chem. Soc. <u>1934</u>, 56, 2554.

- 1. Sulfur dioxide; SO₂; [7746-09-5]
- 2. Water; H₂O; [7732-18-5]
- Cadmium chloride; CdCl₂;
 [10043-52-4]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

Temperature, concentration of salt

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

Equivalent taken by authors as 2CdCl2 "Normality" 3 2.5 2 1.5 0.5 T/K 29.46 27.09 30.55 31.66 26.06 28.16 298 Ostwald coefficient, L

(L for water given as 32.76) 308 Ostwald coefficient, 18.68 19.23 20.02 20.55 21.23 21.73 $_L$

(L for water given as 22.43)

The following arithmetic was shown by the original author:

- $\alpha = {\rm cm}^3$ SO₂ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = \text{cm}^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂.

1/2 sx = a/22.4, for one cm³ of the saturated solution. For e cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/e (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the L values are about 2% too large.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO₂, 0.2% water, commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Water; H₂O; [7732-18-5]

Cadmium bromide; CdBr2; [7789-42-6]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

Temperature, concentration of salt.

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES: Equivalent taken by the author as $1/2 \text{ CdBr}_2$

T/K	"Normality"	3	2.5		1.5	1	0.5
298	Ostwald coefficient,	27.46	28.15	29.27	30.17	31.01	31.91
	L						
	(L for water given as	32.76)					
308	Ostwald coefficient,	19.17	19.70	20.60	20.81	31.46	21.88
1	L						
	(L for water given as	22.43)					

The following arithmetic was shown by the original author:

- $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm^3 ; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂.

1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/cThe coefficient L was taken to be equal to a (760/b). (T/K / 273 K). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm⁻³ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm³ and not 22.4 dm³ under these conditions; therefore all the L values are about 2% too large.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm3), and the amount of SO₂ determined by iodinethiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide, 99.8% SO₂, 0.2% water, commercial.
- 2. Presumably conductivity grade.
- 3. Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Cadmium iodide; CdI₂; [7790-80-9]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

PREPARED BY:

Temperature, concentration of salt

W. Gerrard

EXPERIMENTAL VALUES: Equivalent taken by the author as 1/2 CdI₂

"Normality" 2.5 0.5 T/K 33.76 34.98 34.74 34.16 33.27 35.77 Ostwald coefficient, 298 (L for water given as 32.76) Ostwald coefficient, 23.71 23.38 23.06 22.75 308 24.30 23.99

(L for water given as 22.43)

The following arithmetic was shown by the original author:

- $\alpha = {\rm cm^3~SO_2}$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂.

1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO $_2$ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO₂, 0.2% water, commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

- Sulfur dioxide; SO₂; [7446-09-5]
- Water; H₂O; [7732-18-5]
 Cadmium sulfate; CdSO₄; [10124-36-4]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

Temperature, concentration of salt

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES: Equivalent given by the author as 1/2 CdSO4

T/K	"Normality"	3	2.5	2	1.5	1	0.5
298	Ostwald coefficient,	23.76	25.14	26.58	28.24	29.71	31.11
	L						
	(L for water given as						
308	Ostwald coefficient,	16.25	17.41	18.31	19.42	20.43	21.45
•	L						
	(L for water given as	22.43)					

The following arithmetic was shown by the original author:

- $a = cm^3 SO_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2.

1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K / 273 K). The coefficient L was taken to be equal to α (760/b). (See evaluation)

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO₂ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm3), and the amount of SO₂ determined by iodinethiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO2, 0.2% water, commercial.
- Presumably conductivity grade. 2.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Jager (Jaeger), L. 1. Sulfur dioxide; SO₂; [7446-09-5] 2. Water; H₂O; [7732-18-5] Chem. Prumysl. 1957, 7, 601-602. 3. Zinc sulfate; ZnSO4; [7733-02-0] VARIABLES: PREPARED BY: Temperature, concentration of salt W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPag SO₂/dm³ g ZnSO₄/dm³ T/K 84.2 293 88.1 79.6 119.0 156.0 74.3 69.2 194.0 63.5 232.5 55.1 284.0 320.5 48.1 67.8 303 28.75 59.5 65.6 58.9 65.4 87.5 62.8 125.7 59.9 114.0 58.9 156.0 55.1 156.0 55.1 50.6 199.2 194.8 49.4 46.2 231.0 229.0 45.8 41.3 286.0 37.5 316.0 50.6 313 32.6 49.9 30.3 49.0 54.2 56.7 49.6 90.4 47.1 AUXILIARY INFORMATION METHOD APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide may be taken An ount of sulfur dioxide absorbed at the total pressure of about 1 atm was as of satisfactory purity. determined by iodimetric titration. 2. As for (1). 3. As for (1). Content in solution The temperature was controlled to within ±0.1°C. was determined by chelatometric titration. ESTIMATED ERROR: REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
 2. Water; H₂O; [7732-18-5]
- 3. Zinc sulfate; ZnSO₄; [7733-02-0]

ORIGINAL MEASUREMENTS

Jager (Jaeger), L.

Chem. Prumysl. <u>1957</u>, 7, 601-602.

		801-802.	
EXPERIMENTAL VALUES:	760 mmHg = 1 atm	n = 101.325 kPa	
T/K	g ZnSO ₄ /dm ³	g SO ₂ /dm³	
313	159.5	42.3	
4.1 0	157.8	41.6	
	237.0	35.8	
	279.0	32.5	
	282.0	32.7	
	322.0	29.4	
323	28.1	37.4	
	26.8	36.9	
	65.1	36.8	
	66.2	37.2	
	98.2	35.5	
	98.2	35.5	
	160.5	31.7	
	161.2	31.9	
	198.2	30.6	
	284.5	25.6	
	284.5	25.6	
	321.5	22.9	
343	31.7	21.9	
	31.7	21.9	
	62.9	22.1	
	160.0	20.7	
	160.5	20.6	
	188.5	19.5	
	188.4	19.5	
	258.0	17.6	
	331.0	15.2	
	331.0	15.2	
363	60.0	9.08	
- 	60.1	9.08	
	140.3	9.92	
	140.2	9.92	
	220.5	9.78	
	220.0	9.77	
	295.0	8.37	
	352.5	7.67	
373	70.1	3.46	
	124.0	2.69	
	124.1	2.69	
	245.0	3.71	
	293.5	3.46	
			
	•		
<u>NOTE:</u> g	SO ₂ /dm³ presumably	means g SO₂ absorbed	
h	1 dm3 of the emissi	mal galution of the	

NOTE: g SO₂/dm³ presumably means g SO₂ absorbed by 1 dm³ of the original solution of the salt.

84 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Peisakhov, I. L.; Karmazina, V. D. Zh. Priklad. Khim. 1959, 32, 70-78. 2. Water; H₂O; [7732-18-5] Zinc bisulfite; Zn(HSO₃)₂; [15457-98-4] 4. Zinc sulfate; ZnSO4; [7733-02-0] VARIABLES: PREPARED BY: Temperature, concentration of W. Gerrard components 3 and 4 EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa $SO_2(T)$ = total sulfur dioxide $SO_2(F)$ = free sulfur dioxide = density of solution

Conc. of Zn(HSO ₃) ₂ /g dm ⁻³	ZnSO.				т/к	^p SO₂ /mmHg
5.31	4.52	2.98	0	1.006	293 313 323 333	0.057 0.126 0.160 0.241
	log p _{SO:}	/mmHg =	3.94 - 1	520/(T/K)		
10.2	3.52	5.84	0	1.009	293 313 323 333	0.149 0.393 0.597 0.954
	log p _{SO;}	/mmHg =	4.88 - 19	60/(T/K)		
13.9	8.1	7.97	0.19	1.016	293 313	0.465 0.679
	Zn(HSO ₃) ₂ /g dm ⁻³ 5.31	$\frac{\text{Zn}(\text{HSO}_3)_2}{/\text{g dm}^{-3}}$ $\frac{\text{ZnSO}_4}{/\text{g dm}^{-3}}$ 5.31 4.52 $\frac{\log p_{\text{SO}_2}}{3.52}$	$\frac{\text{Zn} (\text{HSO}_3)_2}{/\text{g} \text{ dm}^{-3}}$ $\frac{\text{ZnSO}_4}{/\text{g} \text{ dm}^{-3}}$ $\frac{\text{Jg dm}^{-3}}{}$ $\frac{\text{Jg dm}^{-3$	$\frac{\text{Zn}(\text{HSO}_3)_2}{/\text{g} \text{ dm}^{-3}} = \frac{\text{ZnSO}_4}{/\text{g} \text{ dm}^{-3}$	$2n (HSO_3)_2 / g dm^{-3} / g dm^{-3} / g dm^{-3} / g dm^{-3} / g cm^{-3}$ 5.31 4.52 2.98 0 1.006 $\log p_{SO_2} / mmHg = 3.94 - 1520 / (T/K)$ 10.2 3.52 5.84 0 1.009 $\log p_{SO_2} / mmHg = 4.88 - 1960 / (T/K)$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Nitrogen from a cylinder was passed through a rheometer, and then through five consecutive absorption flasks containing the solution, the procedure being that of Kuzminykh and Kuznetsova (1). Presumably the sulfur dioxide solution was prepared separately. The absorption flasks were held in a thermostat. pressure, p_{SO_2} was measured by the

determination of the volume content of the gas emerging from the last flask, iodine titrations being used. Likewise the sulfur dioxide content of the solutions in the last three flasks was determined. To obtain a pulp of solid zinc sulfite, crystals of the latter were added to each flask. The rate of passage of nitrogen was 0.5 liter/minute.

SOURCE AND PURITY OF MATERIALS:

Not stated.

ESTIMATED ERROR:

REFERENCES:

1. Kuzminykh, I. N.; Kuznetsova, Zh. Priklad. Khim. 1954, 27, 816.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Zinc bisulfite; Zn(HSO₃)₂;
 [15457-98-4]
- 4. Zinc sulfate; ZnSO4; [7733-02-0]

ORIGINAL MEASUREMENTS:

Peisakhov, I. L.; Karmazina, V. D. Zh. Priklad. Khim. 1959, 32, 70-78.

(cont.)

EXPERIMENTAL VALUES:

Expt.	Conc. of Zn(HSO ₃) ₂ /g dm ⁻³	Conc. of ZnSO ₄ /g dm ⁻³	SO ₂ (T) /g dm ⁻³	$SO_2(F)$ /g dm ⁻³	ρ /g cm ⁻³	T/K	^p so₂ /mmHg
3	13.9	8.1	7.97	0.19	1.016	323 333	1.29
		$\log p_{SO_2}$	/mmHg =	6.43 - 20	040/(T/K)		
4	13.9	4.44	7.83	0	1.012	293 313 323 333	0.302 0.767 1.26 2.02
		log p _{SO2}	/mmHg =	6.23 - 20	040/(T/K)		
5	24.2	3.71	14.0	0.26	1.018	293 313 323 333	1.68 3.34 4.61 8.77
		log p _{SO2}	/mmHg =	7.28 - 21	.10/(T/K)		
6	25.6	6.6	15.0	0.58	1.025	293 313 323 333	1.67 3.74 5.70 7.62
		log p _{SO2}	/mmHg =	5.77 - 16	20/(T/K)		
7	39.3	11.4	23.65	1.54	1.041	293 313 323 333	3.8 8.52 12.2 18.5
		log p _{SO2} /	mmHg = 6	.04 - 160	0/(T/K)		
8	41.4	9.35	25.0	1.73	1.04	293 313 323 333	3.6 9.34 14.57 19.73
		log $p_{\cdot \text{SO}_2} /$	mmHg = 6	.92 - 186	5/(T/K)		
9.	5.56	24.8	3.36	0.23	1.026	293 313 323 333	0.206 0.319 0.356 0.50
		$\log p_{SO_2}$	mmHg = 2	.22 - 880	/(T/K)		
10	41.3	26.8	23.7	0.45	1.051	293 313 323 333	6.70 13.2 16.8 21.5
		log $p_{SO_2}/$	mmHg = 5	.06 - 124	0/(T/K)		

COMPONENTS: ORIGINAL MEASUREMENTS: Peisakhov, I. L.; Karmazina, V. D. 1. Sulfur dioxide; SO₂; [7446-09-5] Zh. Priklad. Khim. 1959, 32, 70-78. 2. Water: H₂O; [7732-18-5] Zinc bisulfite; Zn(HSO₃)₂; [15457-98-4] 4. Zinc sulfate; ZnSO4; [7733-02-0] **EXPERIMENTAL VALUES:** Expt. Conc. of Conc. of $SO_2(T)$ $SO_2(F)$ T/K ρ p_{SO2} $Zn (HSO_3)_2$ ZnSO4 $/g dm^{-3}$ $/g cm^{-3}$ /g dm⁻³ /g dm /g dm⁻³ /mmHq 3.86 1.055 293 11 55.0 2.21 0.32 0.07 313 0.134 323 0.175 333 0.259 $\log p_{SO_2}/mmHg = 1.85 - 850/(T/K)$ 12 6.14 53.2 3.5 293 0.363 0.05 1.057 313 0.723 323 0.843 1.035 333 $\log p_{SO_2}/mmHg = 3.5 - 1150/(T/K)$ 13 42.3 49.6 25.0 1.15 1.080 293 8.44 15.7 313 323 20.5 333 27.5 $log p_{SO_2}/mmHg = 5.38 - 1300/(T/K)$ 1.088 293 0.256 14 3.64 88.2 2.63 0.58 313 0.289 323 0.30 0.395 333 15 3.64 88.2 293 2.63 0.58 1.088 0.188 0.258 313 323 0.311 333 0.468 $\log p_{SO_2}/mmHg = 2.09 - 830/(T/K)$ 14 and 15 293 16 10.9 82.6 6.9 1.21 1.090 0.948 313 1.78 323 2.52 333 3.58 $log p_{SO_2}/mmHg = 4.76 - 1400/(T/K)$ 17 22.9 82.0 13.7 1.10 293 1.02 2.68 313 5.46 323 6.96 333 9.41 $log p_{SO_2}/mmHg = 4.92 - 1320/(T/K)$ 18 35.4 77.5 22.2 2.3 1.106 293 9.35 313 16.77 323 18.73 333 21.3 19 35.4 77.5 22.2 2.3 1.106 293 8.64 313 14.78 323 17.6 333 22.3 $\log p_{SO_2}/mmHg = 3.88 - 850/(T/K)$ 18 and 19 (cont.)

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- Zinc bisulfite; Zn(HSO₃)₂; [15457-98-4]
- 4. Zinc sulfate; ZnSO4; [7733-02-0]

ORIGINAL MEASUREMENTS:

Peisakhov, I. L.; Karmazina, V. D. Zh. Priklad. Khim. 1959, 32, 70-78.

EXPERIMENTAL VALUES:

Expt.	Conc. of Zn(HSO ₃) ₂ /g dm ⁻³	7-00			p /g cm ⁻³	T/K	^p so₂ /mmHg
20	3.64	104	2.06	0	1.088	293 313 323 333	0.187 0.299 0.329 0.472
		log p_{S^0}	O_2 /mmHg =	2.68 - 10	00/(T/K)		
21	5.67	103	3.44	0.24	1.099	293 313 323 333	0.373 0.726 0.933 1.25
		$\log p_{S($	O_2 /mmHg =	4.01 - 13	00/(T/K)		٠
22	42.7	101.4	24.5	0.45	1.122	293 313 323 333	7.83 17.0 22.5 32.5
		log $p_{S($	O ₂ /mmHg =	6.16 - 15	50/(T/K)		
23	3.28	194	3.01	1.65	1.825	293 313 323 333	0.274 0.573 0.740 1.08
		log p _{SC}	D_2 /mmHg =	4.38 - 14	50/(T/K)		1.00
24	38.1	198	21.5	0	1.216	293 313 323 333	5.93 14.94 20.53 28.7
		$\log p_{SC}$	mmHg = 0	6.66 - 170	00/(T/K)		

The smoothing equations given were calculated by the authors. Care should be taken in using these equations as there are significant discrepancies between values calculated from the equations and the experimental values. The equations for experiments nos. 2, 4, 9 and 24 appear to be in error.

88 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. Water; H₂O; [7732-18-5] Z. Phys. Chem. 1902, 41, 458-482. 2. Sodium chloride; NaCl; 3. [7647-14-5] VARIABLES: PREPARED BY: Concentration of salt. W. Gerrard EXPERIMENTAL VALUES: 2,5 0.5 T/K "Normality" 3 1.5 Ostwald coefficient, 31.36 31.51 31.76 31.96 32.25 32.46 298 (L for water given as 32.76)The following arithmetic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2. 1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, $a = (11.2 \ sx)/c$ (T/K / 273 K). The coefficient L was taken to be equal to α (760/b). (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm and not 22.4 ${ m dm}^3$ under these conditions; therefore all the L values are about 2% too large. AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by ripet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Sulfur dioxide, 99.8 SO₂, 0.2% water, commercial.
- (2) Presumably conductivity grade.
- (3) Salt of Kahlbaum grade, recrystallised and analytically attested.

COLLINITED DIVIDION	ESTIMATED ERROR	1
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Aqueous electrolyte solutions 89 COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. Water; H₂O; [7732-18-5] Z. Phys. Chem. 1902, 41, 458-482 З. Sodium bromide; NaBr; [7647-15-6] VARIABLES: PREPARED BY: Concentration of salt W. Gerrard EXPERIMENTAL VALUES: T/K "Normality" 3 2.5 2 1.5 1 0.5 298 Ostwald coefficient, 37.74 36.84 36.26 35.27 34.54 33.76 (L for water given as 32.76) The following arithmetic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2(273 \text{ K}, 760 \text{ mmHg}) \text{ in } 1 \text{ cm}^3 \text{ of "solution," presumably meaning}$ the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂. 1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c (T/K / 273 K). The coefficient L was taken to be equal to α (760/b). (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO $_2$ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large. AUXILIARY INFORMATION " METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The absorption vessel was fitted with 1. Sulfur dioxide, 99.8% SO2, 0.2% electrodes for the measurement of water, commercial. conductance, data not herein recorded, Sulfur dioxide was passed through 2. Presumably conductivity grade. the solution to saturation at barom-3. Salt of Kahlbaum grade, reetric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. crystallised and analytically attested. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 \mbox{cm}^3), and the amount of \mbox{SO}_2 determined by iodine-thiosulfate ESTIMATED ERROR: titration.

Sulfur Dioxide Solubilities 90 ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. 2. Water; H₂O; [7732-18-5] Sodium sulfate; Na₂SO₄; 3. Z. Phys. Chem. 1902, 41, [7757-82-6] 458-482. VARIABLES: PREPARED BY: Temperature, concentration of salt. W. Gerrard EXPERIMENTAL VALUES: Equivalent taken by the author as $1/2 \text{ Na}_2\text{SO}_4$ "Normality" 3 2.5 T/K 28.44 29.51 30.45 28.66 31.14 Ostwald coefficient, 298 (L for water given as 32.76) Ostwald coefficient, 20.20 20.81 21.35 308 19.27 19.79 (L for water given as 22.43) The following arithmetic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm^3 ; 0.001 mole I_2 taken to be equivalent to 0.001 mole SO_2 . 1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, $\alpha = (11.2$ sx)/c(T/K / 273 K). The coefficient L was taken to be equal to α (760/b) (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm3), and the amount of SO2 determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

Sulfur dioxide, 99.8% SO2, 0.2% water, commercial.

0.5

31.96

21.88

- Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERRO	R	:
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20.00

9.17

0.0258

0.0252

20.01

7.006

0.0197

0.0193

20.01 .

5.630

0.0158

0.0156

Aqueous electrolyte solutions COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Hudson, J.C. 2. Water; H₂O; [7732-18-5] J. Chem. Soc. 1925, 127, 1332-1347 Sodium sulfate; Na2504; [7757-82-6] VARIABLES: PREPARED BY: Temperature, concentration of salt W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaT/K 293.15 g salt/100 g 0 1.94 4.93 7.95 10.00 15.00 water g SO₂ 100 g 10.64 10.66 10.57 10.36 10.07 9.66 water *Mole ratio 0.0299 0.0300 0.0297 0.0291 0.0283 0.0272 0.0289 0.0283 0.0275 ***SO2 0.0265 0.0290 0.0291 5.47 7.83 2.04 3.99 10.00 303.15 g salt/100 g water 7.608 g SO₂/100 g 7.709 7.776 7.773 7.716 7.586 water *Mole ratio 0.0214 0.0217 0.0219 0.0219 0.0217 0.0213 ***SO2 0.0209 0.0212 0.0214 0.0214 0.0212 0.0209 313.15 g salt/100 g 2.49 5.04 7.95 10.00 14.94 water $g SO_2/100 g$ 5.585 5.812 5.910 5.927 5.882 5.802 water

0.0163

0.0160

2.49

4.508

0.0125

0.01185 0.0127

AUXILIARY INFORMATION

0.0166

0.0163

5.04

4.678

0.0132

0.0130

METHOD / APPARATUS / PROCEDURE:

*Mole ratio

g salt/100 g

*xso2

water g SO₂/100 g

water *Mole ratio

**so2

323.15

0.0157

0.0155

4.214

0.0117

Sulfur dioxide was bubbled through a weighed amount of salt solution in a tube immersed in a thermostat. The pressure was measured on a manometer. The saturated solution was weighed and the SO₂ content was determined by an iodine titration. It was stated that the calculated value of the partial pressure of the gas Over the solution was within 10 mmHg of 760 mmHg; the final weight of gas was given as for 760 mmHg the basis of Henry's law." A tentative allowance was made for the lowering of the vapor pressure of water by the dissolved salt and gas.

Calculated by compiler

SOURCE AND PURITY OF MATERIALS:

0.0167

0.0164

10.04

4.728

0.0133

0.0131

(1) Sulfur dioxide was from a cylinder; the purity was stated to be high; the chief impurity being water, less than 0.4%.

0.0165

0.0162

14.94

4.730

0.0133

0.0131

0.0163

0.0160

19.99

4.648

0.0131

0.0129

(2) and (3) may be taken as of analytical purity.

ESTIMATED ERROR:

ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Kobe, K.A.; Kenton, F.H. Water; H₂O; [7732-18-5] Sodium bisulfate; NaHSO4; Ind. Eng. Chem., Anal. Edit. 1938, 10, 76-77. [7681-38-1] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa $p_{SO_2} = 760 \text{ mmHg}.$ T/K = 298.15The aqueous solution was made up by dissolving 200 g anhydrous sodium sulfate in 800 g of distilled water, and adding 40 cm of "concentrated, 36N sulfuric acid." Volume of solution Volume of gas Volume of gas Bunsen (original) / cm3 absorbed /cm3 dissolved in coefficient one volume of solution 131.2 9.54 13.6 12.5 24.54 392.2 NOTE: The absorption coefficient, 13.6, is based on the volume of the final solution; the so-called Bunsen coefficient, α , was obtained by 13.6 x (273/298) = 12.46. However, the Bunsen α is usually referred to the volume of the original liquid, and not the final volume. The following results are supplied by compiler. $131.2/9.54 = 13.75 : \alpha = 12.60$ $329.2/24.54 = 13.41 : \alpha = 12.29$ AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: A mine-air buret was used. See 1. Not specified. Ref. (1). 2. and 3. Analytical grade compounds were used. ESTIMATED ERROR: REFERENCES: 1. Kobe, K.A.; Williams, J.S. Ind. Eng. Chem. Anal. Ed. 1935, 7, 37.

ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Otuka, Y. J. Soc. Chem. Ind. Japan., Suppl. 2. Water; H₂O; [7732-18-5] 1939, 42, 205B-209B 3. Sodium bisulfite; NaHSO₃; [7631-90-5] VARIABLES: PREPARED BY: W. Gerrard Temperature, pressure EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaMoles SO_2/dm^3 T/K $p_{\text{Total}}/\text{atm}$ $p_{\text{SO}_2}/\text{atm}$ H solution 1.58 0.1594 0.266 373 0.60 1.94 0.97 0.2670 0.275 0.1563 1.86 0.69 0.226 378 2.27 1.11 0.2618 0.236 2.18 0.1531 0.191 0.80 383 2.62 1.25 0.2567 0.205 0.1498 2.55 0.91 0.165 388 2.99 1.36 0.2529 0.186 2.94 0.144 393 1.02 0.1468 3.43 1.52 0.2479 0.163 0.1438 0.127 1.13 3.37 398 3.90 1.67 0.2432 0.146 0.1413 3.83 0.116 1.22 403 4.41 1.81 0.2387 0.132 4.35 1.33 0.1384 0.104 408 4.98 1.98 0.2336 0.118 4.96 1.47 0.1347 0.092 413 5.56 2.09 0.2304 0.110 5.55 0.1331 0.086 418 1.54 6.15 2.17 0.2282 0.105 0.1328 6.14 0.085 1.56 423 6.75 2.20 0.2274 0.103 "Solution" appears to mean the final solution. The author defined the "solubility" as $H=({\rm H_2SO_3})/p_{{\rm SO_2}}$, the pressure being in atm. (H_2SO_3) evidently means moles SO_2/dm^3 of solution. The concentration of NaHSO₃ was given as 0.3000 mol/dm⁻³. NOTE: The author refers to "pure sulfurous acid, H_2SO_3 ." METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The total vapor pressure, $p_{\rm Total}$ was determined by means of a glass spring manometer. It was stated that Not stated. the partial pressures were approximated from the dimensions of the apparatus, but details were not given. ESTIMATED ERROR: REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- Sodium bisulfite;
 NaHSO3;

[7631-90-5]

ORIGINAL MEASUREMENTS:

Kubelka, V.

Chem. Zvesti 1959, 13, 430-435.

VARIABLES:

AKIADEED.

Temperature, concentration

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

760~mmHg = 1~atm = 101.325~kPa Solubility was expressed as g SO₂/100 g of solution at 760 mmHg.

						-/		
"Normality"			293	303	313	333	353	363
of NaHSO ₃ 0.2	SO₂,	Total Combined Free	10.71 1.26 9.45	7.80 1.26 6.54	5.69 1.26 4.43	3.53 1.26 2.27	1.68 1.26 0.42	1.44 1.26 0.18
0.3		T C F	11.31 2.10 9.21		6.38 2.10 4.28	4.17 2.10 2.07		2.33 2.10 0.23
0.5		T C F	11.85 3.13 8.72		6.89 3.13 3.76	5.14 3.13 2.01		3.43 3.13 0.30
1.0		T C F	14.27 6.12 8.15		9.66 6.12 3.54	7.62 6.12 1.50		6.98 6.12 0.86
2.0		T C F	18.70 11.72 7.98		15.20 11.72 3.48	13.27 11.72 1.55		12.43 11.72 0.71

For each normality a small diagram was given to show that for a stated temperature the plot of $p_{\rm SO_2}$ vs. g, ${\rm SO_2(Total)/100}$ g solution was linear, although the numerical data were not given. These lines were presumably used to indicate the g ${\rm SO_2(Total)}$ for 1 atm.

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The method of Domansky and Rendos (1) was used. The sulfur dioxide was determined by an iodine titration.

SOURCE AND PURITY OF MATERIALS:

- 1. May be taken of satisfactory purity.
- 2 and 3. Sodium carbonate was used as a basis of the sodium bisulfite.

ESTIMATED ERROR:

REFERENCES:

Domansky, R.; Rendos, F.
 Chem. Zvesti 1957, 11, 453.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- Sodium thiocyanate; NaCNS;
 [540-72-7]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

PREPARED BY:

Concentration of salt.

W. Gerrard

EXPERIMENTAL VALUES:

T/K "Normality" 3 2.5 2 1.5 1 0.5 298 Ostwald coefficient, 48.34 45.86 43.37 40.78 38.24 35.44 L (L for water given as 32.76)

The following arithmetic was shown by the original author:

- $a={\rm cm^3~SO_2}$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂.

1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO₂ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO₂, 0.2% water commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:
	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] Water; H₂O; [7732-18-5] 	Hansen, C.J.
 Sodium thiocyanate; NaCNS; [540-72-7] 	Ber. 1933, 66B,447-450.
[540-72-7]	<u> </u>
VARIABLES:	PREPARED BY:
	W. Gerrard.
EXPERIMENTAL VALUES:	
At 282.15 K, 106.3 g of the ori	ginal solution containing
28.75 g NaCNS (27% by weight, d	$l = 1.13 \text{ g cm}^{-3}$), i.e. 0.355
mole, and 94 cm ³ , absorbed 29.9 total pressure equal to the uns	g SO ₂ , presumably at a specified barometric pressure.
The number of moles of SO ₂ was the correct value is 0.467. The	stated to be 0.477, whereas,
correctly stated to be 1.32. T	The mole fraction, x_{00} ,
calculated by compiler is 0.569	302
	•
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known amount of salt solution	1. Pure sulfur dioxide was stated to be used.
was treated in measuring cylinder with sulfur dioxide. The final	to be used.
solution was weighed, and its volume determined.	2. and 3. Satisfactory purity may be assumed.
Volume determined.	be assumed.
	ESTIMATED ERROR:
	REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Potassium chloride; KCl; [7447-40-7]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482

VARIABLES:

Temperature, concentration of salt

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K		-		2			0.5
298	Ostwald coefficient,	42.27	40.96	39.32	37.76	36.05	34.42
	L (L for water given as	32.76)					
308	Ostwald coefficient,		28.93	27.94	26.54	25.15	23.74
	(L for water given as	22.43)					

The following arithmetic was shown by the original author:

- $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm 3 of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I_2 taken to be equivalent to 0.001 mole SO_2 .

1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO $_2$ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO₂, 0.2% water, commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Potassium chloride; KCl [7447-40-7]

ORIGINAL MEASUREMENTS:

Hudson, J.C.

J. Chem. Soc. 1925, 127, 1332-1347

VARIABLES:

Temperature, concentration of salt

PREPARED BY:

W. Gerrard

EXPERIMENTA	L VALUES:	1	atm = 76	60 mmHg =	101.32	5 kPa	*Mole
T/K	$P_{ t Total}$	p _{SO 2}	y KCl	s_{1}	${\mathcal S}$	*Mole ratio	fraction
1/10	/mmHg	/mmHg	/g	/g	/g	SO ₂ /H ₂ O	$1 \text{ atm}, x_{SO_2}$
283.15			0		15.39	0.0433	0.0415
	780.3	772.0	5.55	17.32	17.05	0.0479	0.0458
	780.3	772.2	10.22	18.88	18.58	0.0522	0.0497
	766.2	758.3	15.85	20.23	20.28	0.0570	0.0539
	766.2	758.4	20.78	21.92	21.96	0.0618	0.0582
	768.2	761.4	29.90	25.45	25.40	0.0714	0.0667
288.15			0		12.66	0.0356	0.0344
	772.2	760.8	10.39	15.30	15.32	0.0431	0.0413
	771.9	761.0	19.91	17.67	17.64	0.0496	0.0473
	772.2	761.9	30.71	20.64	20.59	0.0579	0.0547
293.15			0		10.64	0.0299	0.0290
	773.9	757.9	5.14	11.60	11.62	0.0327	0.0317
	774.6	758.9	10.30	12.50	12.52	0.0352	0.0340
	778.0	761.7	15.61	13.58	13.55	0.0381	0.0367
	774.0	759.4	24.98	15.37	15.38	0.0433	0.0415
	779.0	764.8	30.38	16.76	16.65	0.0468	0.0447
303.05			0		7.58	0.0213	0.0209
	788.6	759.3	5.19	8.204	8.21	0.0231	0.0226
	789.4	760.7	10.11	8.810	8.80	0.0247	0.0241
	784.0	756.7	20.82	10.00	10.05	0.0283	0.0275
	782.8	756.8	29.86	11.21	11.26	0.0317	0.0307

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled through the weighed amount of salt solution in a tube immersed in a thermostat, and attached to a manometer assembly for the measurement of the total pressure at the saturation stage. After saturation, the tube was weighed and the sulfur dioxide content determined by oxidation with hydrogen peroxide in sodium hydroxide solution, and the gravimetric estimation of sulfate as barium sulfate.

For the estimation of the vapor pressure of water over the solution, see end of the complete table.

SOURCE AND PURITY OF MATERIALS:

- (1) Sulfur dioxide was from a cylinder; the purity was stated to be high, the chief impurity being water, less than 0.4%.
- (2) and (3) may be taken as analytically pure.

ESTIMATED ERROR:

- Sulfur dioxide; SO₂; [7446-09-5]
 Water; H₂O; [7732-18-5]
- 3. Potassium chloride; KCl; [7447-40-7]

ORIGINAL MEASUREMENTS:

Hudson, J.C.

J. Chem. Soc. 1925, 127, 1332-

EXPERIMENT	ral Values	S:	l atm =	760 mmHg	= 101.32	kPa	*Mole
T/K	Protal /mmHg	^p sO₂ /mmHg	^y ĸCl ∕g	^S 1 /g	s *1	Mole ratio SO ₂ /H ₂ O	fraction 1 atm, ^x SO ₂
313.15	816.7 818.1 810.4 818.1 810.4 803.7	764.3 766.9 759.2 768.1 761.6 756.0 757.0	0 5.17 10.20 10.40 15.44 20.14 24.83 28.95	5.994 6.380 6.380 6.869 7.086 7.415 7.721	5.54 5.96 6.32 6.39 6.675 7.07 7.45 7.75	0.0156 0.0168 0.0178 0.0180 0.0188 0.0199 0.0210 0.0218	0.0154 0.0165 0.0175 0.0177 0.0185 0.0195 0.0206 0.0213
321.30	841.8 841.8 826.9 839.8 826.9 839.8	761.7 763.6 750.7 765.7 754.0 769.7	0 5.06 10.14 15.82 21.11 25.09 32.72	4.712 4.968 5.180 5.521 5.703 6.258	4.39 4.70 4.945 5.24 5.48 5.74 6.18	0.0123 0.0132 0.0139 0.0147 0.0154 0.0161 0.0174	0.0122 0.0130 0.0137 0.0145 0.0152 0.0159 0.0171
333.15	889 888 896 890.5	746 748 763.5 764	0 5.30 10.67 21.12 30.98	3.384 3.468 3.943 4.258	3.25 3.45 3.52 3.92 4.24	0.0091 0.0097 0.0099 0.0110 0.0119	0.0090 0.0096 0.0098 0.0109 0.0118
343.15	969 960.5 960	747.5 752 757	0 8.74 21.68 30.73	2.756 3.016 3.251	2.61 2.80 3.05 3.26	0.0073 0.0079 0.0086 0.0092	0.00725 0.0078 0.0085 0.0091
353.15	958 961 961	620 643 656	0 8.66 21.35 29.68	1.850 2.043 2.179	2.13 2.27 2.415 2.52	0.0060 0.0064 0.0068 0.0071	0.0060 0.0063 0.0067 0.0070
363.15	967.5 958 965.5	468 482 520	0 9.23 19.49 32.75	1.142 1.248 1.445	1.81 1.855 1.97 2.11	0.0051 0.0052 0.0055 0.0059	0.0051 0.0052 0.0055 0.0059

Calculated by compiler.

P_{Total} = total pressure.

= partial pressure of SO2. p_{SO₂}

= g of KCl in 100 g of water. y_{KCl}

"Solubility" $S_1 = g$ of SO₂ per 100 g of water at p_{SO_2}

= g of SO₂ per 100 g of water at 760 mmHg

 $= S_1 \times 760/p_{SO_2}$

Allowance for the vapor pressure of water, ${\bf p}$. It was assumed that lowering of the vapor pressure of water was equal to the sum of the depressions that would be caused by SO_2 and salt separately. Data for for the salt were taken from the literature; the lowering due to the gas was estimated by Raoult's law on the assumption that water is bimolecular. The correction was deemed to be small, 0.1% at 283 K, 1.25% at 363 K. Uncertainty was attributed to the combination of sulfur dioxide with water and with the salt, see the evaluation.

COMPONENTS: ORIGINAL MEASUREMENTS: Fox, C.J.J. Sulfur dioxide; SO₂; [7446-09-5] Z. Phys. Chem. 1902, 41, 458-482. Water: H₂O: [7732-18-5] Potassium bromide; KBr; [7758-02-3] VARIABLES: PREPARED BY: Temperature, concentration of salt W. Gerrard EXPERIMENTAL VALUES: "Normality" 3 2.5 2 1.5 0.5 T/K 52.26 48.87 44.96 42.41 39.11 35.94 Ostwald coefficient, 298 (L for water given as 32.76) 31.93 29.64 27.49 308 Ostwald coefficient, 36.14 34.12 24.83 (L for water given as 22.43) The following arithmetic was shown by the original author: $a = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm^3 ; 0.001 mole I₂ taken to be equivalent to 0.001 mole SO₂. 1/2 $sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, $a = (11.2 \ sx)/c$ (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm 3 and not 22.4 dm^3 under these conditions; therefore all the L values are about 2% too large. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: The absorption vessel was fitted with l. electrodes for the measurement of Sulfur dioxide, 99.8% SO2, 0.2% water commercial. conductance, data not herein recorded Sulfur dioxide was passed through the 2. Presumably conductivity grade. solution to saturation at barometric pressure, the apparatus being held in 3. Salt of Kahlbaum grade, rea thermostat, controlled at 25.05 to 25.1°C or 35 to 35.05°C. A volume crystallised and analytically attested. of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm3), and the amount of SO₂ determined by iodine-thiosulfate titration. ESTIMATED ERROR: REFERENCES:

Aqueous electrolyte solutions COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Fox, C.J.J. Water; H₂O; [7732-18-5] Potassium iodide; KI; Z. Phys. Chem. 1902, 41, 458-482. [7681-11-0] VARIABLES: PREPARED BY: W. Gerrard. Temperature, concentration of salt. EXPERIMENTAL VALUES: T/K "Normality" 2.5 2 1.5 0.5 68.36 62.63 56.75 50.58 44.76 298 Ostwald coefficient, 38.66 (L for water given as 32.76) 45.43 41.87 38.04 34.64 30.25 26.30 308 Ostwald coefficient, (L for water given as 22.43) The following arithmetic was shown by the original author: $\alpha = cm^3 SO_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2.

 $1/2 sx = \alpha/22.4$, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation).

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15K and 1 atm, the molar volume of SO_2 is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The absorption vessel was fitted with 1. electrodes for the measurement of conductance, data not herein recorded Sulfur dioxide was passed through the 2. solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to $1.436~{\rm cm}^3$), and the amount of SO₂ determined by iodine-thiosulfate titration.

- SOURCE AND PURITY OF MATERIALS:
- Sulfur dioxide, 99.8% SO2, 0.2% water, commercial.
- Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

102 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. 2. Water; H₂O; [7732-18-5] 3. Potassium sulfate; K2SO4; Z. Phys. Chem. 1902, 41, 458-482. [7778-80-5] **VARIABLES:** PREPARED BY: Concentration of salt W. Gerrard. EXPERIMENTAL VALUES: Equivalent taken by the author as 1/2 K2SO4 T/K "Normality" 0.5 33.61 298 Ostwald coefficient, 33.20 (L for water given as 32,76). The following arithmetic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2. 1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15K and 1 atm, the molar volume of SO₂ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the L values are about 2% too large. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: The absorption vessel was fitted Sulfur dioxide, 99.8% SO2, 0.2% with electrodes for the measurement water, commercial. of conductance, data not herein 2. Presumably conductivity grade.

recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus 3. Salt of Kahlbaum grade, rebeing held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO₂ determined by iodine-thiosulfate titration.

- crystallised and analytically attested.

ESTIMATED	ERROR

- Sulfur dioxide; SO2; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- З. Potassium nitrate; KNO3; [7757-79-1]

ORIGINAL MEASUREMENTS:

Fox, C.J.J.

Z. Phys. Chem. 1902, 41, 458-482.

VARIABLES:

PREPARED BY:

Temperature, concentration of salt

W. Gerrard.

EXPERIMENTAL VALUES:

T/K	"Normality"	3	2.5	2	1.5	1	0.5
298	Ostwald coefficient,	38.52	37.57	36.66	35.77	34.79	33.80
	L	20 561					
308	(L for water given as		26 54	25 72	24 70	04.00	02 05
308	Ostwald coefficient, L	21.33	20.54	25.72	24.79	24.03	23.21
	(L for water given as	22.43)					

The following arithmetic was shown by the original author:

- $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas.
- $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I2 taken to be equivalent to 0.001 mole SO2.

1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, a = (11.2 sx)/c(T/K /273 K). The coefficient L was taken to be equal to α (760/b). (See evaluation.)

NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO $_2$ is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the $\it L$ values are about 2% too large.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel was fitted with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was Withdrawn by pipet (0.9181 to 1.436 ${\mbox{cm}}^3)$, and the amount of ${\mbox{SO}}_2$ determined by iodine-thiosulfate titration.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide, 99.8% SO2, 0.2% water, commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

104 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Fox, C.J.J. Z. Phys. Chem. 1902, 41, 458-482. Water; H₂O; [7732-18-5] 3. Potassium thiocyanate; KCNS; [333-20-0] VARIABLES: PREPARED BY: Temperature, concentration of salt. W. Gerrard EXPERIMENTAL VALUES: "Normality" 3.0 2.5 2.0 1.5 1.0 0.5 T/K 55.87 47.02 37.57 61.26 51.86 42.38 298 Ostwald coefficient, (L for water given as 32.76) 32.03 28.79 25.63 308 Ostwald coefficient, 42.94 38.13 35.05 (L for water given as 22.43) The following arithmetic was shown by the original author: $\alpha = \text{cm}^3 \text{ SO}_2$ (273 K, 760 mmHg) in 1 cm³ of "solution," presumably meaning the salt solution before absorption of gas. $x = cm^3$ of iodine solution containing s equivalents per dm³; 0.001 mole I, taken to be equivalent to 0.001 mole SO2 . 1/2 sx = a/22.4, for one cm³ of the saturated solution. For c cm³ of the solution taken for titration, at T/K and b mmHg pressure, $a = (11.2 \ sx)/c$ (T/K / 273 K). The coefficient L was taken to be equal to a (760/b). (See evaluation). NOTE by compiler: based on the published density of sulfur dioxide, 2.9266 g dm $^{-3}$ at 273.15 K and 1 atm, the molar volume of SO_2 is 21.87 dm 3 and not 22.4 dm 3 under these conditions; therefore all the L values are about 2% too large. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The absorption vessel was fitted Sulfur dioxide, 99.8% SO2, 0.2%

with electrodes for the measurement of conductance, data not herein recorded. Sulfur dioxide was passed through the solution to saturation at barometric pressure, the apparatus 3. being held in a thermostat, controlled at 25.05 to 25.1°C, or 35 to 35.05°C. A volume of the saturated solution was withdrawn by pipet (0.9181 to 1.436 cm³), and the amount of SO_2 determined by iodinethiosulfate titration.

- water, commercial.
- 2. Presumably conductivity grade.
- Salt of Kahlbaum grade, recrystallised and analytically attested.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Hansen, C.J. 2. Water; H₂O; [7732-18-5] Ber, 1933, 66B, 447-450. 3. Potassium thiocyanate; KCNS; [333-20-0] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: At 281.15 K, 50 g of the original solution of potassium thiocyanate (25 g, 0.258 moles) absorbed 32.2 g SO₂ to give 82.2 g of final solution of 58 cm³ (density, * 1.42 g cm⁻³. The mole ratio, SO₂/KCNS was given as 0.503/0.258 = 1.95; mole fraction, x_{SO_2} , calculated by compiler is 0.661. *The density was given as 1.48. At 285.15 K 60 g of the original solution containing 50 g of KCNS (0.515 mole) absorbed 52.5 g of SO₂(0.820 mole) to give 112.5 g (68 cm³, density 1.65 g cm⁻³) of final solution. The mole ratio, SO₂/KCNS was given as 0.820/0.515 = 1.59. The corresponding mole fraction, x_{SO_2} , = 0.614. The total pressure appears to have been the unspecified barometric pressure. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Pure SO₂ was stated to be used. A known amount of the salt solution was treated in a measuring cylinder with sulfur dioxide. The final solution was weighed, and its 2. and 3. Satisfactory purity may be assumed. volume was determined. ESTIMATED ERROR: REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:			
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	McCrae, J.; Wilson, W. E.			
2. Water; H ₂ O; [7732-18-5]	Z. anorg. Chem. 1903, 35, 11-15.			
<pre>3. Trichloromethane (Chloroform); CHCl₃; [75-43-4]</pre>				
VARIABLES:	PREPARED BY:			
	W. Gerrard			

EXPERIMENTAL	VALUES:	T/K	= 293.15			
g SO ₂ /dm ³ (soln.)	Water phase *Equiv. SO ₂ /dm ³ (soln.) e ₁	^x SO ₂ ** (water)	Chlo g SO ₂ /dm ³ (soln.)	*Equiv. SO ₂ /dm ³ (soln.)	xSO ₂ ** (CHCl ₃)	e ₁ /e ₂
1.738 1.753 2.326 2.346 2.628 3.039 3.058 3.686 3.735 4.226 5.269 5.372 6.588 31.92 33.26	0.05426 0.05473 0.07263 0.07324 0.08206 0.09488 0.1151 0.1166 0.1319 0.1645 0.1678 0.2057 0.9968 1.038	0.000489 0.0089 0.0093	1.123 1.122 1.704 1.703 1.897 2.395 2.385 3.063 3.062 3.626 4.798 4.813 6.183 33.84 37.25	0.03505 0.03503 0.05320 0.05320 0.05924 0.07478 0.07478 0.09563 0.09561 0.1132 0.1498 0.1503 0.1930 1.056 1.163	0.00140 0.0407 0.0445	1.55 1.56 1.37 1.38 1.38 1.27 1.28 1.20 1.22 1.17 1.10 1.12 1.07 0.94 0.89

- * As 1/2 SO₂.
- ** The mole fraction, $x_{\rm SO_2}$, water, is based on 1 dm³ of water, *i.e.*, on the assumption that there was no change in volume when SO₂ dissolved. Likewise for CHCl₃.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: A freshly prepared aqueous solution (50 cm³) of sulfur dioxide was shaken thoroughly with chloroform (50 cm³) in a separatory funnel in a thermostat at 293 K. The amount of SO₂ absorbed at equilibrium in a measured volume of each liquid phase was determined by titration (iodinethiosulfate).

NOTE: Pressure was not mentioned. The results merely provide so-called distribution coefficients as ratios of mole/l in the aqueous phase/mole/l in the chloroform phase for a range of concentrations in the aqueous phase.

SOURCE AND PURITY OF MATERIALS:

Not specified.

ESTIMATED ERROR:

1. Sulfur dioxide; SO₂; [7446-09-5]

Adueous phase

- 2. Trichloromethane (Chloroform); CHCl₃; [75-43-4]
- 3. Water; H₂O; [7732-18-5]
- 4. Hydrogen chloride; HCl;

ORIGINAL MEASUREMENTS:

McCrae, J.; Wilson, W. E.

Chloroform phage

Z. anorg. Chem. 1903, 35, 11-15.

[7647-01-0]

PREPARED BY:

W. Gerrard

VARIABLES:

EXPERIMENTAL VALUES:

T/K = 293.15

* As 1/2 SO₂

	Aqueous pna	se	Cn.	rorororm bua	ıse
N HCl	g SO ₂ /dm ³ (soln.)	*Equiv. SO ₂ /dm ³ (soln.) e ₁	g SO ₂ /dm ³ (soln.)	*Equiv. SO ₂ /dm ³ (soln.) e ₂	Distribution Coefficient e_1/e_2
0.05 0.05 0.05 0.05 0.1 0.1 0.1 0.1 0.2 0.2	1.86 3.076 4.277 5.340 1.25 1.324 2.78 3.86 5.161 1.268 1.914 2.464 3.967	0.0581 0.0960 0.1336 0.1667 0.0390 0.0413 0.0868 0.1199 0.1612 0.0396 0.0597 0.0769 0.1239	1.46 2.830 4.07 5.420 1.410 1.416 3.080 4.08 5.715 1.509 2.274 3.040 4.898	0.0456 0.0884 0.1271 0.1692 0.0440 0.0442 0.0962 0.1275 0.1784 0.0471 0.0710 0.0949 0.1530	1.28 1.08 1.04 0.96 0.88 0.93 0.90 0.94 0.90 0.84 0.84 0.81
0.4	1.202 1.894	0.0375 0.0591	1.614 2.263	0.0504 0.0706	0.79 0.83

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

A freshly prepared aqueous solution of sulfur dioxide and HCl was shaken thoroughly with chloroform in a separatory funnel in a thermostat at After attainment of equi-293.15 к. librium, the amount of sulfur di-Oxide in each phase was determined by iodine-thiosulfite titrations. NOTE: Pressure was not mentioned. The results merely provide so-called distribution coefficients as ratios of mole/1 in the aqueous phase divided by mole/l in the chloroform phase, for a range of concentrations in the aqueous phase.

SOURCE AND PURITY OF MATERIALS:

Not specified.

ESTIMATED ERROR:

108 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur Dioxide, SO₂; [7446-09-5] Tokunaga, J. J. Chem. Engng. Data. 1974, 19, 2. Water; H₂O; [7732-18-5] 3. Methanol; CH₄O; [67-56-1] 162-165. VARIABLES: PREPARED BY: C.L. Young Temperature EXPERIMENTAL VALUES: T/K Mole fraction Total Partial s§ s+ pressure Pressure of alcohol in P/bar of sulfur soln. (before dioxide absorption). P/bar 15.66 15.66 283.15 0.0000 1.024 1.012 0.0608 1.030 1.013 16.06 16.06 16.91 16.92 0.0813 1.032 1.013 0.1415 1.019 20.55 20.42 1.044 24.98 0.2066 1.043 1.015 25.04 1.045 1.015 43.60 43.50 0.3428 0.4161 1.053 1.017 51.75 51.53 1.056 56.63 56.26 0.4620 1.019 0.5862 1.049 1.010 75.96 76.17 90.85 1.023 91.79 0.6792 1.063 1.058 1.016 97.44 97.07 0.7490 112.18 110.97 1.066 1.024 0.8694 0.9263 1.059 1.016 120.38 120.02 131.85 131.56 1.015 1.0000 1.060 10.90 1.013 10.90 0.0000 1.036 293.15 1.013 10.45 10.44 0.0107 1.037 0.0675 1.048 1.014 11.14 11.12 14.48 14.51 1.011 0.1835 1.061 1.074 19.05 18.99 0.2659 1.016 24.56 0.3503 1.076 1.011 24.51 31.40 1.013 31.41 0.4233 1.082 0.5080 1.084 1.022 38.64 38.27 AUXILIARY INFORMATION METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide bubbled through 1. High purity sample with purity aqueous solution. Saturated solution analysed by iodometric of 99.96 mole per cent. titration. Details in source. 2. No details given. Partial pressure of sulfur dioxide calculated from known vapor pressure 3. Fractionated. of water + alcohol mixture and assuming Raoult's law for the lowering of vapor pressure of aqueous alcohol solution owing to dissolved sulfur dioxide. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta P/bar = \pm 0.001$;

 $\delta x_{\mathrm{SO}_2} = \pm 1$ %. (estimated by compiler)

- 1. Sulfur Dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Methanol; CH₄O; [67-56-1]

ORIGINAL MEASUREMENTS:

Tokunaga, J.

J. Chem. Engng. Data, 1974, 19,

162-165.

EVDED	IMENTAL	TATTIEC	
CAPER	TWINIAL	VALUES	

T/K	Mole fraction of alcohol in soln. (before absorption).	Total pressure P/bar	Partial pressure of sulfur dioxide P/bar	s [§]	s ⁺ _o
293.15	0.5798 0.6694 0.7638 0.8996 1.0000	1.095 1.097 1.096 1.089	1.019 1.018 1.014 1.002 1.012	45.87 53.02 63.57 75.33 86.11	45.58 52.74 63.44 76.15 86.19
303.15	0.0000 0.0811 0.1890 0.2849 0.4193 0.4679 0.6197 0.6760 0.7506 0.8734 0.9673 1.0000	1.057 1.079 1.102 1.120 1.132 1.133 1.147 1.153 1.157 1.168 1.169	1.016 1.014 1.010 1.010 1.006 1.009 1.009 1.008 1.011 1.007	7.79 8.35 10.80 14.13 21.18 23.41 32.69 35.69 40.36 49.09 56.60 57.63	7.77 8.33 10.88 14.16 21.23 23.56 32.82 35.79 40.53 49.19 56.92 57.53
313.15	0.0000 0.0830 0.1402 0.3185 0.4041 0.5332 0.5822 0.6354 0.6740 0.7957 0.8400 0.9165 1.0000	1.086 1.125 1.153 1.201 1.221 1.242 1.240 1.232 1.262 1.271 1.288 1.290 1.301	1.013 1.011 1.016 1.012 1.015 1.017 1.007 1.010 1.016 1.010 1.011 1.013 1.013	5.76 6.26 7.22 11.98 14.88 20.94 22.21 24.69 26.33 31.96 33.56 37.46 40.82	5.76 6.26 7.20 11.98 14.85 20.85 22.33 24.75 26.23 32.05 33.62 37.44 40.80

 $[\]mathcal{S}^{\S}$ - grams of sulfur dioxide per 100 grams of solution (solute gas free) at total pressure.

Original gives pressure in units of mmHg 760 mmHg = 1 atm = 1.01325 bar

 $S_{\rm O}^{+}$ - grams of sulfur dioxide per 100 grams of solution (solute gas free) at 1 atm. partial pressure.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Sulfur dioxide, SO ₂ ; [7466-09-5] (2) Water, H ₂ O; [7732-18-5] (3) Acetonitrile; C ₂ H ₃ N; [75-05-8]	Byerley, J.J.; Rempel, G.L.; Le, V.T J. Chem. Eng. Data. <u>1980</u> ,25, 55-56
VARIABLES: T/K: 298.15, 323.15 Total p/kPa 101.3 (1 atm) CH ₃ CN/wt% 0-100	PREPARED BY: H.L. Clever
EXPERIMENTAL VALUES: 298.15 : Liquid components SO ₂ solubility CH ₃ CN H ₂ O Single Two Wt % phase CH ₃ CH	, ^d g/100g SO₂ solubility, g/100g o phase

	ſ	CAL VALUES: COMPONENTS H ₂ O Wt %		298.15 K lubility, d g/100g SO ₂ solubility, g/100g Two phase single phase CH ₃ CN H ₂ O rich rich
į	0 5	100	8.24	3.77
	5	95	8.37	-
	10	90	9.03	3.95
	15	85	10.0	-
	20	80	b	a a 5.08
	30	70	b	59.4 (0.25) ^C 12.4 (0.74) ^C 6.85
	40	60	b	59.4 (0.45) 12.4 (0.55) 8.33
	50	50	b	59.4 (0.60) 12.4 (0.40) 11.09
	60	40	b	59.4 (0.74) 12.4 (0.25) 13.75
	70	30	b	59.4 (0.87) 12.4 (0.13) 15.60
	80	20	b	a a 18.67
	90	10	73.8	23.10
	95	5	78.7	-
	100	0	84.6	25.64

- a. Phase separation. ill defined reading to poor reproducibility.
- b. Two phases.
- c. Number in c) is the phase fraction. The total composition of the CH₃CN rich phase is 12.9 wt% $\rm H_2O$, 37.3 wt % $\rm SO_2$, and 49.8 wt % acetonitrile with density 0.975 g cm⁻³. The water rich phase is 73.0 wt % $\rm H_2O$, 11.0 wt % $\rm SO_2$ and 16.0 wt % acetonitrile with density 1.005 g cm⁻³
- d. The SO_2 solubility is expressed as g $SO_2/100$ g of gas free solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The mixed solvent was placed in a 50 ml water jacketted buret. Sulfur dioxide was bubbled at a rate of 60 $ml m^{-1}$ from the bottom of the buret. A spiral condenser at the top prevented excessive loss of acetonit-The sulfur dioxide concentration after saturation was measured by titrating excess iodine with standard thiosulfate solution using starch as the indicator. In the cases where there was phase separation upon saturation with SO2, the composition of both phases was determined by gas chromatography. The column, 0.91m long and 0.4 cm i.d., stainless steel was packed with 50-80 mesh Porapak Q. The carrier gas was a helium hydrogen mixture.

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide. Union Carbide Canada. Ltd. Anhydrous.
- Water, distilled, carbon dioxide free.
- Acetonitrile. J.T. Baker Co. Reagent grade. Used as received.

ESTIMATED ERROR:

 $\delta T/K = 0.1$

-

COMPONENTS:			ORIGINAL MEASUREMENT	S:	
1. Sulfur Dioxide; SO ₂ ; [7446-09-5]			Tokunaga, J.	•	
				David a	1074 40
	H ₂ O; [7732-18-5]		J. Chem. Engng.	Data.	1974, 19,
3. Ethano	1; C ₂ H ₆ O; [64-17-	5]	162-165.		
VARIABLES:			PREPARED BY:		
т	emperature		C.L. Young		1
EXPERIMENTAL	VALUES:				
T/K	Mole fraction of alcohol in soln. (before adsorption).	Total Pressure P/bar	Partial pressure of sulfur dioxide P/bar	S [§]	<i>s</i> ⁺ °
283.15	0.0000 0.0628 0.0986 0.1722 0.2423 0.3325 0.3827 0.4728 0.6010 0.6650 0.7955 0.8730	1.024 1.029 1.035 1.036 1.036 1.037 1.039 1.038 1.038 1.043	1.012 1.012 1.016 1.014 1.013 1.015 1.015 1.015 1.019 1.019	15.66 14.44 14.87 20.18 26.88 35.76 39.73 47.06 57.08 60.83 65.55 67.60	14.45 14.82 20.15 26.84 35.73 39.62 46.98 56.94 60.46 65.44 67.61
293.15	1.0000 0.0000 0.0563 0.0986 0.2168 0.2781 0.3399 0.4753 0.5923 0.6832	1.034 1.036 1.048 1.043 1.043 1.064 1.064 1.060 1.059	1.014 1.013 1.015 1.005 0.998 1.017 1.016 1.013 1.012	70.58 10.90 9.21 9.78 15.08 19.00 23.09 30.88 35.73 39.15	10.90 9.19 9.86 15.30 18.92 23.00 30.88 35.76
		AUXILIARY	INFORMATION		
METHOD /API	PARATUS/PROCEDURE:		SOURCE AND PURITY OF	MATERIA	LS:
Sulfur dioxide bubbled through aqueous solution. Saturated solution analysed by iodometric titration. Details in source. The partial pressure of sulfur dioxide was calculated from the known vapor pressure of water + alcohol mixture and assuming Raoults law for the lowering of vapor pressure due to			1. High purity s of 99.96 mole 2. No details gi 3. Fractionated.	ample w per ce	th purity
dissoluti	on of sulfur diox	ide	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta$ $\delta x_{SO} = \pm 1\%. \ ($	P/bar = estimat compile	ed by

- 1. Sulfur Dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Ethanol; C₂H₆O; [64-17-5]

ORIGINAL MEASUREMENTS:

Tokunaga, J.

J. Chem. Engng. Data. 1974,19,

162-165.

EXPERIMENTAL VALUES:

T/K	Mole fraction of alcohol in soln. (before adsorption).	Total pressure <i>P/</i> bar	Partial pressure of sulfur dioxide P/bar	s [§]	s ⁺ _o	
293.15	0.7927 0.8941 1.0000	1.059 1.059 1.059	1.014 1.014 1.016	42.37 44.91 46.95	42.33 44.83 46.81	
303.15	0.0000 0.0651 0.1159 0.1992 0.3004 0.3663 0.4684 0.5004 0.6082 0.7307 0.8182 0.8807 0.9551	1.057 1.074 1.080 1.093 1.096 1.101 1.102 1.100 1.102 1.101 1.099 1.098 1.098	1.016 1.010 1.007 1.012 1.011 1.014 1.014 1.011 1.013 1.013 1.011 1.011 1.011	7.79 6.63 7.22 10.32 14.20 16.46 19.98 20.47 23.04 26.21 28.10 28.79 30.33 31.76	7.77 6.44 7.27 10.32 14.22 16.43 19.96 20.49 23.02 26.19 28.14 28.84 30.32 31.62	
313.15	0.0000 0.0644 0.1035 0.1900 0.3000 0.3982 0.5111 0.6055 0.7294 0.8205 0.9152 1.0000	1.086 1.118 1.135 1.156 1.157 1.159 1.168 1.167 1.169 1.167	1.013 1.007 1.012 1.019 1.011 1.009 1.004 1.013 1.011 1.014	5.76 5.29 5.99 7.99 10.01 12.60 15.07 17.13 18.30 20.33 21.69 23.80	5.76 5.32 6.09 7.94 10.02 12.64 15.19 17.12 18.32 20.31 21.68 23.80	

grams of sulfur dioxide per 100 grams of solution (solute gas free) at total pressure.

Original gives pressure in units of mmHg 760 mmHg = 1 atm = 1.01325 bar

 $S_{\rm O}^{+}$ - grams of sulfur dioxide per 100 grams of solution (solute gas free) at 1 atm. partial pressure.

Aqueous org	panic solutions 113
 COMPONENTS: Sulfur dioxide; SO₂; [7746-09-5] Water; H₂O; [7732-18-5] Sulfinybismethane, (Dimethylsulfoxide); C₂H₆OS; [67-68-5] 	ORIGINAL MEASUREMENTS: Smedslund, T.H. Finska Kemistsamfundets Medd. 1950, 59, 40-43.
VARIABLES: Temperature	PREPARED BY: W. Gerrard
EXPERIMENTAL VALUES: Dimethylsulfoxide	containing "10%" water.
T/K SO2, Weight %	Presumably for total pressure of 1 atm.

292.15 54.3 350.15 22.1 408.15 6.0 420.15 2.5 293.15 5.2 $p_{SO_2} = 11.2 \text{ mmHg}$ 293.15 12.1 $p_{SO_2} = 31 \text{ mmHg}$ 293.15 16.1 $p_{SO_2} = 46 \text{ mmHg}$	T/K	SO ₂ , weight	70	riesume	, DI	l atr	pressur
293.15	350.15 408.15	22.1 6.0					
293.15 $16.1 p_{SO_2}^2 = 46 mmHg$							
	293.15	16.1	p_{SO_2}	= 46	mmHo	j .	

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The first set of data are for saturation at 1 atm; details are not available for the second set.	(1) Information not available (2) Dimethylsulfoxide was prepared by the catalytic oxidation of dimethyl sulfide in the vapor state (1). The purified product had b.p. 63°C/6 mmHg.
	REFERENCES: 1. Smedslund, T.H. U.S. Patent, 2,581,050, 1952

114 COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] 1. Tokunaga, J. Water; H₂O; [7732-18-5] J. Chem. Engng. Data. 1974,19, 3. 1-Propanol; C_3H_8O ; [71-23-8] 162-165. VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: s § s+ Mole fraction Total T/K Partial of alcohol in Pressure soln. (before P/bar Pressure of sulfur adsorption). dioxide P/bar 283.15 0.0000 1.024 1.024 15.66 15.66 0.0124 1.030 1.017 14.59 14.52 0.0352 14.28 14.28 1.027 1.013 0.0651 15.51 15.53 1.026 1.011 0.1036 19.04 1.030 19.02 1.011 0.2000 1.028 1.012 26.56 26.58 33.27 38.36 33.29 38.35 0.3026 1.027 1.012 1.027 1.013 0.3960 0.4986 1.027 1.013 42.09 42.06 1.027 1.014 45.54 45.46 0.5927 47.77 47.80 0.7068 1.025 1.013 0.8160 1.023 1.012 48.96 48.97 49.43 0.9286 1.023 1.014 49.52 1.013 49.63 49.60 1.0000 1.020 1.013 10.90 10.90 0.0000 1.036 293.15 1.040 9.96 0.0218 1.013 9.95 10.16 10.15 0.0501 1.042 1.013 1.014 12.24 12,22 0.0922 1.045 0.1882 1.051 1.019 17.22 17.11 1.013 18.21 18.21 0.2172 1.044 1.014 21.04 21.02 0.2967 1.044 AUXILIARY INFORMATION METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide bubbled through 1. High purity sample with purity of 99.96 mole per cent. aqueous solution. Saturated solution analysed by iodometric titration. 2. No details given. Details in source. 3. Fractionated. The partial pressure of sulfur dioxide was calculated from the known vapor pressure of water + alcohol mixture and assuming Raoults law for the lowering of vapor pressure due to dissolution of sulfur dioxide. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta P/bar = \pm 0.001$; $\delta x_{SO_2} = \pm 1$ %. (estimated by compiler). REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Water; H₂O; [7732-18-5]
- 3. l-Propanol; C₃H₈O; [71-23-8]

ORIGINAL MEASUREMENTS :

Tokunaga, J.

J. Chem. Engng. Data. 1974, 19,

162-165

EXPERIMENTAL VALUES :

T/K	Mole fraction of alcohol in soln. (before adsorption).	Total pressure <i>P/</i> bar	Partial pressure of sulfur dioxide P/bar	S [§]	<i>S</i> + 0	
293.15	0.3980 0.4846 0.5960 0.6948 0.7860 0.8941 1.0000	1.044 1.043 1.041 1.038 1.036 1.033 1.027	1.014 1.014 1.013 1.013 1.013 1.013	24.28 26.55 28.47 29.38 30.27 30.37 30.68	24.24 26.50 28.47 29.39 30.27 30.36 30.68	
303.15	0.0000 0.0223 0.0516 0.0761 0.1964 0.3009 0.3976 0.4900 0.5984 0.7077 0.7732 0.9026 1.0000	1.057 1.064 1.069 1.071 1.073 1.058 1.071 1.068 1.066 1.065 1.061 1.052	1.017 1.014 1.014 1.012 1.014 1.000 1.014 1.012 1.012 1.014 1.013 1.013	7.79 7.34 8.04 8.79 12.78 15.28 17.67 18.98 20.43 21.32 21.53 21.91 22.05	7.77 7.34 8.03 8.80 12.77 15.49 17.66 18.99 20.45 21.29 21.53 21.92 22.06	
313.15	0.0000 0.0186 0.0355 0.0763 0.1043 0.1974 0.2992 0.3950 0.4994 0.6068 0.7108 0.7824 0.9112 1.0000	1.087 1.085 1.107 1.116 1.119 1.118 1.116 1.116 1.116 1.112 1.106 1.097 1.088 1.071	1.014 1.009 1.012 1.016 1.014 1.013 1.013 1.015 1.014 1.014 1.010 1.015	5.76 5.57 5.59 6.49 7.21 9.30 11.22 12.39 13.60 14.53 15.15 15.54 15.69	5.76 5.60 5.60 6.47 7.20 9.30 11.22 12.39 13.58 14.52 15.14 15.59 15.66 15.95	

 s^{\S} - grams of sulfur dioxide per 100 grams of solution (solute gas free) at total pressure.

Original gives pressure in units of mmHg 760 mmHg = 1 atm = 1.01325 bar

⁻ grams of sulfur dioxide per 100 grams of solution (solute gas free) at 1 atm. partial pressure.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Alkanes

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia. November 1980

CRITICAL EVALUATION:

Although these systems have been investigated by several workers, there are very serious discrepancies between solubilities reported by different authors. The most extensive studies are those of Makranczy $et\ al.$ (1) and Sololev $et\ al.$ (2) and values of their mole fraction solubilities at 298.15 K and 101.3 kPa are contrasted below.

Alkane	x_{SO_2} (Sololev et al.)	x_{SO_2} (Makranczy et αl .)
Octane	0.0319	0.0586
Dodecane	0.0378	0.0662
Hexadecane	-	0.0745
Heptadecane	0.0372	-

The evaluator is of the opinion that the values of Sololev et al. (2) are probably in error whereas those of Makranczy et al. (1) are moderately reliable. The value of Gerrard (3) for decane at 293.15 K and 273.15 K extrapolate to 298.15 K to give a value of about 35% higher than the value of Makranczy et al. (1). The mole fraction solubilities for hexadecane of Tremper and Prausnitz (4), Lenoir et al. (5), Sano (6) and Makranczy et al. (1) agree within about 15% whereas the value of Sololev et al. (2) is approximately have of the average value of the other workers.

Therefore the values of Sololev et αl . (2) and Gerrard (3) are classified as doubtful whereas those of Makranczy et αl . (1), Lenoir et αl . (5), Sano (6) and Tremper and Prausnitz (4) are classified as tentative.

The data of Makranczy et al. for the alkanes can be represented as a function of carbon number, \mathcal{C}_n , by the equation

$$\ln x_{SO_2} = 0.02933C_n - 3.068$$

well within the experimental error of 3 per cent. A plot of $\ln x_{\rm SO_2}$ against $C_{\rm n}$ is given on the following page.

The value of Lenoir $et\ al$. (5) was determined from gas chromatographic retention volume data and is effectively at infinite dilution of sulfur dioxide. The extrapolation to 101.3 kPa pressure assumes Henry's law holds up to that pressure and consequently involves considerable approximation.

The data presented by Komissarov $et\ al.$ (7) on the system sulfur dioxide + tetradecane appears to be greatly in error, the mole fraction solubility calculated from their data being about double the value of Makranczy $et\ al.$ (1).

References

- Makranczy, J.; Megyerg-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. <u>1976</u>, 4, 269.
- Sololev, I. A.; Kukarin, V. A.; Dzhagatspanyan, R. V.; Kosorotov, V. I.; Zogarets, P. A.; Popov, A. I. Khim. Prom. 1970, 46, 668.
- Gerrard, W. Solubility of Gases and Liquids, Plenum Press, New York, <u>1976</u>, p.239.
- Tremper, K. K.; Prausnitz, J. M. J. Chem. Engng. Data 1976, 21, 295.
- Lenoir, J. Y.; Renault, P.; Renon, H. J. Chem. Engng. Data 1971, 16, 340.
- 6. Sano, H. Nippon Kagaku Zasshi 1968, 89, 362.
- Komissarov, V. D.; Saitova, M. A.; Timirova, R. G. Khim. Prom. 1973, 49, 738.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Alkanes

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

November 1980

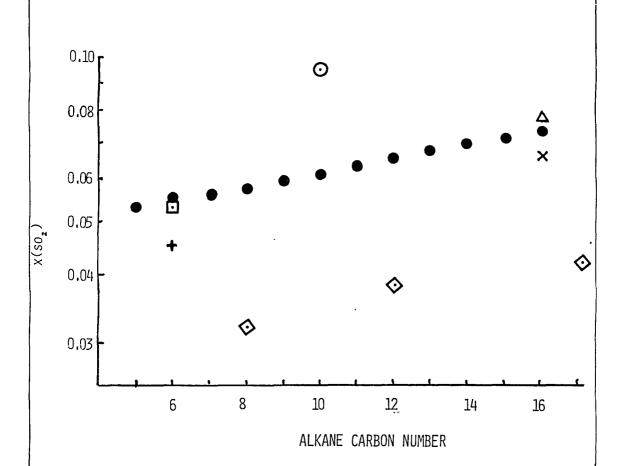


Figure 1. Comparison of mole fraction solubilities for sulfur dioxide in alkanes.

- Makranczy, Megyery-Balog, Rusz and Patyi (1)
- Gerard (3)
- Sololev, Kukarin, Dzhagatspanyan, Kosorotov, Zogarets and Popov (2)
- Patyi, Furmer, Makranczy, Sadilenko, Stepanova and Berengarten
- Δ Lenoir, Renault, Renon (5)
- × Tremper and Prausnitz (4)
- + Sano (6)

COMPONENTS: 1. Sulfur Dioxide; SO₂; Makranczy, J.; Megyery-Balog, K.; [7446-09-5]; Rusz, L.; Patyi, L. 2. Pentane; C₅H₁₂; [109-66-0] Hung. J. Ind. Chem. 1976, 4(2), 269-280. VARIABLES: T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES:

T/K	Mole fraction x SO $_2$	Bunsen coefficient $lpha$	Ostwald coefficient L
298.15	0.0543	10.880	11.876
313.15	0.0402	7.76	8.90

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

Bodor, E.; Bor, Gy.; Mohai, B.;
 Sipos, G. Veszprémi Vegyipari
 Egyetem Kösleményei 1957, 1, 55;
 CA 55, 3175h.

1. Sulfur dioxide; SO2;

[7446-09-5]

2. Hexane; C₆H₁₄; [110-54-3]

ORIGINAL MEASUREMENTS:

Sano, H.

Nippon Kagaku Zasshi

1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$ T/K = 303

Vapor pressure of hexane, $p_s^{\circ} = 0.240$ atm

Absorption coefficient,	Bunsen b coefficient, b	Bunsen coefficient, c	_l c,d	Mole ratio	Mole fraction ^e
6.8	8.1	8.2	6.5	0.047	0.0449

- ^a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature at a total pressure of 1 atmosphere.
- b Determined by static absorption method.
- C Determined by flow method.
- d $\alpha = \ell(1 p_s^o)$ where p_s^o is vapor pressure of solvent.
- e Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: (a) static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5$ %

(estimated by compiler).

120 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur Dioxide; SO₂; [7446-09-5] Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. 2. Hexane; C_6H_{14} ; [110-54-3] Hung. J. Ind. Chem. 1976, 4(2), 269-280. VARIABLES: PREPARED BY: T/K: 298.15 - 313.15 S. A. Johnson/ H. L. Clever P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES: Mole fraction Bunsen coefficient Ostwald coefficient T/K xso, 0.0562 9.964 10.876 298.15 0.0408 313.15 7.00 8.02 Mole fractions and Bunsen coefficients were calculated by the compiler. AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

DATA CLASS:

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

Alkanes 121

Veszpremi. Vegyip. Egy. Kosl.

<u>1957</u>, 1, 55.

A.	indities 12
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] Hexane; C₆H₁₄; [110-54-3] 	Patyi, L.; Furmer, I. E. Makranczy, J.; Sadilenko, A. S.; Stepanova, Z. G.; Berengarten, M. G. Zh. Prikl. Khim. 1978, 51, 1296- 1300.
WARTARY	
VARIABLES:	PREPARED BY:
	C. L. Young
EXPERIMENTAL VALUES:	
T/K α [†]	Mole fraction of sulfur dioxide at a partial pressure of 101.325 kPa $^x{ m SO}_2$
298.15 9.38	0.05336
AUXILIAR	Y INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method. Pressure measured when known amounts of gas were added, in increments, to a	COURSE AND PORTIE OF PATERIALS,
	Purity better than 99 mole per cent as determined by gas chromatography.
known amount of liquid in a vessel of known dimensions. Corrections were made for the partial pressure of solvent. Details in ref. (1).	cent as determined by gas

COMPONENTS: 1. Sulfur Dioxide; SO₂; [7446-09-5] Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. 2. Heptane; C₇H₁₆; [142-82-5] Hung. J. Ind. Chem. 1976, 4(2), 269-280. VARIABLES: T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES:

т/к	Mole fraction $^x{ m SO}_2$	Bunsen coefficient $\boldsymbol{\alpha}$	Ostwald coefficient L
298.15	0.0567	8.969	9.790
313.15	0.0417	6.40	7.34

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

Alkanes 123 COMPONENTS: ORIGINAL MEASUREMENTS: Sobolev, I.A.; Kukarin, V.A.; 1. Sulfur dioxide; SO₂; [7446-09-5] Dzhagatspanyan, R.V.; Kosorotov, V.I. 2. Octane; C₈H₁₈; [111-65-9] Zogorets, P.A.; Popov, A.I. Khim. Prom. 1970, 46,668-70. VARIABLES: PREPARED BY: C.L. Young. Temperature. EXPERIMENTAL VALUES: Solubility Mole fraction of + T/K sulfur dioxide in /mol 1 in liquid, x SO2 0.283 0.044 283.15 0.040 288.15 0.254 293.15 0.227 0.036 0.032 0.201 298.15 303.15 0.182 0.029 + calculated by compiler. * at atmospheric pressure. ln S = 830/(T/K) - 6.35 (where S is in units of mol 1^{-1} atm⁻¹). AUXILIARY INFORMATION .-METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Bubbler method. Samples of saturated liquid taken and added to sodium 1. Purity at least 95 mole per cent. hydroxide solution and then excess 2. Chemically pure. Dried. alkali back titrated. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; δ (Solubility) = $\pm 2\%$; $\delta x_{SO_2} = \pm 0.001$, (estimated by compiler) REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur Dioxide; SO₂; [7446-09-5] Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4(2), 2. Octane; C₈H₁₈; [111-65-9] 269-280. VARIABLES: PREPARED BY: T/K: 298.15 - 313.15 S. A. Johnson / H. L. Clever P/kPa: 101.325 (1 atm) EVDEDIMENTAL MALUEC.

EXPERIMEN	TAL VALUES:			
т/к	Mole fraction x SO $_2$	Bunsen coefficient α	Ostwald coefficient L	
298.15 313.15	0.0583 0.0429	8.330 5.95	9.092 6.82	

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

 $\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

ORIGINAL MEASUREMENTS:		
Sobolev, I.A.; Kukarin, V.A.; Dzhagatspanyan, R.V.; Kosorotov, V.I; Zogorets, P.A.; Popov, A.I. Khim. Prom. 1970, 46,668-70.		
PREPARED BY: C.L. Young		
y*, S Mole fraction + of sulfur dioxide **SO2		
0.0355		
essure		
piler		
ARY INFORMATION		
SOURCE AND PURITY OF MATERIALS: 1. Purity at least 95 mole per cent. 2. Chemically pure. Dried.		

COMPONENTS:		ORIGINAL MEASUREMENTS:		
1. Sulfur dioxide; SO ₂	; [7446-09-5]	Nitta, T.; Kido. O.; Katayama, T.;		
2. 2,2,4-Trimethylpents [540-84-1]	ane; C ₈ H ₁₈ ;	J. Chem. Engng. Japan, <u>1976</u> , 9,317-8.		
VARIABLES: Pressure		PREPARED BY: C.L. Young		
EXPERIMENTAL VALUES:				
T/K	P/bar	Mole fraction of sulfur dioxide in liquid, x_{SO_2}		
293.15	0.7021 1.031 1.516 2.042 2.521 2.796 3.170 3.193 3.200	0.0445 0.0710 0.1184 0.1847 0.2706 0.3362 0.6412 0.7897 0.8506		
	AUXILIARY	INFORMATION		
METHOD: Static method liquid composition estimated Few details given in similar to that used	by iodometry. source. Method	SOURCE AND PURITY OF MATERIALS: 1. Seitetsu Chemical Co.sample, purity better than 99.9 mole per cent. 2. Nakarai Chemicals Ltd. sample, guaranteed grade.		
		ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta P/bar = \pm 0.001 \ (below 1.3 \ bar) \ \pm 0.005 \ (above 1.3 \ bar); \\ \delta x_{SO_2} = 1.5 \%$ REFERENCES: Quitzich, K.; Ulbrecht, H.; Geiseler, G. Z. Physik Chem. 1967, 234, 33.		

Alkanes 127

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur Dioxide; SO₂; [7446-09-5] Nonane; C₉H₂₀; [111-84-2] 	Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4(2), 269-280.
VARIABLES: T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm)	PREPARED BY: S. A. Johnson / H. L. Clever

EXPERIMENTAL VALUES:

T/K	 fraction ^x SO ₂	Bunsen	coefficient α	Ostwald	coefficient L
298.15 313.15	0.0602 0.0441		7.840 5.58		.558 .40

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

Bodor, E.; Bor, Gy.; Mohai, B.;
 Sipos, G. Veszprémi Vegyipari
 Egyetem Kösleményei 1957, 1, 55;
 CA 55, 3175h.

- 1. Sulfur Dioxide; SO₂; [7446-09-5]
- 2. Decane; $C_{10}H_{22}$; [124-18-5]

ORIGINAL MEASUREMENTS:

Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L.

Hung. J. Ind. Chem. 1976, 4(2),

269-280.

VARIABLES:

T/K: 298.15 - 313.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson/ H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mole fraction x SO ₂	Bunsen coefficient α	Ostwald coefficient L
298.15	0.0620	7.430	8.110
313.15	0.0456	5.30	6.08

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

- Sulfur dioxide; SO₂; [7446-09-5]
- 2. Decane; $C_{10}H_{22}$; [124-18-5] or Decahydronaphthalene; (Decalin); $C_{10}H_{16}$; [91-17-8] or 1,2,3,4- Tetrahydronaphthalene; (Tetralin); $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1976, p.239.

VARIABLES:

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

EXPERIMENTAL	VALUES:			
T/K	Weight of Component(2) g	Weight of So₂ absorbed,g		Mole fraction **SO2
		Decane		
			(Total press	ure, l atm)
273.15	3.8122	0.3040	0.179	0.151
293.15	3.8122	1.7832	0.105	0.095
		(cis-trans) D	ecalin	
			(Total press	ure, l atm)
293.15	7.2121	0.2090	0.062	0.060
		Tetralin		
		10014111	(Total press	ure, l atm)
293.15	7.5100	1.0732	0.295	0.228
		760 mmHg = 1 atm	= 101.325 kPa	

AUXILIARY INFORMATION

METHOD:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube. The amount of gas absorbed was determined by re-weighing the tube. The total pressure was barometric, very nearly 1 atm. See ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high degree of purity was attested by the measurement of vapor pressure from 258-268 K.
- 2. The best commercial specimen was purified and attested.

ESTIMATED ERROR:

REFERENCES:

1. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22,623.

298.15

313.15

130 Sulfur Dioxide Solubilities ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur Dioxide; SO₂; [7446-09-5] Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. 2. Undecane; C₁₁H₂₄; [1120-21-4] Hung. J. Ind. Chem. 1976, 4(2), 269-280. VARIABLES: PREPARED BY: T/K: 298.15 - 313.15 S. A. Johnson / H. L. Clever P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES: T/K Mole fraction Bunsen coefficient Ostwald coefficient x_{SO₂}

Mole fractions and Bunsen coefficients were calculated by the compiler.

7.170

5.07

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

0.0647

0.0471

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

7.826

5.81

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

Alkanes 131

AIK	anes
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] Dodecane; C₁₂H₂₆; [112-40-3] 	Sobolev, I.A.; Kukarin, V.A.; Dzhagatspanyan, R.V.; Kosorotov, V.I Zogorets, P.A.; Popov, A.I.
	Khim. Prom. <u>1970</u> , 46, 668-670.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES:	
T/K Solubility / mol 1-1	, S Mole fraction of the sulfur dioxide in liquid, x_{SO_2}
283.15 0.243	0.052
288.15 0.214	0.046 0.042
293.15 0.191 298.15 0.172	0.038
303.15 0.153	0.034
+ calculated by compiler.	
* at atmospheric pressure relationship between pr up to 1 atmosphere part	essure and solubility .
$ \ln S = 852 / (T/K) - 6.50 \text{mol } 1^{-1} \text{atm}^{-1}) $	(where S is in units of
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Bubbler method. Samples of saturated liquid taken and added to sodium hydroxide solution and	1. Purity at least 95 mole per cent.
then excess alkali back titrated	2. Chemically pure. Dried. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; δ (Solubility) = $\pm 2\%$; $\delta x_{SO_2} = \pm 0.001$; (estimated by compiler). REFERENCES:
	MITARENCES;

298.15

313.15

132 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur Dioxide; SO₂; [7446-09-5] Makranczy, J.; Magyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4(2), 2. Dodecane; C₁₂H₂₆; [112-40-3] 269-280. VARIABLES: PREPARED BY: T/K: 298.15 - 313.15 S. A. Johnson / H. L. Clever P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES: Ostwald coefficient T/K Mole fraction Bunsen coefficient ^xso₂

Mole fractions and Bunsen coefficients were calculated by the compiler.

6.820

4.85

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

0.0662

0.0484

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

7.444

5.56

ESTIMATED ERROR:

$$\delta x_{\mathrm{SO}_2}/x_{\mathrm{SO}_2} = \pm 0.03.$$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

- 1. Sulfur Dioxide; SO₂; [7446-09-5]
- 2. Tridecane; C₁₃H₂₈; [629-50-5]

ORIGINAL MEASUREMENTS:

Makranczy, J.; Megyery-Balog, K.;
Rusz, L.; Patyi, L.

Hung. J. Ind. Chem. <u>1976</u>, 4(2), 269-280.

VARIABLES:

T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson/ H. L. Clever

EXPERIMENTAL VALUES:

T/K	 fraction ^x SO ₂	Bunsen	coefficient a	Ostwald	coefficient L
298.15 313.15	0.0682 0.0500		5.580 4.68		.182 .36

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

Bodor, E.; Bor, Gy.; Mohai, B.;
 Sipos, G. Veszprémi Vegyipari
 Egyetem Kösleményei 1957, 1, 55;
 CA 55, 3175h.

ORIGINAL MEASUREMENTS: 1. Sulfur Dioxide; SO₂; [7446-09-5] Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. 2. Tetradecane; C₁₄H₃₀; [629-59-4] Hung. J. Ind. Chem. 1976, 4(2), 269-280. VARIABLES: T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4(2), 269-280.

EXPERIMENTAL VALUES:

T/K	Mole fraction ^x SO ₂	Bunsen coefficient α	Ostwald coefficient L
298.15	0.0702	6.360	6.942
313.15	0.0514	4.52	5.18

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

 Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

- 1. Sulfur Dioxide; SO₂; [7446-09-5]
- 2. Pentadecane; $C_{15}H_{32}$; [629-62-9]

ORIGINAL MEASUREMENTS:

Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L.

Hung. J. Ind. Chem. 1976, 4(2), 269-280.

VARIABLES:

T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson / H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mole fraction	Bunsen coefficient	Ostwald coefficient
	^x so₂	α	L

0.0722 298.15 6.170 6.735 313.15 0.0531 4.40 5.04

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszprémi Vegyipari Egyetem Kösleményei 1957, 1, 55; CA 55, 3175h.

COMPONENTS: ORIGINAL MEASUREMENTS: Tremper, K.K.; Prausnitz, J.M. Sulfur dioxide; SO₂; [7446-09-5] J. Chem. Engng. Data 1976, 21,295-9 2. Hexadecane; $C_{16}H_{34}$; [544-76-3] VARIABLES: PREPARED BY: C.L. Young Temperature EXPERIMENTAL VALUES: Mole fraction b of Henry's Constanta T/K sulfur dioxide at /atm 1 atm partial pressure, xSO2 15.1 0.0662 300 0.0448 325 22.3 0.0325 350 30.8 0.0249 375 40.2 0.0200 400 50.1 60.1 0.0166 425 69.8 0.0143 450 0.0130 77.1 475 Authors stated measurements were made at several pressures and values of solubility used were all within the Henry's-Law region. Calculated by compiler assuming linear relationship between mole fraction and pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Volumetric apparatus similar to that described by Dymond and Hildebrand Solvent degassed, no other details (1). Pressure measured with a null given. detector and precision gauge. Details in ref. (2). NOTE It was stated that "while all measurements were made at low pressures, experiments were made at several pressures. The total pressures were always less than 1000 mm Hg and usually much less." ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta x_{SO_2} = \pm 1%.$ REFERENCES: EFERENCES: 1. Dymond, J.; Hildebrand, J.H. Ind. Eng. Chem. Fundam. 1967, 6, 130. 2. Cukor, P.M.; Prausilozi, J.M.

Ind. Eng. Chem. Fundam. 1971, 10, 638.

1. Sulfur Dioxide; SO₂; [7446-09-5]

2. Hexadecane; $C_{16}H_{34}$; [544-76-3]

ORIGINAL MEASUREMENTS:

Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4(2), 269-280.

VARIABLES:

T/K: 298.15 - 313.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson / H. L. Clever

EXPERIMENTAL VALUES:

т/к	fraction ^x SO ₂	Bunsen coefficient α	Ostwald	coefficient L
298.15 313.15	0.0745 0.0545	6.020 4.27		.571 .90

Mole fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Apparently the volumetric apparatus described in ref.(1) was modified for use at temperatures above 0°C. The apparatus was designed to be operated at a partial pressure of sulfur dioxide of 760 torr.

SOURCE AND PURITY OF MATERIALS:

Analytical grade reagents of Hungarian and foreign origin were used (both liquids and gases). No further information.

ESTIMATED ERROR:

$$\delta x_{SO_2}/x_{SO_2} = \pm 0.03.$$

REFERENCES:

Bodor, E.; Bor, Gy.; Mohai, B.;
 Sipos, G. Veszprémi Vegyipari
 Egyetem Kösleményei 1957, 1, 55;
 CA 55, 3175h.

- . Sulfur dioxide, SO₂; [7446-09-5]

ORIGINAL MEASUREMENTS:

Lenoir, J-Y.; Renault, P.; Renon, H.

J. Chem. Eng. Data. 1971, 16, 340-342

VARIABLES:

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES: SOLVENT	т/к	HENRY'S CONSTANT H SO ₂ /ATM	MOLE FRACTION * AT 1 ATM	
Hexadecane	298	12.9	0.0775	
Heptadecane	323	16.4	0.0610	

* Calculated by compiler assuming a linear function of p_{SO_2} vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$.

The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x_{SO_2} \to 0} \frac{f_{SO_2}(P,T)}{x_{SO_2}}$

 x_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition" of pressure and temperature. H_{SO_2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit was used. The chromatograph was an IGC 12 M Intersmat model, equipped with a thermal conductivity detector. The temperature control was stated to be within ±0.1° C. The pressure drop in the column, was measured by a mercury manometer. Helium was the carrier gas.

There is serious uncertainty in the estimation of accuracy.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was provided by l'Air Liquide, and had a stated purity of 99.9%. It was used as provided.
- Provided by Touzart & Matignon and Serlabo, and stated to have a minimum purity of 99%. Distillation was carried out when necessary, and the refractive index was measured.

ESTIMATED ERROR:

Alk	ranes 139
COMPONENTS: 1. Sulfur dioxide; SO ₂ ; [7446-09-5] 2. Heptadecane; C ₁₇ H ₃₆ ; [629-78-7]	ORIGINAL MEASUREMENTS: Sobolev, I.A.; Kukarin, V.A.; Dzhagatspanyan, R.V.; Kosorotov, V.I.; Zogorets, P.A.; Popov, A.I.; Khim, Prom. 1970, 46,668-70
VARIABLES: Temperature	PREPARED BY: C.L. Young
EXPERIMENTAL VALUES:	L
T/K Solubility /mol 1-1	*,S Mole fraction of ⁺ sulfur dioxide in liquid,x _{SO2}
303.15 0.124 313.15 0.104 323.15 0.0902 333.15 0.0768	0.037 0.031 0.027 0.023
+ calculated by compiler	•
* at atmospheric pressur	e.
$\ln S = 565/(T/K) - 5.67$ (mol 1^{-1} atm ⁻¹).	where S is in units of \cdot
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Bubbler method. Samples of saturated liquid taken and added to sodium hydroxide solution and then excess alkali back titrated.	SOURCE AND PURITY OF MATERIALS: 1. Purity at least 95 mole per cent. 2. Chemically pure. Dried.

ESTIMATED ERROR:

REFERENCES:

 $\delta \text{T/K} = \pm 0.1; \ \delta \text{(Solubility)} = \pm 2\$; \\ \delta x_{\text{SO}_2} = \pm 0.001; \ \text{(estimated by compiler)}.$

- Sulfur dioxide; SO₂; [7446-09-5]
- 2. Cyclohexane; C_6H_{12} ; [110-82-7] Decahydronaphthalene (decalin); $C_{10}H_{18}$; [91-17-8] 1,2,3,4-Tetrahydronaphthalene (tetralin); $C_{10}H_{12}$; [119-64-2]

Sano, H. Nippon Kogaku Zasshi 1968, 89, 362-368.

ORIGINAL MEASUREMENTS:

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of cyclohexane, $p_s^{\circ} = 0.140$ atm

Absorption coefficient, s^a , b	Bunsen coefficient, b	Bunsen coefficient, c,f	_l c,d	Mole ratio	Mole fraction ^e
	Сус	lohexane			
8.0	8.5	8.6	7.25	0.041	0.0394
	Decahydronaphth	alene (mixed isor	mers)		
7.0	6.4	6.2	6.2	0.045	0.0431
	1,2,3,4-Tetr	ahydronaphthalene	9		
45.6	41.4	42.0	42.0	0.253	0.202

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: (a) static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

c Determined by flow method.

 $[\]alpha = \ell(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

Assuming vapor pressure of decahydronaphthalene and tetrahydronaphthalene are negligible.

Alkanes COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO2; Patyi, L.; Furmer, I. E.; Makranczy, J.; Sadilenko, A. S.; [7446-09-5] Stepanova, Z. G.; Berengarten, 2. Cyclohexane; C₆H₁₂; [110-82-7] M. G. Zh. Prikl. Khim. 1978, 51, 1296-1300. **VARIABLES:** PREPARED BY: C. L. Young EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide α† at a partial pressure of 101.325 kPa T/K x_{SO_2} 0.06251 298.15 10.71

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric method. Pressure measured when known amounts of gas were added, in increments, to a known amount of liquid in a vessel of known dimensions. Corrections were made for the partial pressure of solvent. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

Purity better than 99 mole per cent as determined by gas chromatography.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta \alpha = \pm 4\%$ or less.

REFERENCES:

Bodor, E.; Bor, G. J.; Mohai,
 B,; Sipos. G.
 Veszpremi. Vegyip. Egy. Kozl.
 1957, 1, 55.

[†] volume of gas (measured at 101.325 kPa and 273.15 K) dissolved by one volume of cyclohexane.

COMPONENTS	Inner
COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Benoit, R.L.; Milanova, E.
2. Cyclohexane, C ₆ H ₁₂ ; [110-82-7]	Can. J. Chem., <u>1979</u> , 57, 1319-1323
VARIABLES:	PREPARED BY:
	C.L. Young
EXPERIMENTAL VALUES:	
T/K	Henry's law constant + H/atm
298.15	28.3
$^+$ Defined in original as $_H = \frac{\text{partial pressure of su}}{\text{mole fraction of sul}}$	<u>lfur dioxide</u> fur dioxide
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Few details given. Pressure measured with quartz spiral gauge. Partial pressure calculated assuming Raoult's law. Concentration of sulfur dioxide determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.05 to 0.10 mol 1-1	1. Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per cent. 2. Dried over 4A molecular sieve
	ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 4\%$ (estimated by compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	
 Decahydronaphthalene, (decalin); C₁₀H₁₈; [91-17-8] 	Z. angew. Chem. <u>1927</u> , 40, 734-736.
VARIABLES:	PREPARED BY:
	W. Gerrard
EXPERIMENTAL VALUES:	
T/K Volume of Volume of Comp.(2)/cm³ absorbed	of SO ₂ *Mole ratio *Mole fraction /cm ³ SO ₂ /Comp.(2)
	(pressure assumed to be barometric)
293.15 157.5 1181. ("Molar volume")	25 0.0503 0.0479
AIIVII I ADV	INFORMATION
AUXILIARY METHOD 'APPARATUS / PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
	SOURCE AND PURITY OF MATERIALS:
METHOD APPARATUS/PROCEDURE: Used an absorption vessel of 200 cm ³ capacity, and a vessel with a two- way tap. Simply stated that the absorptiometer was like that used by Manchot, but the reference was not	SOURCE AND PURITY OF MATERIALS:

COMPONENTS: 1. Sulfur dioxide, SO₂; [7446-09-5] 2. Decahydronaphthalene, (decalin); C₁₀H₁₈; [91-17-8]

ORIGINAL MEASUREMENTS:

Lenoir, J-Y.; Renault, P.; Renon, H.

2. Decahydronaphthalene, (decaIin); J. Chem. Eng. Data 1971, 16,340-342.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa.

T/K Henry's constant

HSO2/atm

*Mole fraction at l atm

298 323 18.8

0.0532

* Calculated by compiler assuming a linear function of p_{SO_2} vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$.

The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x_{SO_2} \to 0} \frac{f_{SO_2}(P,T)}{x_{SO_2}}$

 x_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition" of pressure and temperature. H_{SO_2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit was used. The chromatog graph was an IGC 12M Intersmat model equipped with a thermal conductivity detector. The temperature control was stated to be within ±0.1°C. The pressure drop in the column was measured by a mercury manometer. Helium was the carrier gas.

There is serious uncertainty in the estimation of accuracy.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was provided by l'Air Liquide, and had a stated purity of 99.9%. It was used as provided.
- Provided by Touzart & Matignon and Serlabo, and stated to have a minimum purity of 99%. Distillation was carried out when necessary, and the refractive index was measured.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Aromatic hydrocarbons and Hydronaphthalenes

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

November 1980

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CRITICAL EVALUATION:

Benzene; C_6H_6 ; [71-43-2]

This system has been studied by six groups. Lloyd's (1) data for benzene are in the form of concentration of sulfur dioxide in units of grams per litre of solution for a total pressure equal to the barometric pressure. The calculated mole fraction is based on the assumption that the volume of solution after absorption is the same as that before absorption. Calculation of the mole fraction at a partial pressure of sulfur dioxide of 101.3 kPa (1 atm) entails further uncertainty as the partial pressure of benzene becomes larger and increasingly uncertain for the higher temperatures.

Ipatiev and Monroe (2) made measurements at pressures between 120 kPa and 250 kPa for temperatures between 298 K and 300 K. extensive data for this system are those of Horiuti (3) who studied the system at temperatures between 283.15 K and 333.15 K. The table below compares the mole fraction solubility from the six groups extrapolated, where necessary, to 298.15 K and a partial pressure of 101.3 kPa. data of Horiuti (3) were used to give an approximate estimate of the temperature dependence of the solubility for the purpose of this extra-The data of Benoit and Milanova (4) were determined at low polation. pressure and the mole fraction at a partial pressure of 101.3 kPa was Obtained assuming Henry's law is obeyed. There is reasonable agreement between the data of Lloyd (1), Horiuti (3), Benoit and Milanova (4), Sano The result of Patyi et al. (5) is about (6) and Ipatiev and Monroe (2). 10 per cent smaller and is classified as doubtful.

Mole fraction solubility at 298 K and 101.3 kPa partial pressure

Patyi et $al.$ (5)	0.202
Benoit and Milanova (4)	0.221
Lloyd (1)	0.21
Horiuti (3)	0.23
Ipatiev and Monroe (2)	0.23
Sano (6)	0.21

Although Horiuti (3) and Ipatiev and Monroe (2) data agree at 298 K and 101.3 kPa when the complete mole fraction data at 298 K are plotted against pressure, the plot of Horiuti, which covers the pressure range up to 135 kPa total pressure, has a slightly different slope from that obtained by plotting Ipatiev and Monroe's data. Therefore no data are recommended but the data of Horiuti (3), Ipatiev and Monroe (2), Lloyd (1), Sano (6), and Benoit and Milanova (4) are all classified as tentative.

Methylbenzene; C₇H₈; [108-88-3]

This system has been studied in detail by Lorimer $et\ al.$ (7) at 227.6 K, 237.4 K and 249.8 K. In this temperature range sulfur dioxide is a liquid at atmospheric pressure. (The normal boiling point is

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Aromatic hydrocarbons and Hydronaphthalenes

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

November 1980

CRITICAL EVALUATION:

Lloyd's data (1) cover the temperature range 293.15 K to 333.15 ∿ 263 K.) Since conversion of the mass of sulfur dioxide per unit volume of solution to a mole fraction value required an approximation for the density of solution, Lloyd's data must be assessed with caution. Gerrard (8) has determined the solubility of sulfur dioxide at 273.15 K and a total pressure of 101.3 kPa. The mole fraction solubility value of Sano (6) is somewhat (\sim 10 per cent) larger than the value of Lloyd at the same However, in view of the different range of temperature covered it is impossible to make any precise comparisons between the work of the four groups. The results of Lorimer et al. (7) appear to be selfconsistent and are probably the most accurate and therefore are classified as tentative. The data of Sano (6), Gerrard (8) and Lloyd (1) are probably less reliable.

1,3-Dimethylbenzene; C₈H₁₀; [108-38-3]

This system has also been studied by Lorimer et al. (7) at 227.6 K, 237.4 K and 249.9 K and by Gerrard (9) over the temperature range 273.15 to 298.15 K. In this case there is better agreement between these two groups' results than in the case of methylbenzene and both are classified as tentative. The isolated value of Sano (6) for a mixture or xylenes appears to be slightly small compared with the value obtained by extrapolation of the values of Gerrard (9) to the same temperature.

1,3,5-Trimethylbenzene; C9H12; [108-67-8]

This system has also been investigated by Lorimer $et\ al.$ (7) at $_27.6\ K$, 237.4 K and 250.0 K and by Gerrard (9) over the temperature range 273.15 to 293.15 K. The temperature dependence of Gerrard's data indicates that the mole fraction solubility at the temperatures studied by Lorimer $et\ al.$ (7) would be less than that given by Raoult's law, whereas the opposite was found experimentally. This could arise because of small errors in weighing in Gerrard's measurements when large amounts of gas are absorbed. The data of both groups are classified as tentative but the measurement of Gerrard at 273.15 K is doubtful.

1,1'-Methylenebis(l-methylethyl)benzene; $C_{19}H_{24}$; [25566-92-1]

1,1'-Methylenebis (methylbenzene); C₁₅H₁₆; [1335-47-3]

The solubility of sulfur dioxide in these two compounds has been studied by Gel'perin $et\ al.\ (10)$. The temperature dependence of the solubility is more or less as would be expected for a system which shows only moderate deviations from Raoult's law. In the absence of any other evidence as to the reliability of these data, they are classified as tentative.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Aromatic hydrocarbons and Hydronaphthalenes

EVALUATOR:

Colin L. Young School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

November 1980

CRITICAL EVALUATION:

Hydronaphthalenes

The mole fraction solubility of sulfur dioxide in tetrahydronaphthalene given by Gerrard (9) at 293.15 K and 101.3 kPa total pressure is 0.228 and 0.202 at 303 K and a partial pressure of 101.3 kPa according to Sano (6), where as Weissenberger and Hadwiger (11) reported that the solubility of sulfur dioxide in this compound was too small to be of Gerrard's value for decahydronaphthalene is 0.060 at 298.15 consequence. K and 101.3 kPa total pressure whereas the value based on Weissenberger and Hadwiger's primary data is 0.0479 under the same conditions. (6) obtained a value at 303 K and 101.3 kPa of 0.0431. It is to be expected that the value for decahydronaphthalene should be much less than that for the tetrahydro-compound (cf. the solubility in cyclohexane which is much smaller than in benzene). It is therefore suggested that the data of Weissenberger and Hadwiger should be rejected. Lenoir et al. (12) gave solubility data at 298 K which, with some approximation, lead to a mole fraction solubility of sulfur dioxide in decahydronaphthalene of In view of the approximation made, this must be regarded as in good agreement with Gerrard's value.

Turpentine

Gerrard's mole fraction solubility values for pinene (representing turpentine) are 0.200 at 273 K and 0.110 at 293 K for a total pressure of 101.3 kPa. Weissenberger and Hadwiger's (11) value of 0.055 for turpentine at 293 K appears to be unacceptable.

References

- 1. Lloyd, S. J. J. Phys. Chem. 1918, 22, 300.
- Ipatiev, V. N.; Monroe, G. S. Ind. Eng. Chem. Anal. Ed. <u>1942</u>, 14, 166.
- 3. Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. Tokyo 1931, 17, 125.
- 4. Benoit, R. L.; Milanova, E. Can. J. Chem. 1979, 57, 1319.
- 5. Patyi, L.; Furmer, I. E.; Makranczy, J.; Sadilenko, A. S.; Stepanova , Z. G.; Berengarten, M. G. Zh. Prikl. Khim. 1978, 51, 1296.
- 6. Sano, H. Nippon Kagaku Zasshi 1968, 89, 362.
- 7. Lorimer, J. W.; Smith, B. C.; Smith, G. H. J. C. S. Faraday I 1975, 71, 2232.
- 8. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
- 9. Gerrard, W. Solubility of Gases and Liquids, Plenum Press,
 New York, 1976, p. 239.
- New York, 1976, p.239.

 10. Gel'perin, N. I.; Matveev, I. G.; Bil'shau, K. V. Zh. Prikl. Khim. 1958, 31, 1323.
- 11. Weissenberger, G.; Hadwiger, H. Z. Angew. Chem. 1927, 40, 734.
- 12. Lenoir, J.-Y.; Renault, P.; Renon, H. J. Chem. Engng. Data 1971, 16, 340.

COMPONENTS: ORIGINAL MEASUREMENTS: Lloyd, S.J. Sulfur dioxide; SO₂; [7446-09-5] J. Phys. Chem. 1918, 22, 300-302. Benzene; C_6H_6 ; [71-43-2] VARIABLES: PREPARED BY: Temperature W. Gerrard. EXPERIMENTAL VALUES: Weight of SO₂ per dm³ of T/K *Speculative values *Mole ratio, SO₂/ Comp. (2) *Mole fraction (as solution /g. for 1 atm) x_{SO2} 127.5 0.210 0.174 303.15 313.15 82.9 0.131 0.115 323.15 0.093 0.085 60.3 0.049 333.15 34.0 0.052 760 mmHg = 1 atm = 101.325 kPa. * Calculated by compiler by assuming that the volume of solution is the same as the volume of the component (2) before absorption of gas. AUXILIARY INFORMATION METHOD:/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Gas was bubbled through component (2) (1) Prepared from concentrated in a long graduated tube of small sulfuric acid and a saturated aqueous solution of sodium bisuldiameter. After equilibrium had been attained at a total pressure of about 1 atm (barometric pressure, 756-760 mmHg), the volume of the solution (about 5 cm³) was measured, and the fite. Dried by sulfuric acid and phosphorus pentoxide. (2) Distilled, dried by calcium chloride, and redistilled before weight of absorbed sulfur dioxide use. was determined by an iodometric titration. ESTIMATED ERROR: REFERENCES:

Aromatic compounds 149 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Horiuti, J., Sci. Pap. Inst. Phys. Chem. Res. 2. Benzene; C_6H_6 ; [71-43-2] (Jpn.), 1931/32, 17, 125-256. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction Mole fraction οf οf Ostwald P\$/bar sulfur dioxide T/K P†/bar sulfur dioxide coefficient, T/K in liquid, in liquid, 298.15 0.1248 0.0000 283.15 0.9749 0.3764 126.4 0.9592 0.3833 0.0592 288.15 0.3107 103.2 0.9390 0.2549 0.3921 0.0618 293.15 84.81 0.9136 70.01 0.1247 298.15 0.6577 0.2079 0.1275 0.6730 303.15 0.8829 0.1722 59.50 0.1783 50.37 0.8842 308.15 0.8452 0.1405 0.9350 0.1910 313.15 0.7999 0.1139 43.01

1.078

1.147

1.230

1.301

1.348

318.15

323.15

328.15

333.15

0.7457

0.6806

0.6062

0.5172

Ostwald coefficient (as $x \rightarrow 0$, T/K = 298.15) = 60.3.

0.2252

0.2401

0.2605

0.2796

0.2909

Henry's law constant, dp/dx (as $x \rightarrow 0$, T/K = 298.15) = 3454 mmHg = 4.605 bar.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus consisted of a gas buret, a solvent reservoir, and an absorption pipet. Dry gas introduced into degassed solvent. System mixed using a magnetic stirrer until saturation occurred. to prevent solvent vapor from mixing With gas in the gas buret. Volume of gas determined from gas buret reading; volume of liquid deter-mined from height of meniscus in the absorption pipet.

SOURCE AND PURITY OF MATERIALS:

1. Sample obtained from Nippon Sulphuric Acid Manufacturing Co. Dried and fractionated several times.

0.0921

0.0737

0.0570

0.0435

37.25

32.63

28.28

25.36

Care was taken 2. Merck, extra pure sulfur-free sample refluxed over sodium amalgam. B. pt. 80.18 °C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta P/\text{bar} = \pm 0.001;$

 $\delta x_{\rm SO_2} = \pm 0.001$ (estimated by compiler)

total pressure.

partial pressure, total pressure = 1 atmosphere = 1.01325 × 10⁵ Pa.

COMPONENTS: 1. Sulfur dioxide; SO ₂ ; [7446-09-5]				ORIGINAL MEASUREMENTS: Ipatieff, V.N.; Monroe, G.S.		
 Sulfur dioxide; SO₂; [7446-09-5] Benzene; C₆H₆; [71-43-2] 				Anal. Edn. <u>1942</u> ,14,		
ssure			PREPARED BY: C.	L. Young		
LUES:						
т/к				Mole fraction * of sulfur dioxide, x _{SO2}		
299 299 300 298	1.75	1.77	24.7 37.6 84.8 125.5	0.231 0.314 0.508 0.605		
	C ₆ H ₆ ; essure LUES: T/K 299 299 300	C ₆ H ₆ ; [71-43-2] essure LUES: T/K Total p p/atm 299 1.20 299 1.75 300 2.40	C ₆ H ₆ ; [71-43-2] essure LUES: T/K Total pressure p/atm p/kPa 299 1.20 1.22 299 1.75 1.77 300 2.40 2.43	LUES: T/K Total pressure p/atm p/kPa g SO2/100g H2O 299 1.20 1.22 24.7 299 1.75 1.77 37.6 300 2.40 2.43 84.8		

^{*} calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Rotating bomb of 3.5 dm³ capacity. Pressure measured with a Bourdon gauge and temperature measured with thermocouple. Samples of liquid phase analysed by removing sulfur dioxide by a stream of air and absorption into potassium hydroxide solution. Benzene determined gravimetrically.

SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Baker C.P. thiophene free sample, $n^{20}_{\ D} \ 1.5012.$

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Benzene; C₆H₆; [71-43-2]
 Methylbenzene (toluene); C₇H₈;
 [108-88-3]
 Dimethylbenzene (xylene, mixture
 of isomers); C₈H₁₀; [1330-20-7]

ORIGINAL MEASUREMENTS:

Sano, H. Nippon Kagaku Zasshi 1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of benzene, $p_s^{\circ} = 0.117$ atm Vapor pressure of methylbenzene, $p_s^{\circ} = 0.037$ atm Vapor pressure of dimethylbenzene (mixture of isomers), $p_s^{\circ} = 0.013$ atm

Vapor pressu	TE OF GIMECHAIN	enzene (mixture	OT TROME	13/, P _S -	O.OIS acm
Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c	_l c,d	Mole ratio	Mole fraction ^e
_S a,b	α	α			
		Benzene			
52.0	53.4	54.2	45.2	0.213	0.176
	Met	hylbenzene			
61.8	58.0	59.2	56.2	0.276	0.216
	Dime	thylbenzene			
58.05	53.5	54.1	53.8	0.294	0.227

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of Passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

d $\alpha = \ell(1 - p_s^{\circ})$ where p_s° is the vapor pressure of solvent.

e Calculated by compiler.

Sulfur Dioxide Solubilities				
[7446-09	ioxide; SO ₂ ; -5] C ₆ A ₆ ; [71-43-2]	ORIGINAL MEASUREMENTS: Patyi, L.; Furmer, I. E.; Makranczy, J.; Sadilenko, A. S.; Stepanova, Z. G.; Berengarten, M. G. Zh. Prikl. Khim. 1978, 51, 1296- 1300. PREPARED BY: C. L. Young		
EXPERIMENTAL VAI	LUES: α [†]	Mole fraction of sulfur dioxide at a partial pressure of 101.325 kPa $^x\mathrm{SO}_2$		
298.15	62.05	0.2020		
	volume of gas (measure dissolved by one volum	ed at 101.325 kPa and 273.15 K) ne of benzene.		
	AUXILI	IARY INFORMATION		
METHOD/APPARATU Volumetric	S/PROCEDURE: method. Pressure	SOURCE AND PURITY OF MATERIALS: Purity better than 99 mole per		

measured when known amounts of gas were added, in increments, to a known amount of liquid in a vessel of known dimensions. Corrections were made for the partial pressure of solvent. Details in ref. (1).

cent as determined by gas chromatography.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta \alpha = \pm 4\%$ or less.

REFERENCES:

1. Bodor, E.; Bor, G. J.; Mohai, B.; Sipos, G. Veszpremi. Vegyip. Egy. Kozl. 1957, 1, 55.

Aromatic	compounds	ı
OMPONENTS:	ORIGINAL MEASUREMENTS:	
. Sulfur dioxide; SO ₂ ;	Benoit, R.L.; Milanova, E.	
[7446-09-5]	Can. J. Chem., <u>1979</u> , 57, 1319-1323	
• Benzene; C ₆ H ₆ ; [71-43-2]	,	
ARIABLES:	PREPARED BY:	
	C.L. Young	
·	L. Toung	
XPERIMENTAL VALUES:		
T/K	Henry's law constant +	
	H/atm	
298.15	4.51	_
$H = \frac{\text{partial pressure of su}}{\text{mole fraction of sul}}$	fur dioxide	
<pre>H = partial pressure of su mole fraction of sul</pre>	fur dioxide	
mole fraction of sul	fur dioxide	
mole fraction of sul	SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per cent.	

COMPONENTS:		ORIGINAL MEASUREMENTS:		
1. Sulfur	dioxide; SO ₂ ; [7446-09-5]	Lloyd, S.J.		
2. Methylbenzene; C ₇ H ₀ ; [108-88-3]		J. Phys. Chem. <u>1918</u> , 22,300-302.		
VARIABLES:		PREPARED BY:		
		W. Gerrard		
EXPERIMENTAL	WAT HEC.			
T/K		tivo valvos		
1/1	per dm³ of	tive values $0.50_2/\text{Comp.}$ (2) *Mole fraction (as for 1 atm) x_{SO_2}		
293.15	217.5 0	.482 0.325		
298.15		.354 0.261		
303.15 313.15		.244 0.196 .178 0.151		
323.15	77.2	.145 0.127		
333.15	54.7 0	.101 0.092		
	760 mmHg = 1 atm = 101	.325 kPa		
		s the same as the volume before absorption of		
	AUXILIARY	INFORMATION		
METHOD:/APPA	RATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
in a long of diameter. attained at latm (bard 756-760 mm) solution (and the weddioxide was	beled through component (2) graduated tube of small After equilibrium had been t a total pressure of about ometric pressure, Hg), the volume of the about 5 cm ³) was measured, ight of absorbed sulfur s determined by an titration.	 (1) Prepared from concentrated sulfuric acid and a saturated aqueous solution of sodium bisulfite. Dried by sulfuric acid and phosphorus pentoxide. (2) Distilled, dried by calcium chloride and redistilled before use. 		
		ESTIMATED ERROR:		
		REFERENCES:		

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W. J. Appl. Chem. Biotechnol. 2. Methylbenzene (toluene); C7H8; [108-88-3] 1972, 22, 623-650. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa*Mole fraction T/K Pressure, total Mole ratio SO₂/toluene /mmHg xso2 0.646 273.15 760 1.82

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the com-The refractive index, ponent (2). and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- 2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

50		Juliui Dioz	ide Joidpliftles		
COMPONENTS:			ORIGINAL MEASURE	MENTS:	
1. Sulfur dioxide; SO ₂ ;[7446-09-5]			Lorimer, J.W.; Smith, B.C.; Smith, G.H.		
<pre>2. Methylbenzene, (Toluene);C7H8; [108-88-3]</pre>			J.C.S. Faraday I, <u>1975</u> , 71,2232-50.		
VARIABLES:			PREPARED BY:		
Tem	perature, pro	essure		C.L. Young	
EXPERIMENTAL V	ALUES:				
T/K	p /mmHg $^{\mathrm{a}}$	p/kPa ^{a,b}	Mole fraction in liquid, "SO ₂	of sulfur dioxide in vapor, ${}^y\mathtt{SO}_2$	
			SO ₂	[▽] SO ₂	
227.6	0.42 7.88 14.83 30.19	0.056 1.051 1.977 4.025	0.0000 0.0864 0.1949 0.2879	0.000 0.952 0.979 0.991	
	43.59 61.73 75.19 81.78 93.38	5.812 8.230 10.025 10.903 12.450	0.3834 0.5135 0.6031 0.6557	0.995 0.997 0.998 0.999	
	104.17 116.67	13.888 15.555	0.7623 0.8812 1.0000	0.999 1.000 1.000	
237.4	0.83 14.48 30.55 56.03	0.111 1.931 4.073 7.470	0.0000 0.0830 0.1850 0.2794	0.000 0.948 0.979 0.990	
	78.34 110.59 131.91 143.80	10.444 14.744 17.587 19.172	0.3625 0.4904 0.5900 0.6369	0.994 0.997 0.998 0.998	
	166.33 186.12 208.43	22.176 24.814 27.788	0.7517 0.8782 1.0000	0.999 0.999 1.000	
		AUXILIAR	Y INFORMATION		
ŒTHOD/APPARAT	•		SOURCE AND PURIT	TY OF MATERIALS:	
apparatus. using mercur cathetometer using a sulf pressure the in source, to coefficients calculated ipressure and	r-liquid equi Total pressury manometers Temperature fur dioxide vermometer. Stogether with S. Vapor conferment total from the total d liquid compers technique	are measured and measured vapor some details a activity ompositions al vapor cosition	No de	tails given	
			δ ^x SO ₂ , δ ^y SO ₂	; $\delta p/kPa = \pm 0.01;$	
			REFERENCES:	т л	
			1. Barker, Aust. J		
			<u>1953</u> , 6	, 207.	

- 1. Sulfur dioxide; SO₂; [7746-09-5]
- 2. Methylbenzene, (Toluene); C₇H₈;
 [108-88-3]

ORIGINAL MEASUREMENTS:

Lorimer, J.W.; Smith, B.C.; Smith, G.H.

J.C.S. Faraday I, <u>1975</u>, 71, 2232-50

EXPERIMENTAL	VALUES:			35 313-
T/K	p/mmHg a	p/kPa ^{a,b}	Mole fraction of su in liquid, "SO ₂	in vapor, ySO2
249.8	1.85 28.82 65.48 107.02 139.74 202.40 245.28 265.84 306.92 363.40 405.40	0.247 3.842 8.730 14.268 18.630 26.984 32.701 35.442 40.919 48.449 54.049	0.0000 0.0762 0.1745 0.2632 0.3248 0.4525 0.5585 0.5947 0.7289 0.8695 1.0000	0.000 0.941 0.977 0.988 0.992 0.995 0.997 0.997 0.998 0.999 1.000

a total pressure.

b calculated by compiler.

EXPERIMENTAL VALUES:

T/K	Pressure, total /mmHg	Mole ratio SO ₂ /Xylene.	*Mole fraction ^x SO ₂	
273.15	765	2.15	0.683	•
283.15	765	0.895	0.472	
293.15	765	0.51	0.338	1
298.15	765	0.40	0.286	,

760 mmHg = 1 atm = 101.325 kPa.

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Lorimer, J.W.; Smith, B.C.; Smith, G.H. 1,3-Dimethylbenzene, (m-xylene); J.C.S. Faraday I, <u>1975</u>, 71, 2232-50 C_8H_{10} ; [108-38-3] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide $p/mmHg^a$ p/kPa^{a,b} T/K in liquid, in vapor, ^xSO₂ y_{SO2} 0.029 0.000 227.6 0.0000 0.22 1.017 0.0893 0.974 7.63 2.138 0.2020 0.989 16.04 23.95 3.193 0.3040 0.994 38.22 5.096 0.3695 0.997 52.36 0.4704 0.998 6.981 0.5724 0.999 67.18 8.957 10.696 80.23 0.6250 0.999 12.418 93.14 0.7595 1.000 105.16 14.020 0.8760 1.000 15.555 116.67 1.0000 1.000 0.000 237.4 0.35 0.047 0.0000 1.944 14.58 0.0854 0.978 30.57 4.076 0.1955 0.991 46.76 0.2962 0.995 6.234 67.73 9.030 0.3516 0.997 92.90 12.386 0.4525 0.998 121.07 16.141 0.5565 0.999 0.999 17.871 0.6046 134.04 0.7477 1.000 166.71 22.226 1.000 188.58 25.142 0.8725 1.000 209.13 27.882 1.0000 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static vapor-liquid equilibrium apparatus. Total pressure measured using mercury manometers No details given. and cathetometer. Temperature measured using a sulfur dioxide vapor pressure thermometer. Some details in source, together with activity coefficients. Vapor compositions calculated from the total vapor pressure and liquid composition using Barker's technique (ref. 1). ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.01$; δx_{SO_2} , $\delta y_{SO_2} = \pm 1$ %. REFERENCES: 1. Barker, J. A. Aust. J. Chem. 1953, 6, 207.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 1,3-Dimethylbenzene, (m-xylene); $C_{\theta}H_{10}$; [108-38-3]

ORIGINAL MEASUREMENTS:

Lorimer, J.W.; Smith, B.C.; Smith, G.H.

J.C.S. Faraday I, <u>1975</u>, 71, 2232-50.

T/K	p/mmHg ^a	p/kPa ^{a,b}	Mole fraction in liquid, xSO2	of sulfur dioxide in vapor, ^y SO ₂
249.9	0.47	0.063	0.0000	0.000
249.9	28.21	3.761	0.0000	0.000
	60.19	8.025	0.1826	0.994
	92.18	12.290	0.2805	0.996
	119.30	15.905	0.3188	0.997
	168.48	22.462	0.4163	0.999
	222.02	29.600	0.5233	0.999
	240.60	32.077	0.5560	0.999
	312.50	41.663	0.7195	1.000
	363.18	48.420	0.8639	1.000
	408.08	54.405	1.0000	1.000

^a total pressure.

b calculated by compiler.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Lorimer, J.W.; Smith, B.C.; Smith, G.H. 1,3,5-Trimethylbenzene, J.C.S. Faraday I, 1975, 71, 2232-50. (mesitylene); C_9H_{12} ; [108-67-8] VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide p/kPa^{a,b} $p/mmHg^a$ T/K in liquid, in vapor, y_{SO2} y_{so₂} 0.023 0.0000 0.000 0.17 227.6 0.871 0.1124 0.977 6.53 0.1940 0.990 1.884 14.13 24.29 3.238 0.2956 0.995 0.3970 0.998 5.141 38.56 7.349 0.4882 0.999 55.12 0.999 0.5903 9.779 73.35 11.584 0.6860 1.000 86.89 0.7975 1.000 100.25 13.366 0.9012 1.000 108.69 14.491 1.000 1.0000 116.67 15.555 0.000 0.0000 0.23 0.031 237.4 12.57 1.676 0.1084 0.984 0.993 0.1880 25.30 3.373 46.06 6.141 0.2868 0.997 0.998 0.3781 66.72 8.895 95.21 0.999 12.694 0.4682 0.5725 0.999 127.27 16.968 0.6604 1.000 19.877 149.09 0.7845 1.000 176.06 23.473 1.000 26.014 0.8977 195.12 1.000 208.65 27.818 1.0000 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static vapor-liquid equilibrium apparatus. Total pressure measured using mercury manometers and No details given. cathetometer. Temperature measured using a sulfur dioxide vapor pressure thermometer. Some details in source, together with activity coefficients. Vapor compositions calculated from the total vapor pressure and liquid composition using Barker's technique (ref. 1). ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.01$; δx_{SO_2} , $\delta y_{SO_2} = \pm 1$ %. REFERENCES: 1. Barker, J. A. Aust. J. Chem. 1953, 6, 207.

- 1. Sulfur dioxide; SO₂; [7446-09-5]

ORIGINAL MEASUREMENTS:

Lorimer, J.W.; Smith, B.C.; Smith, G.H.

J.C.S. Faraday I, 1975, 71, 2232-50.

KPERIMENTAL T/K	p/mmHg a	p/kPa ^a ,b	Mole fraction o in liquid, "SO2	f sulfur dioxide in vapor, ^y SO ₂
250.0	0.48	0.064	0.0000	0.000
	25.29	3.372	0.1004	0.983
	50.73	6.763	0.1742	0.992
	89.13	11.883	0.2676	0.996
	119.25	15.899	0.3403	0.998
	170.08	22.675	0.4267	0.999
	231.39	30.849	0.5328	0.999
	264.15	35.217	0.5987	0.999
	334.28	44.567	0.7490	1.000
	377.45	50.323	0.8888	1.000
	410.55	54.735	1.0000	1.000

a total pressure.

b calculated by compiler.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 1,3,5-Trimethylbenzene, (Mesitylene); C₉H₁₂; [526-73-8]

ORIGINAL MEASUREMENTS:

Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1976, p.239.

VARIABLES:

PREPARED BY:

Temperature

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Weight of Component(2)	Weight of SO_2 absorbed, g	Mole ratio SO ₂ /Comp.(2)	Mole fraction ^x SO ₂
			(Total press	sure, 1 atm)
273.15 283.15 293.15	3.8690 3.8690 3.8690	3.5828 1.9450 1.2539	1.740 0.944 0.610	0.635 0.485 0.380

760 mmHg = 1 atm = 101.325 kPa.

AUXILIARY INFORMATION

METHOD:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube. The amount of gas absorbed was determined by reweighing the tube. The total pressure was barometric, very nearly 1 atm. See ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high degree of purity was attested by the measurement of vapor pressure from 258-268 K.
- The best commercial specimen was purified and attested.

ESTIMATED ERROR:

REFERENCES:

Gerrard, W. J. Appl. Chem.
 Biotechnol. <u>1972</u>, 22,623.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Bis(1-methylethyl)benzene, (diisopropylbenzene); C₁₂H₁₈; [25321-09-9]

ORIGINAL MEASUREMENTS:

Gel'perin, N. I.; Matveev, I. G.;
Bil'shau, K. V.

Zh. Prikl. Khim.

<u>1958</u>, *31*, 1323-1332.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa

т/к	g SO ₂ /100 g Comp. (2)	*Mole ratio SO ₂ /Comp. (2)	*Mole fraction ^x SO ₂
277.65	26.5	0.672	0.402
298.15	10.7	0.271	0.213
315.15	7.5	0.190	0.160

^{*} Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The amount of gas absorbed "at normal pressure" was determined by weighing, to constant weight. The data expressed as g SO₂/100 g component (2) were stated to agree to within 1-2% with the data obtained by titration with 0.1 N potassium hydroxide solution to a phenol-phthalein end-point.

SOURCE AND PURITY OF MATERIALS:

- 1. Simply referred to as "concentrated 100%" sulfur dioxide.
- 2. Fraction from a cracking plant.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 1,1'-Methylenebismethylbenzene
 (Ditotylmethane);
 C₁₅H₁₆; (a mixture of o-, m-,
 and p- isomers of constant
 composition); [1335-47-3]

ORIGINAL MEASUREMENTS:

Gel'perin, N. I.; Matveev, I. G.;
Bil'shau, K. V.
Zh. Prikl. Khim. 1958, 31, 13231332.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES: The original data appear to be for 1 atm. 760 mmHg = 1 atm = 101.325 kPa

	760 11411	Hg = 1 atm = 101.325	Kra •
T/K	g SO ₂ for 100 g of Comp.(2)	*Mole ratio SO ₂ /Comp.(2)	*Mole fraction [#] SO ₂
277.65 282.15 290.65 298.15 307.65 315.15 327.65 333.15 348.15 348.15 362.65 403.15 413.15	59 45 19.9 14.5 10.8 9.17 5.92 5.19 3.96 3.79 3.27 2.06 1.65 0.95	1.810 1.380 0.610 0.445 0.331 0.281 0.182 0.159 0.121 0.116 0.100 0.0632 0.0506 0.0291	0.644 0.580 0.379 0.308 0.249 0.220 0.154 0.137 0.108 0.104 0.0912 0.0594 0.0482 0.0283

Presumably to demonstrate the effect of a change in partial pressure of SO_2 , a mixture of air and SO_2 of stated % SO_2 by volume was used. It appeared to be understood that y/100 was the partial pressure of SO_2 in atm, y being the % by volume of SO_2 in the SO_2 + air mixture. Data are given below.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The amount of gas absorbed "at normal pressure" was determined by weighing, to constant weight. The data, expressed as g SO₂/100 g component (2), were stated to agree to within 1-2% with the data obtained by titration with 0.1 N potassium hydroxide solution to a phenolphthalein end-point.

SOURCE AND PURITY OF MATERIALS:

- 1. Simply referred to as "concentrated 100%" sulfur dioxide.
- From the method of preparation ditolylmethane was a mixture of o-, m-, and p- isomers of constant composition. Various properties such as density, viscosity, and vapor pressure were stated.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 1,1'-Methylenebismethylbenzene
 (Ditotylmethane);
 C₁₅H₁₆; (a mixture of o-, m-,
 and p- isomers of constant
 composition); [1335-47-3]

ORIGINAL MEASUREMENTS:

Gel'perin, N. I.; Matveev, I. G.;
Bil'shau, K. V.
Zh. Prikl. Khim. 1958, 31, 13231332.

T/K	у	Solubility /(g SO ₂ / 100 g solvent)	Mole ratio * SO ₂ /solvent	Mole fraction * ^x SO ₂
276.15 287.65 298.95 308.75 322.15 347.15 276.65 298.15 308.75 322.75 347.75 281.65 287.65 299.15 316.95 316.95 329.45 339.15	57.75 21.00 7.08	21.9 14.2 9.14 6.46 4.22 2.32 9.68 5.69 3.8 3.02 1.97 0.94 2.95 1.92 1.34 0.932 0.716 0.516 0.408 0.354 0.385	0.672 0.436 0.280 0.198 0.129 0.0712 0.297 0.175 0.117 0.0926 0.0604 0.0288 0.0905 0.0589 0.0411 0.0286 0.0220 0.0158 0.0125 0.0109 0.0118	0.402 0.303 0.219 0.165 0.115 0.0664 0.229 0.149 0.105 0.0848 0.0570 0.0280 0.0830 0.0556 0.0395 0.0278 0.0278 0.0215 0.0156 0.0124 0.0107
298.15 308.15		0.32 0.180	0.00982 0.00552	0.0972 0.00549

^{*} Calculated by compiler.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. (1-Methylethyl)-1,1'-methylenebisbenzene, (Dicumylmethane), (diisopropylphenylmethane); C₁₉H₂₄;
 [25566-92-1]

ORIGINAL MEASUREMENTS:

Gel'perin, N.I.; Matveev, I.G.;
Bil'shau, K.V.

Zh. Prikl. Khim. 1958, 31, 1323-1332.

VARIABLES:

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa.

T/K	g SO ₂ /100 g component(2)	*Mole ratio SO ₂ /Comp. (2)	*Mole fraction ^x SO ₂	(Appears to be for 1 atm)
 276.15	35.2	1.389	0.581	
277.65	29.2	1.152	0.535	
282.15	21.5	0.848	0.459	
290.65	13.3	0.525	0.344	
298.15	10.8	0.426	0.299	
307.65	8.25	0.326	0.246	
315.15	7.58	0.299	0.230	
327.65	3.87	/ 0.153	0.132	
338.15	3.54	0.140	0.123	
348.15	2.62	0.103	0.0934	
362.65	1.65	0.0651	0.0611	

Presumably to demonstate the effect of a change in partial pressure of SO_2 , a mixture of air and SO_2 of stated % SO_2 by volume was used. It appeared to be understood that y/100 was the partial pressure in atm of SO_2 in these mixtures, y being the % SO_2 by volume. Data are given on continuation sheet.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The amount of gas absorbed "at normal pressure" was determined by weighing, to constant weight. The data expressed as g SO₂/100 g component (2) were stated to agree to within 1-2% with the data obtained by titration with 0.1% potassium hydroxide solution to a phenolphthalein end-point.

SOURCE AND PURITY OF MATERIALS:

- Simply referred to as "concentrated 100%" sulfur dioxide.
- From the method of preparation component (2) was a mixture of o-, m- and p- isomers of constant composition.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. (1-Methylethyl)-1,1'-methylenebisbenzene, (Dicumylmethane),
 (diisopropyl-phenylmethane);
 C₁₉H₂₄; [25566-92-1]

ORIGINAL MEASUREMENTS:

Gel'perin, N.I.; Matveev, I.G.; Bil'shau, K.V.

Zh. Prikl. Khim. <u>1958</u>, 31,1323-1332

EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa. Mole ratio* Mole fraction* T/K Solubility y /(gSO₂/100g SO₂/Solvent x_{SO_2} solvent) 0.370 14.9 0.588 276.15 57.75 287.65 10.8 0.426 0.299 6.62 0.261 0.207 298.95 4.77 308.75 0.188 0.158 0.112 322.15 3.18 0.125 0.0663 347.15 1.80 0.0710 21.00 6.95 0.274 0.215 276.65 0.158 287.95 4.74 0.187 3.11 0.123 0.109 298.15 308.75 2.21 0.0872 0.0802 1.46 0.0576 0.0550 322.75 0.70 0.0276 0.0269 347.75 2.17 0.0856 0.0789 281.65 7.08 0.0612 0.0576 287.65 1.55 299.15 1.058 0.0417 0.0401 0.0277 309.15 0.721 0.0284 316.95 0.589 0.0232 0.0227 0.0153 329.45 0.393 0.0155 0.0129 339.15 0.0128 0.328 348.35 0.275 0.0109 0.0107 293.45 1.7 0.321 0.0127 0.0125 0.0102 0.0103 298.15 0.26 308.15 0.119 0.0047 0.0047

^{*} Calculated by compiler.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Pinene; C₁₀H₁₆; (isomer not specified, used as representing turpentine).

ORIGINAL MEASUREMENTS:

Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1976, p. 239.

VARIABLES:

Temperature

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

T/K	Weight of Pinene g.	Weight of SO ₂ absorbed,g	Mole ratio SO ₂ /Pinene	Mole fraction x SO $_2$
-----	------------------------	--------------------------------------	---------------------------------------	----------------------------

(Total Pressure, 1 atm)

273.15 3.4166 293.15 3.4166 0.4009 0.2201 0.250 0.124 0.200

760 mmHg = 1 atm = 101.325 kPa.

AUXILIARY INFORMATION

METHOD:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube. The amount of gas absorbed was determined by reweighing the tube. The total pressure was barometric, very nearly l atm. See ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high degree of purity was attested by the measurement of vapor pressure from 258-268 K.
- 2. The best commercial specimen was purified and attested.

ESTIMATED ERROR:

REFERENCES:

1. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623

COMPONENTS:		ORIGINAL MEASUREMENTS:
l. Sulfu	r dioxide; SO ₂ ; [7446-09	0-5] Weissenberger, G.; Hadwiger, H.
2. Terpe	ntin	Z. Angew. Chem. <u>1927</u> , 40,734-736.

VARIABLES:		PREPARED BY:
		W. Gerrard
EXPERIMENTAL	VALUES:	
T/K	Volume of Volume	of SO ₂ *Mole ratio *Mole fraction
	component(2) absorb	ped,/cm ³ SO_2 /Comp.(2) x_{SO_2}
	/ Cili	(pressure assumed to be baro- metric).
293	1 8	.3 *0.056 0.053
ļ	* Calculated by o	rama () au
	ourouruccu s,	compiler
	* Based on pinene	••
	IXUA	LIARY INFORMATION
METHOD/APPAR	ATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Used an a	bsorption vessel of 200c	em ³
	and a vessel with a two	
Simply st meter was	ated that the absorption like that used by Manch	ot,
but the r	eference was not cited,	
propably	rer.(r).	
		ESTIMATED ERROR:
		1
		REFERENCES:
		1. Manchot, W. Z. anorg. Chem.
		1924, 141, 38.
		<u>1924</u> , <i>141</i> , 38.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Weissenberger, G.; Hadwiger, H. Z. angew. Chem. 1927, 40,734-736. 2. Hydroterpin. VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: Volume of SO₂ absorbed, /cm³ T/K *Mole fraction Volume of *Mole ratio $SO_2/Comp.(2)$ component xso2 (2) $/cm^3$ (pressure assumed to be barometric) 293.15 14.3 * 0.108 0.097 1 14.8 Calculated by compiler "Hydroterpin" was stated to be obtained by the hydrogenation of "Terpentinol" In Chem. Abs. 21,3052, the compound is named hydroterpinol. The authors state that 1 g has a volume of 1.133cm³. The mole ratio given above is based on an assumed molar weight of 154, the assumed formula being $C_{1\,0}H_{1\,8}O$. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Used an absorption vessel of 200cm³ No details given. capacity, and a vessel with a twoway tap. Simply stated that the absorptiometer was like that used by Manchot, but the reference was not cited, probably ref. (1). ESTIMATED ERROR: REFERENCES: 1. Manchot, W. Z. anorg. Chem. 1924,

141, 38.

COMPONENTS:		ORIGINAL MEASUREMENT	ïS:
1. Sulfur dic	oxide; SO ₂ ; [7446-09-5]	Yuferev, R.F.;	Maluigin, P.V.
2. Kerosene (range unsp	petroleum, boiling becified).	Z. Chim. Prom.	<u>1930</u> , 7, 553-555
VARIABLES:	nperature	PREPARED BY:	Gerrard
EXPERIMENTAL VALUE	ES:		
T/K	Weight of SO ₂ per V cm ³ of solvent g c	olume of SO ₂ per m ³ of solvent cm ³	* Mole fraction, $x_{\rm SO_2}$, approximate, based on an assumed molecular weight of 200, and a density of 0.7 for the solvent.
273.15 292.15	0.0771 0.0439	26.98 15.36	0.256 0.164
Kerosene s	aturated with water		
273.15 292.15	0.0801 0.04472	28.03 15.65 *Calc	ulated by compiler.
	AUXILIAR	Y INFORMATION	
METHOD/APPARATUS/	PROCEDURE:	SOURCE AND PURITY O	F MATERIALS:
the kerosene (saturation was whole was then aqueous soluti formed sulfuri	reached. The transferred to an on of I2 + KI. The cacid was determined y. The pressure was	sulfuric ac	ide was dried by id. s dried over , without distill- stored over sodium.
		ESTIMATED ERROR:	
		i	

Aromatic	compunds 1/
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] Soft paraffin (see note). 	Sobolev, I.A.; Kukarin, V.A.; Dzhagatspanyan, R.V.; Kosorotov, V.I. Zogorets, P.A.; Popov, A.I.
	Khim. Prom. 1970, 46, 668-70.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES:	
т/к 5	Solubility*, S /mol l-!
303.15 313.15	0.15 0.128
323.15 333.15	0.115 0.0937
<pre>* at atmospheric pressure (a between pressure and soluk pressure of SO₂)</pre>	authors claim linear relationship bility up to l atmosphere partial
$\ln S = 690/(T/K) - 5.98 (v$	where S is in units of mol $l^{-1}atm^{-1}$)
AUXILIARY	'INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Bubbler method. Samples of, saturated liquid taken and added to sodium hydroxide solution and then excess alkali back titrated.	1. Purity at least 95 mole per cent.
NOTE: Mixture of C_{12} - C_{22} hydrocarbons (86.7% normal paraffins, 11.3% branched paraffins, 0.4% aromatic and 1.6% naphthenic hydrocarbons).	
	ESTIMATED ERROR: $\delta T/K = \pm 0.1$; δ (Solubility) = $\pm 2\%$
•	(estimated by compiler).
	REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Methanol; CH,O; [67-56-1]

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria, 3052 AUSTRALIA

June, 1981

CRITICAL EVALUATION:

The data of Lobry de Bruyn (1) and that of Gerrard (2) are in reasonable agreement and are deemed acceptable. These data are for a total pressure of 1 atmosphere. The vapor pressures of pure methanol are 29.6 mmHg (273 K) 54.7 mmHg (283 K) 96.0 mmHg (293. K) 160.0 (303 K) 260.5 mmHg (313 K). Obviously as the temperature increases there will be an increasingly important difference between the mole fraction at 1 atmosphere total pressure and 1 atmosphere partial pressure. Bekarek and Hala (3) give their data as mole fractions in gas and liquid phases for a series of total pressures, these being considerable less than 1 atmosphere. It is possible to calculate so called Henry's constants from these data (see Table 1) by assuming the partial pressure of methanol in the vapor phase is equal to the vapor pressure of pure methanol times the mole fraction in the liquid phase. From inspection of Table 1 it is immediately apparent that in the present situation these vary and there is not a linear relationship between partial pressure and mole fraction of gas dissolved in the liquid.

Table 1. Henry's law constants calculated from the data of Bekarek and Hala (3)

T/K	p/mmHg	^x so ₂	y _{SO2}	H/atm	H-1/atm-1
293.2	101.40	0.0043	0.0508	1.580	0.634
	136.20	0.0314	0.3100	1.769	0.565
303.2	169.40	0.0050	0.0542	2.416	0.414
	294.30	0.0619	0.4370	2.734	0.366
313.2	278.60	0.0058	0.0567	3.641	0.275
	418.70	0.0518	0.3990	4.144	0.236

Tokunaga (4) reported data for pure water, pure methanol and mixtures of these, as grams of sulfur dioxide "per 100g of solution (solute gas free) at 1 atm. partial pressure". The evaluator has calculated the mole fractions for 1 atm partial pressure as follows: 283.15K (0.397); 293.15K (0.301); 303.15 (0.223); 313.15K (0.169). There is fair agreement of these data for a partial pressure of 1 atmosphere with those of Lobry de Bruyn (1) and Gerrard (2) at 283.15 K for a total pressure of 1 atmosphere. The increasing difference between partial and total pressure causes the two lines to diverge more and more as the temperature increases. The datum of Sano and Nakamoto (5) is considerably smaller than those of Gerrard (2) and Lobry de Bruyn (1) and is classified as doubtful.

- 1. Lobry de Bruyn, C.A. Rec. Trav. Chim. 1892, 11, 112.
- 2. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
- 3. Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. 1968 33, 2598.
- 4. Tokunaga, J. J. Chem. Eng. Data. 1974, 19, 162.
- 5. Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Methanol; CH₄O; [67-56-1]

ORIGINAL MEASUREMENTS:

Lobry de Bruyn, C.A.

- (a) Rec. Trav. Chim. 1892, 11, 112-157.
- (b) Z.Phys. Chem. 1892, 10, 782-789.

VARIABLES:

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

EXPERIME	NTAL	VALUES:				
		T/K	Weight %, SO ₂	Mole ratio, ROH/SO ₂	*Mole ratio SO ₂ /ROH	Mole fraction* xSO2
Ref. (a)	273.15 280.15 285.45 290.95 299.15	71.1 59.9 52.2 44 31.7	0.81 1.33 1.83 2.55 4.25	1.23 0.747 0.546 0.393 0.232	0.552 0.428 0.353 0.282 0.188
Ref. (b)	273.15 299.15		2/100 g CH ₃ OH 2/100 g CH ₃ OH	1.235 0.235	0.553 0.190

* Calculated by compiler, from wt %.

Total pressure = atmospheric pressure.

AUXILIARY INFORMATION "-

METHOD/APPARATUS/PROCEDURE:

The dry gas was passed into a weighed amount of methanol in a bulb of 2-3 cm³ capacity until equilibrium had been reached at the observed temperature and at a total pressure (barometric, 760-770 mmHg). The bulb was sealed "a la lampe", and weighed. A titration was also mentioned, but the statement is vague.

SOURCE AND PURITY OF MATERIALS:

- 1. Simply stated that the dry gas was used.
- It was stated that the pure alcohol was used.

ESTIMATED ERROR:

1,0				
COMPONENTS: 1. Sulfur dioxide 2. Methanol; CH Ethanol; C ₂ H		ORIGINAL MEASUREMENTS: Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369-373.		
VARIABLES:		PREPARED BY: C. L. Young		
EXPERIMENTAL VALUES:	Vapor pressure of	T/K = 303 methanol = 0.125 atm ethanol = 0.069 atm		
Absorption	Bunsen b Buns	sen c c.d Mole Mole e		

		sure of ethanol			
Absorption coefficient,	Bunsen coefficient,	Bunsen coefficient, c	ℓc,d	Mole ratio	Mole fraction ^e
s ^a ,b	α	α			
	М.	lethanol			
116.2	122.1	124.5	99.9	0.241	0.194
		Ethanol			
88.1	85.9	84.0	75.9	0.227	0.185

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR: $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

^c Determined by flow method.

 $[\]alpha = \ell(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Methanol; CH4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. 1968, 33, 2598-2607.

VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

т/к	P/Torr ⁺	P/kPa ⁺	Mole fraction of in liquid, "SO ₂	sulfur dioxide in gas, ^y SO ₂
293.2	101.40	13.519	0.0043	0.0508
	109.10	14.545	0.0111	0.1230
	113.50	15.132	0.0144	0.1570
	136.20	18.159	0.0314	0.3100
303.2	169.40	22.585	0.0050	0.0542
	182.6	24.34	0.0118	0.1230
	183.00	24.398	0.0122	0.1260
	186.00	24.798	0.0135	0.1390
	208.6	27.81	0.0248	0.239
	234.20	31.224	0.0375	0.3310
	294.30	39.237	0.0619	0.4370
313.2	278.60	37.144	0.0058	0.0576
	298.30	39.770	0.0134	0.1280
	300.80	40.103	0.0139	0.1320
	344.50	45.930	0.0288	0.2480
	418.70	55.822	0.0518	0.3990

Total pressure 760 Torr = 760 mmHg = 1 atm = 101.325 kPa

AUXILIARY INFORMATION .-

METHOD/APPARATUS/PROCEDURE:

A modified Gillespie still was used. Sulfur dioxide in liquid and gaseous Phases estimated by iodometric titration. A small bulb containing a sample of the solution (0.5-1g) was broken in a solution of iodine and potassium iodide. Details in source and ref. (1). Same data given in ref. (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Dried with sulfuric acid and phosphorus pentoxide.
- 2. Analytical grade, fractionally distilled; $d_{20}^{4} = 0.7915$.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta P/kPa = \pm 0.1$ % δx_{SO_2} , $\delta y_{SO_2} = \pm 0.5$ %. (estimated by compiler.

- 1. Dvorak, K.; Boublik, T. Coll. Czech. Chem. Comm. 1963, 28, 1252.
- 2. Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. 1968, 33, 2608.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Methanol; CH₄O; [67-56-1]
- 2-Propanone (Acetone); C₃H₆O; [67-64-1]

ORIGINAL MEASUREMENTS:

Bekarek, V.

Coll. Czech. Chem. Comm. 1968, 33, 2608-2619.

VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

Molo	frac	++10	nc

EXPERIMENTAL VALUES:				Mole fr	actions	
			in liquid		in o	gas
T/K	p/Torr	p/kPa	^x SO₂	^ж С 3 Н 6 О	y _{SO2}	^y C₃H ₆ O
293.2	161.80 174.20 198.70 206.00 222.30 245.70	21.572 23.225 26.491 27.464 29.638 32.757	0.0407 0.0547 0.0732 0.0797 0.0918 0.1410	0.1500 0.1050 0.3600 0.2010 0.0942	0.2330 0.3450 0.2670 0.3840 0.5216 0.3960	0.2380 0.1640 0.3880 0.2390 0.1090 0.4460
303.2	278.70 278.70 264.70 268.80 311.60 316.50 335.70 403.20	37.064 35.290 35.837 41.543 42.197 44.756 53.756	0.1419 0.0457 0.0462 0.0722 0.0737 0.0930 0.1620	0.2620 0.0975 0.1570 0.2120 0.1280 0.4190	0.1880 0.2950 0.2510 0.3330 0.4100 0.3010	0.3300 0.1550 0.2260 0.22510 0.1600 0.3950 0.4180
313.2	390.20 390.20 452.50 533.00 524.10 583.50 634.20	52.022 52.022 60.328 71.060 69.874 77.794 84.553	0.0348 0.0590 0.0579 0.0915 0.1020 0.1190	0.1440 0.1920 0.3140 0.1420 0.4190 0.2440 0.6020	0.1930 0.2800 0.2200 0.4520 0.3200 0.4600 0.4690	0.2160 0.2430 0.3560 0.1510 0.3660 0.2110 0.4150

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A modified Gillespie still was used. Sv!fur dioxide in liquid and gaseous phases estimated by iodometric titration. Details in source and ref. (1).

To determine the acetone concentration a bulb containing (0.5 - 1.0g) of mixture was broken in a solution containing iodine just sufficient to convert sulfur dioxide to sulfuric acid. Acetone was then determined by Messinger's method (ref.(2))

SOURCE AND PURITY OF MATERIALS:

- Dried with sulfuric acid and phosphorus pentoxide.
- Analytical grade, fractionally distilled; d⁴₂₀ = 0.7915.
- 3. Analytical grade, fractionally distilled; $d_{20}^{\pm} = 0.7902$.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.1$ %; δx_{SO_2} , $\delta x_{C_3H_6O}$, δy_{SO_2} , $\delta y_{C_3H_6O}$ = ± 1 %. (estimated by compiler).

- Dvorak, K.; Boublik, T. *Coll. Czech. Chem. Comm.* <u>1963</u>, 28, 1252.
- Goodwin, L.F.; J. Am. Chem. Soc., 1920, 42, 39.

- Sulfur dioxide; SO₂; [7446-09-5]
- Methanol; CH₄O; [67-56-1]
- Acetic acid, methyl ester (Methyl acetate); C₃H₆O₂; [79-20-9]

ORIGINAL MEASUREMENTS:

Bekarek, V.

Coll. Czech. Chem. Comm. 1968, 33, 2608-2619

VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

		I.			
VALUES:			Mole	fractions	
p/Torr	p/kPa	in l	iguid	in	gas
		^x so₂	^ж С ₃ Н ₆ О ₂	y _{SO2}	y C ₃ H ₆ O ₂
131.00 134.80 153.00 148.00 158.80 160.60 181.10	17.465 17.972 20.398 19.732 21.172 21.412 24.145	0.0130 0.0144 0.0245 0.0249 0.0107 0.0390 0.0448	0.0544 0.0591 0.0939 0.0685 0.1970 0.0572	0.1070 0.1130 0.1630 0.1850 0.0552 0.2870 0.2420	0.2000 0.2100 0.2620 0.2230 0.4300 0.1640 0.3070
222.10 234.10 228.00 246.60 260.60 269.50 306.50	29.611 31.211 30.397 32.877 34.744 35.930 40.863	0.0162 0.0112 0.0173 0.0300 0.0306 0.0447 0.0547	0.0653 0.1170 0.0696 0.0747 0.1170 0.0594 0.1820	0.1210 0.0693 0.1230 0.2060 0.1820 0.3080 0.2650	0.3290 0.2060 0.3100 0.2160 0.2040 0.2650 0.1540 0.3150 0.2610
358.90 367.70 357.00 399.40 428.10 440.50 508.30 597.10	47.849 49.023 47.596 53.249 57.075 58.729 67.768 79.607	0.0123 0.0207 0.0210 0.0358 0.0374 0.0521 0.0699 0.1080	0.0960 0.0799 0.0847 0.0692 0.1410 0.0573 0.2320 0.1870	0.0802 0.1360 0.1350 0.2350 0.2010 0.3360 0.2900 0.4450	0.2540 0.2130 0.2200 0.1740 0.2580 0.1170 0.3100 0.2110
	131.00 134.80 153.00 148.00 158.80 160.60 181.10 223.80 222.10 234.10 228.00 246.60 269.50 306.50 368.30 358.90 367.70 357.00 349.40 440.50 508.30	p/Torr p/kPa 131.00 17.465 134.80 17.972 153.00 20.398 148.00 19.732 158.80 21.172 160.60 21.412 181.10 24.145 223.80 29.838 222.10 29.611 234.10 31.211 228.00 30.397 246.60 32.877 260.60 34.744 269.50 35.930 306.50 40.863 368.30 49.103 358.90 47.849 367.70 49.023 357.00 47.596 399.40 53.249 428.10 57.075 440.50 58.729 508.30 67.768	p/Torr p/kPa in 1s xSO2 131.00 17.465 0.0130 134.80 17.972 0.0144 153.00 20.398 0.0245 148.00 19.732 0.0249 158.80 21.172 0.0107 160.60 21.412 0.0390 181.10 24.145 0.0448 223.80 29.838 0.0853 222.10 29.611 0.0162 234.10 31.211 0.0112 228.00 30.397 0.0173 246.60 32.877 0.0300 260.60 34.744 0.0306 269.50 35.930 0.0447 306.50 40.863 0.0547 368.30 49.103 0.0936 358.90 47.849 0.0123 367.70 49.023 0.0207 357.00 47.596 0.0210 399.40 53.249 0.0358 428.10 57.075 0.0374 440.50 58.729 0.0521 508.30 6	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$p/\text{Torr} \qquad p/\text{kPa} \qquad \begin{array}{c} \text{in liquid} \qquad \text{in} \\ x_{\text{SO}_2} x_{\text{C}_3\text{H}_6\text{O}_2} y_{\text{SO}_2} \\ \\ 131.00 17.465 0.0130 0.0544 0.1070 \\ 134.80 17.972 0.0144 0.0591 0.1130 \\ 153.00 20.398 0.0245 0.0939 0.1630 \\ 148.00 19.732 0.0249 0.0685 0.1850 \\ 158.80 21.172 0.0107 0.1970 0.0552 \\ 160.60 21.412 0.0390 0.0572 0.2870 \\ 181.10 24.145 0.0448 0.1570 0.2420 \\ 223.80 29.838 0.0853 0.2660 0.3530 \\ 222.10 29.611 0.0162 0.0653 0.1210 \\ 234.10 31.211 0.0112 0.1170 0.0693 \\ 228.00 30.397 0.0173 0.0696 0.1230 \\ 246.60 32.877 0.0300 0.0747 0.2060 \\ 260.60 34.744 0 0306 0.1170 0.1820 \\ 269.50 35.930 0.0447 0.0594 0.3080 \\ 306.50 40.863 0.0547 0.1820 0.2650 \\ 368.30 49.103 0.0936 0.2140 0.3960 \\ 358.90 47.849 0.0123 0.0960 0.0802 \\ 367.70 49.023 0.0207 0.0799 0.1360 \\ 357.00 47.596 0.0210 0.0847 0.1350 \\ 399.40 53.249 0.0358 0.0692 0.2350 \\ 428.10 57.075 0.0374 0.1410 0.2010 \\ 440.50 58.729 0.0521 0.0573 0.3360 \\ 508.30 67.768 0.0699 0.2320 0.2900 \\ \end{array}$

AUXILIARY INFORMATION -

METHOD/APPARATUS/PROCEDURE:

A modified Gillespie still was used. Sulfur dioxide in liquid and gaseous phases estimated by iodometric titration. Details in source and ref. (1).

To determine the concentration of methyl acetate, a bulb containing a sample of saturated solution was broken in a known amount of sodium hydroxide soln., heated to hydrolyse the ester, sulfur dioxide oxidised to sulfuric acid and the excess alkali was back titrated

SOURCE AND PURITY OF MATERIALS:

- 1. Dried with sulfuric acid and phosphorus pentoxide.
- Analytical grade, fractionally distilled, d₂₀ = 0.7915.
- 3. Added to 5 per cent acetic anhydride and fractionally distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.1$ %. δx_{SO_2} , $\delta x_{C_3H_8O_2}$, $\delta y_{C_3H_8O_2}$, $\delta y_{C_3H_8O_2}$ (estimated by compiler).

REFERENCES:

 Dvorak, K.; Boublik, T. Coll. Czech. Chem. Comm. 1963, 28, 1252.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W.

2. Methanol; CH₄O; [67-56-1]

J. Appl. Chem. Biotechnol.

1972, 22, 623-650.

VARIABLES:

PREPARED BY:

Temperature

C. L. Young

EXPERIMENTAL VALUES:

т/к	P/kPa	Mole ratio SO ₂ /CH ₄ O	* Mole fraction ^x SO ₂
273.15	101.3	1.23	0.581
283.15		0.620	0.383
293.15		0.355	0.262
298.15		0.27	0.21

^{*} Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component 2 in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component 2. The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component 2.

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

P is the total pressure.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Ethanol; C_2H_6O ; [64-17-5]

EVALUATOR:

Colin L. Young School of Chemistry, University of Melbourne Parkville, Victoria, 3052 AUSTRALIA

June, 1981

CRITICAL EVALUATION:

The mole fraction values based on the data of Carius (1), Lobry de Bruyn (2) and Gerrard (3) are for a total pressure of 1 atmosphere. It is again important to distinguish between measurements reported for a total pressure of 1 atmosphere and a partial pressure of 1 atmosphere particularly at the higher temperatures. The vapor pressure of pure ethanol are 12.2 mmHg (273K); 23.8 mmHg (283K); 44.0 mmHg (293K) 78.1 mmHg (303K) and 133.5 mmHg (313K). The data of Tokunaga (4) are for a partial pressure of 1 atm. There is fair agreement between the data of Tokunaga (4) and the above three sets of data at 273 to 283 K. The data of Barclay and Butler (5) are for low partial pressures of sulfur dioxide. These data cannot be extrapolated up to 1 atmosphere pressure because there is not a linear relationship between pressure and mole fraction i.e. Henry's law is not obeyed up to 1 atmosphere. This point is also obvious when the data of Nitta et al (6) are considered. These workers studied the mixture over the whole composition range at 293.15K. The data of Yuferev and Maluigin (7) are in reasonable agreement with the data from references (1), (2), (3), (4) and (6) if it is assumed the mole fraction solubility refers to 101.3kPa total pressure. The data of Nitta et al (6) are thought to be most reliable at 293.15K whereas those of Gerrard (3) are the most reliable at the lower temperatures. The data of de Saussure (8) are of historical interest only. The mole fraction solubility of Sano and Nakamoto (9) is slightly smaller than the value obtained by extrapolation of the data of Gerrard (3) to 303 K.

- 1. Carius, L. Annalen, <u>1855</u>, 94, 129.
- Lobry de Bruyn, C.A. Rec. Trav. Chim. 1892, 11, 112 and Z. Phys. Chem. 1892, 10, 782.
- 3. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
- 4. Tokunaga, J. J. Chem. Eng. Data. 1974, 19, 162.
- 5. Barclay, I.M.; Butler, J.A.V.; Trans Faraday Soc. 1938.34,1445
- 6. Nitta, T.; Itami, J.; Katayama, T.; J. Chem. Engng. Japan. 1973, 6, 303.
- 7. Yuferev, R.F.; Maluigan, P.V. Z. Chim. Prom. 1930,7,553.
- 8. de Saussure, T. Gilbert's Annalen der Physik. 1814,47,113. Annals of Phil, 1815,6,241.
- 9. Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Carius, L. Annalen, 1855, 94,129-166 2. Ethanol: C_2H_6O ; [64-17-5] VARIABLES: PREPARED BY: W. Gerrard.

EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa

Absorption coefficient, Ab.Coef., is the volume of sulfur dioxide absorbed by 1 volume of ethanol or solution at a total pressure of 1 atm. The Ab. coef. refers to the volume of gas after adjustment to 273.15 K. To convert the Ab.coef. into the mole ratio, M.R., the molar volume of sulfur dioxide To convert was taken to be 21887 $\rm cm^3$ at 273.15 K and 1 atm, based on the published density of the gas at 273.15 K and 1 atm. The density of ethanol at the stated temperature was that cited by Timmermans (1). Carius gave a table showing the Ab.Coef. for a saturated solution; the data are combined in the table given here. Carius also gave a table showing density of the solution at a stated temperature, shown below.

T/K	Ab.Coef. m ³ /m ³ (soln)	Ab.Coef.m ³ /m ³ (ethanol)	* M.R. SO ₂ /EtOH	*Mole fraction "SO2	T/K	Density of saturated solution
276.35	188.34	276.76	0.720	0.419	277.15	1.0622
278.95	170.67	239.66	0.625	0.385	284.75	0.9880
284.15	135.48	176.93	0.464	0.317	289.15	0.9527
287.15	120.00	149.98	0.395	0.283	293.25	0.9402
290.15	106.03	129.33	0.342	0.255	296.65	0.9282
293.15	96.34	114.50	0.304	0.233	*Calcula	ated by
297.55	84.03	97.43	0.260	0.206	compi	ller.

Carius plotted the Ab.coef. (volume of saturated solution) vs temperature, and read off values for each degree from 273 to 298 K. These were tabulated and attached to a smoothing equation. From the densities of the saturated solutions, a table showing the Ab.coef. for the volume of alcohol itself was constructed. Again, from a plot of Ab.coef.(ethanol) vs temperature, a table showing the value at each degree was given, and accompanied by a smoothing equation which is not correct.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

was determined by iodometry. The Bunsen absorptiometer was mentioned.

SOURCE AND PURITY OF MATERIALS:

The amount of sulfur dioxide absorbed 1. Sulfur dioxide was stated to be dry.

ŀ

2. Ethanol was water free, density $0.792~\text{g/cm}^3$ at 293 K.

ESTIMATED ERROR:

REFERENCES:

Timmermans, J. "Physico-chemical Constants of Pure Organic Compounds," Elsevier, New York, 1950.

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Lobry de Bruyn, C.A. 2. Ethanol; C₂H₆O: [64-17-5] (a) Rec. Trav. Chim. 1892, 11, 112-157. (b) Z. Phys. Chem. 1892, 10, 782-789. VARIABLES: PREPARED BY: W. Gerrard.

EXPERIMENTAL VALUES:

		т/к	Weight % SO ₂	Mole ratio	*Mole ratio SO ₂ /ROH	Mole fraction* **SO2
Ref.	(a)	273.15 280.15 285.45 291.35 299.15	53.3 45 39.9 32.8 24.4	1.21 1.70 2.09 2.85 4.31	0.827 0.588 0.477 0.351 0.232	0.453 0.370 0.323 0.260 0.188
Ref.	(b)	273.15 299.15		/ 100 g ROH ₂ / 100 g ROH	0.827 0.232	0.453 0.188

(The primary data for expression (b) were probably the same as in (a).)

* Calculated by compiler.

Total pressure = atmospheric pressure.

AUXILIARY INFORMATION ...

METHOD APPARATUS/PROCEDURE: The dry gas was passed into a weighed amount of ethanol in a bulb of 2-3 cm³ capacity until equilibrium had been reached at the observed temperature, and at a total pressure, barometric, 760-770 mmHg. The bulb was sealed "a la lampe," and weighed. A titration was mentioned, but the statement is vague. SOURCE AND PURITY OF MATERIALS: 1. Simply stated that the dry gas was used. 2. Probably purified. ESTIMATED ERROR:

ORIGINAL MEASUREMENTS: COMPONENTS: Yuferev, R.F.; Maluigin, P.V. Sulfur dioxide; SO₂; [7446-09-5] Z. Chim. Prom. 1930, 7, 553-555. 2. Ethanol; C₂H₆O; [64-1705] VARIABLES: PREPARED BY: Temperature W. Gerrard EXPERIMENTAL VALUES: Weight of SO_2 per Volume of SO_2 per *Mole ratio cm³ of solvent g. cm³ of solvent cm³ SO_2 /ethanol *Mole ratio T/K Mole fraction ^xso₂ 273.15 0.9528 333.48 0.851 0.461 0.3036 292.65 106.26 0.276 0.216 "Wet" ethanol 0.9758 273.15 341.53 292.65 0.3066 107.31 * Calculated by compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Sulfur dioxide was passed into 5 cm3 of liquid (component 2) until saturated. The whole solution was then transferred to a stoppered flask 2. Heated over calcium oxide, containing an aqueous solution of I2 + KI. The sulfuric acid formed was determined gravimetrically. The total pressure was presumably 1 atm; but this was not stated.

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide dried by sulfuric acid.
- distilled, and stored over pulverized calcium.

("Wet" ethanol was ethanol dried over calcium oxide, but not distilled.)

ESTIMATED ERROR:

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Barclay, I.M.; Butler, J.A.V.; 2. Ethanol; C₂H₆O; [64-17-5] Trans. Faraday. Soc. 1938,34,1445-1454. VARIABLES: PREPARED BY: W. Gerrard

T/K	Pressure, PSO2, mmHg.	Mole fraction ^x SO ₂	P _{SO₂} /∞ _{SO₂} mmHg*
298.15	4.731	0.002223	2129
	4.699	0.002206	2130
308.15	6.85	0.002259	3035
	6.74	0.002224	3029

760 mmHg = 1 atm = 101.325 kPa.

AUXILIARY INFORMATION

METHOD: /APPARATUS/PROCEDURE:

Dry nitrogen was passed through a bubbler containing the solution at a stated T/K. The saturated vapor emerging was condensed in a tube cooled by solid carbon dioxide and ether. The amount of sulfur dioxide in the condensate was determined by an iodemetric titration.

SOURCE AND PURITY OF MATERIALS:

Stated that the materials were carefully purified and dried.

Ethanol had b.p. 78.47°C at 1 atm.

ESTIMATED	ERROR:

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446~09-5] Gerrard, W. 2. Ethanol; C₂H₆O; [64-17-5] J. Appl. Chem. Biotechnol. 1972, 22, 623-650. VARIABLES: Temperature PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: T/K P/kPa Mole ratio *Mole fraction

T/K	P/kPa	Mole ratio SO₂ / ROH	*Mole fraction $^x\mathrm{SO}_2$
273.15 283.15 293.15	102.5	1.10 0.564 0.357	0.524 0.361 0.263
	* Calculate	ed by compiler.	
	P is the to	otal pressure.	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a we ghed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K
- The best obtainable specimen was carefully purified and rigorously attested.

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EST	ΉΜΑ	TED	FRE	ans.

EXPERIMENTAL VALUES:

T/K	p/mmHg +	p/kPa ⁺	Mole fraction of sulfur dioxide in liquid,
-, -:		•	^x so ₂
293.15	414.8	55.30	0.1415
	796.6	106.2	0.2516
	1223	163.1	0.3866
	1379	183.9	0.4468
	1438	191.7	0.4705
	1526	203.4	0.5042
	1694	225.8	0.5847
	1739	231.8	0.5881
	1846	246.1	0.6507
	2052	273.6	0.7580
	2236	298.1	0.8617
	2452	326.9	1.000

⁺ Total pressure

AUXILIARY INFORMATION -

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with magnetic stirrer. After equilibrium established, pressure measured with Bourdon gauge and approximately 2 cm³ of liquid analysed by iodometric titration.

- SOURCE AND PURITY OF MATERIALS:
- Seitetsu Chemical Co. sample purity better than 99.9 mole per cent.
- Nakarai Chemicals spectrograde sample.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$; $\delta p/kPa = \pm 0.5$; $\delta x_{SO_2} = \pm 1\%$ (estimated by compiler)

188	Sulfur Dioxide Solubilities				
2. Ethanol;	oxide; SO_2 ; [7446-09-5] C_2H_6O ; [64-17-5] C_2H_6O ; $C_2H_$	ORIGINAL MEASUREMENTS: de Saussure, T. Gilbert's Annalen der Physik 1814, 47, 113-183. Annals of Phil. 1815, 6, No. 4, 241.			
VARIABLES:		PREPARED BY: W. Gerrard			
EXPERIMENTAL V	ALUES:				
291.15 K	sulfur dioxide at, pres	absorb 11577 volumes of sumably, the barometric pressure. for pure ethanol, the mole and the mole fraction, x_{SO_2} , ated by compiler).			
NOTE:	The data for water are				

100 volumes of water absorb 4378 volumes of sulfur dioxide at barometric pressure. The mole ratio is 0.338, and the mole fraction, $x_{\rm SO_2}$, is 0.0327 (calculated by compiler).

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The ethanol was freed as much as possible from air by boiling. The gas was held over mercury in a tube of 4 cm internal diameter. The alcohol was added, and the tube was shaken. The final volume was read after several days.	No specific information.
	ESTIMATED ERROR: REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Organic compounds containing oxygen

EVALUATOR:

C. L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

November 1982

CRITICAL EVALUATION:

In general the measurements on these systems are such that a detailed critical evaluation of each system is not possible.

1-Octanol; C₈H₁₈O; [111-87-5]

Gerrard's (1) values of the mole fraction solubility extrapolated to 303 K give a value which is significantly larger than that found by Sano and Nakamoto (2) but it is difficult to assess which is the more accurate. A comparison of the mole fraction solubilities for the alkanes determined by Makranczy $et\ al.$ (3) with data for decane (Gerrard) and hexane (Sano) suggests Gerrard's value (5) to be high and Sano's (4) to be low.

1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

This system has been investigated by four groups of workers (1,2,6,7). The results of Foote and Fleisher (6) and Gerrard (1) are consistent but the degree of overlap in experimental conditions is small. The value of Sano and Nakamoto (2) is again significantly smaller than the value obtained by extrapolation of Gerrard's data.

2-Propanone; C₃H₆O; [67-64-1]

This system has been investigated by five groups (4, 8-11) but detailed comparisons between sets of data are difficult to make in view of the different range of temperatures employed. The data of Bekarek and Hala (10) are in general agreement with those of Horiuti (9). The isolated value of Sano (4) appears to be consistent with those of Bekarek and Hola although extrapolation over such a large range of pressure could obscure any discrepancy. The data of Lorimer $et\ al.$ (11) cannot be meaningfully compared in detail with other data on this system because of the differences in temperature.

Acetic acid, methyl ester; C₃H₆O₃; [79-20-9]

The data of Horiuti (9) at 298.15 K and Bekarek and Hala (10) at 293.2, 303.2 and 313.2 K are consistent and are both classified as tentative. The isolated value of Sano (4) appears to be slightly low compared to a value obtained by extrapolation of the data of Bekarek and Hala (10).

Acetic anhydride; C4H6O3; [108-24-7]

The mole fraction solubilities of Lloyd (12) for this system are considerably lower than the values at comparable temperatures and pressures obtained by Gerrard (1) and Sano (4) and are almost certainly in error. The isolated value of Sano (4) appears to be somewhat low when compared with Gerrard's (1) values. The data of Nitta, Kido and (cont.)

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Organic compounds containing oxygen

EVALUATOR:

November 1982

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

CRITICAL EVALUATION:

Katayama (13) are consistent with those of Gerrard (1).

4-Methyl-1,3-dioxolan-2-one (Propylene carbonate); $C_4H_6O_3$; [108-32-7] The data of Lenoir et αl . (7) and Benoit and Milanova (14) on this system were both determined at low partial pressures of sulfur dioxide. There is a discrepancy of about 25 per cent between the values of the Henry's law constant obtained by these workers at 298 K.

1,1'-Oxybisethane (Diethyl ether); C4H10O; [60-29-7]

There is reasonable agreement between the data of Nitta $et\ al.$ (13) at 293.15 K and the value of Yuferev and Maluigin (15) at 291.65 K. The value of Sano (4) at 303 K appears to be too high.

Cyclohexanone; C₆H₁₀O; [108-94-1]

The value of Weissenberger and Hadwiger (16) at 293.15 K is much too low to be consistent with the data of Sano (4) at 303 K and that of Gerrard (5) at 283.15 K and 293.15 K and is almost certainly in error. Sano's value is somewhat lower than would be expected from any reasonable extrapolation of Gerrard's values but it is not possible to state which of the values are in error.

1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one (Camphor); $C_{10}H_{16}O$; [464-49-3] The data of Bineau (17) and the isolated values of Schulze (8) and Sano (5) are consistent within ± 8 per cent.

References

- 1. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
- 2. Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369.
- Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L.
 Hung. J. Ind. Chem. 1976, 4, 269.
- 4. Sano, H. Nippon Kagaku Zasshi 1968, 89, 362.
- 5. Gerrard, W. Solubility of Gases and Liquids, Plenum Press, New York, 1976, p.239.
- 6. Foote, H. W.; Fleisher, J. J. Am. Chem. Soc. 1934, 56, 870.
- 7. Lenoir, J.-Y.; Renault, P.; Renon, H. J. Chem. Engng. Data 1971, 16, 340.
- 8. Schulze, H. J. Prakt. Chem. 1881, 24, 168.
- 9. Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn.) 1931/32, 17, 125.
- 10. Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. <u>1968</u>, 33, 2598.

(cont.)

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Organic compounds containing oxygen

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

November 1982

CRITICAL EVALUATION:

References (cont.)

- 12. Lloyd, S. J. J. Phys. Chem. 1918, 22, 200.
- Nitta, T.; Kido, O.; Katayama, T. J. Chem. Engng. Japan <u>1976</u>, 9, 317.
- 14. Benoit, R. L.; Milanova, E. Can. J. Chem. 1979, 57, 1319.
- 15. Yuferev, R. F.; Maluigin, P. V. Z. Chim. Prom. 1930, 7, 553.
- 16. Weissenberger, G.; Hadwiger, H. Z. angew. Chem. 1927, 40, 734.
- 17. Bineau, A. Ann. Chim. Phys. 1848 (3), 24, 326.

- 1. Sulfur dioxide; CO₂; [7446-09-5]
- 2. 2-Propanol; C₃H₆O; [67-63-0]
 2-Methyl-2-propanol (tert-butanol);
 C₄H₁₀O; [75-65-0]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of 2-Propanol = 0.035 atm
Vapor pressure of 2-Methyl-2-propanol = 0.041 atm
Vapor pressure of 1-Butanol = 0.008 atm

Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c	ℓc,d	Mole ratio	Mole fraction ^e
_S a,b	α	α			
	2	-Propanol			
53.9	50.7	52.6	48.6	0.184	0.155
н	2-Meth	yl-2-propanol			
47.9	45.7	45.4	42.2	0.191	0.160
	1	-Butanol			
53.8	45.5	49.2	48.4	0.203	0.169

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrcally. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodo-The vapor metric titration. pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

 Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] 2. 3-Methyl-l-butanol (iso-amyl alcohol); C₅H₁₂O; [123-51-3] 1-Hexanol; C₆H₁₄O; [111-27-3] 1-Octanol; C₈H₁₈O; [111-87-5] VARIABLES: ORIGINAL MEASUREMENTS: Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369-373.

EXPERIMENTAL VALU	UES: T/°C	= 30 T/K =	303		
	Vapor pressure o Vapor press	f 3-Methyl-l-buta ure of l-Hexanol	anol = = 0.00	0.006 atm 04 atm	
Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c,f	lc,d	Mole ratio	Mole fraction ^e
sa,b	α	α			
	3-Me	thyl-1-butanol			
40.9	37.4	37.5	37.4	0.183	0.155
		1-Hexanol			
41.5	37.9	37.7	37.6	0.212	0.175
		1-Octanol			
28.7	26.1	25.5	25.5	0.183	0.155

a Volume of sulfur dioxide absorted by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

d $\alpha = l(1 - p_s^{\circ})$ where p_s° is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming the vapor pressure of 1-octanol is negligible.

ORIGINAL MEASUREMENTS:
Albright, L.F.; Shannon, P.T.;
Yu, SN.; Chueh, P.L.
Chem. Engng. Prog. Symp. Ser. 1963,
59, (44), 66-74.
PREPARED BY:
C.L. Young

T/K	P/bar	Mole fraction of sulfur dioxide in liquid, x_{SO_2}
298.15	2.04 3.01 3.48	0.377 0.626 0.831
310.93	2.76 2.83 3.85 4.39 5.21 5.55	0.363 0.373 0.482 0.617 0.831 0.874
338.71	5.36 8.43 10.96	0.363 0.589 0.825
366.48	8.54 14.17 20.13	0.343 0.586 0.824

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).

SOURCE AND PURITY OF MATERIALS:

1. and 2. Commercial grade samples no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta P/bar = \pm 0.3$; $\delta x_{SO_2} = \pm 1$ %.

- Albright, L. F.; Shannon, P. T.; Terrier, F.; Chueh, P. L. Am. Inst. Chem. Engrs. J. 1962, 8, 668.
 Albright, L. F.; Buclez, P. C.;
- 2. Albright, L. F.; Buclez, P. C.; Pluche, C. R.; Doody, T. C. ASHRAE Trans. 1960, 66, 423.

Other organic compounds containing oxygen 195 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W. 2. 1-Octanol; C₈H₁₈O; [111-87-5] J. Appl. Chem. Biotechnol. 1972, 22,623-650. VARIABLES: PREPARED BY: Temperature W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPaT/K Mole ratio *Mole fraction P/kPa SO₂ /ROH [∞]SO₂ 101.3 0.710 0.415 273.15 0.292 0.412 283.15 0.292 0.226 293.15 0.200 298.15 0.250

* Calculated by compiler.

P is the total pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a Weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to Which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- 2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ER	RO	R:
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- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Cyclohexanol; $C_6H_{12}O$; [108-93-0] Benzenemethanol (Benzyl alcohol); C_7H_8O ; [100-51-6]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

0.280

0.219

EXPERIMENTAL VALUES:

66.3

 $T/^{\circ}C = 30$ T/K = 303

Vapor pressure of cyclohexanol = 0.001 atm

Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c,f	ℓc,d	Mole ratio	Mole fraction ^e
38.0	34.6 B	Cyclohexanol 34.3 enzenemethanol	34.3	0.160	0.139

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

59.5

60.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

59.5

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

^C Determined by flow method.

d $\alpha = l(1 - p_s^{\circ})$ where p_s° is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming the vapor pressure of benzenemethanol is negligible.

COMPONENTS: ORIGINAL MEASUREMENTS: Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1. Sulfur dioxide; SO₂; [7446-09-5] 2. Cyclohexanol; $C_6H_{12}O$; [108-93-0] <u>1976</u>, p.239 VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: Mole ratio Weight of SO₂ Mole fraction T/K Weight of Component (2) absorbed, g SO_2 /Comp. (2) x_{SO_2} (Total pressure = 1 atm) 293.15 2.5570 0.4489 0.275 0.216 760 mmHg = 1 atm = 101.325 kPa. AUXILIARY INFORMATION METHOD: SOURCE AND PURITY OF MATERIALS: 1. Sulfur dioxide was the best grade Sulfur dioxide was bubbled into a contained in a small cylinder. Its high degree of purity was attested by the measurement of vapor weighed amount of component (2) in a bubbler tube. The amount of gas absorbed was determined by repressure from 258-268 K. weighing the tube. The total pressure was barometric, very nearly 2. The best commercial specimen was purified and attested. l atm. See ref. (1). ESTIMATED ERROR: REFERENCES: Gerrard, W. J. Appl. Chem. Biotechnol. <u>1972</u>, 22,623.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Schulze, H.; 2. Formic acid; CH₂O₂; [64-18-6] J. Prakt. Chem. 1881, 24, 168-183. orAcetic acid, $C_2H_4O_2$; [64-19-7] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 101.325 kPa.*Mole fraction T/K Weight of SO₂/ g *Mole ratio $SO_2/Comp.(2)$ of comp.(2) x so₂ Formic Acid 0.821 0.590 0.371 273.15 Acetic Acid 0.901 0.474 273.15 0.961 Pressure of SO₂ stated to be 725 mmHg. 1 volume of formic acid absorbed 351 volumes of SO2 1 volume of acetic acid absorbed 318 volumes of SO2 * Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The gas was passed into a known weight of formic acid in a long thin walled test-tube fitted with a rubber stopper carrying an inlet No details given. and an outlet tube. The tube was cooled by melting snow. The amount of gas absorbed was determined by weighing. ESTIMATED ERROR: REFERENCES:

COMPONENTS: 1. Sulfur dioxide; SO₂ Cupr, V. [7446-09-5] 2. Water; H₂O; [7732-18-5] 3. Acetic acid; C₂H₄O₂; [64-19-7] VARIABLES: PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

1 atm = 760 mmHg = 101.325 kPa

The absorption coefficient, designated by Cupr as L, appears to be the Bunsen coefficient; but there is some doubt about the use of the term "solution", which could mean the aqueous solution of acetic acid, i.e., taken as the original liquid; the initial water itself would then be simply the original liquid for that data, and the final acetic acid itself would be the original liquid for its data. However, Seidell and Linke (1) define this L as "cc. SO_2 per 1 cc sat. sol." when reporting this work.

T/K = 300.15 Total pressure = 1 atm

Concentration of acetic acid in aqueous solution * *	SO ₂ in g absorbed by 100 g of acetic acid solution (liquid indicated in col. 1)	"Absorption coefficient"
0.00	7.98	25.7
	. 8.01	25.8
	8.19	26.4
	8.12	26.2
	8.18	26.4
	8.11	26.1
16.72	8.86	31.5
16.74	8.80	31.3
45.58	12.04	44.1
44.73	11.92	43.7
63.51	16.35	61.6
83.59	22.83	84.8
91.89	26.49	97.8
100.00	31.15	112.8
	s a weight or mole per cent.	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was passed into the original liquid (the aqueous solution in the acetic acid + water mixtures) as for a total pressure of 1 atm. The contents of the final solution were determined by chemical titrations, acid-base, and iodine-thiosulfate.

The "absorption coefficient, L" was determined by calculation from the weight data, 22400 being apparently taken as the molar volume in cm³ at 1 atm and 273.15 K. Based on the real molar volume, these L values are 2% too large.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was obtained from Merck, quality sodium sulfite and concentrated sulfuric acid, by which it was dried.
- Water may be taken as of satisfactory purity.
- Acetic acid was of Merck standard, and gave no residue when ignited on a platinum capsule.

ESTIMATED ERROR:

REFERENCES:

Seidell, A.; Linke, W. F.
 Solubilities of Inorganic and
 Organic Compounds,
 1958, 1965.

COMPONENTS:			ORIGINAL	MEASUREME	NTS:	
1. Sulfur diox 2. Acetic acid Formic acid		[64-19-7]	Nippon	H.; Na Kagaku 89, 369		
VARIABLES:			PREPARED		. L. Young	
EXPERIMENTAL VALUE	S:	'/°C = 30	T/K =	: 303		
	Vapor pres	sure of ace	tic acid	1 = 0.01		
Absorption coefficient,	Bunsen coefficient	,b Bunse	en cient, c	_l c,d	Mole ratio	Mole fraction ^e
_S a,b	α	α				,
		Acetic ac	id:			
106.0	97.4	96.	2	95.2	0.251	0.201
		Formic ac	id			
61.2	57.8	60.	0	55.5	0.103	0.094
a	£15 3i-					

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: (a) static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 58$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

^e Calculated by compiler.

COMPONENTS:		long of the second
1. Sulfur dioxide, SO ₂ ; [744	16_00_51	ORIGINAL MEASUREMENTS: Nitta, T.; Kido, O; Katayama, T.;
2. Acetic acid; C ₂ H ₄ O ₂ ; [64-	-19-7]	J. Chem. Engng. Japan. <u>1976</u> , 9,317-8
VARIABLES:		PREPARED BY:
Pressure		C.L. Young
EXPERIMENTAL VALUES:		
т/к	P/bar	Mole fraction of sulfur dioxide in liquid, ω_{SO_2}
293.15	0.0800 0.2758 0.7079 0.9758 1.176 1.537 1.901 2.338 2.613 2.936	0.0207 0.0796 0.1971 0.2651 0.3173 0.4065 0.4981 0.6171 0.7013 0.8238
*		
	AUXILIARY	INFORMATION
METHOD:		SOURCE AND PURITY OF MATERIALS:
Static method liquid phase composition estimated by iodometry. Few details given in source. Method similar to that used in ref. (1).	2	 Seitetsu Chemical Co. sample, purity better than 99.9 mole per cent. Merck analytical grade sample.
		ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta P/bar = \pm 0.001$ (below 1.3 bar) ± 0.005 (above 1.3 bar); δx_{SO_2} = ± 1.5 %
		REFERENCES:
		Quitzich, K.; Ulbrecht, H.; Geiseler, G.
		Z. Physik Chem. <u>1967</u> , 234, 33.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Sano, H.
2. Esters of formic acid	Nippon Kagaku Zasshi
	<u>1968</u> , 89, 362-368.
VARIABLES:	PREPARED BY:
	C. L. Young
EXPERIMENTAL VALUES: T/°C = 30	T/K = 303
Bunsen coefficient, α Mole r	atio Mole fraction ^a
Methyl formate; C ₂ H ₄	O ₂ ; [107-31-3]
331	0.920 0.479
Ethyl formate; C ₃ H ₆	O ₂ ; [109-94-4]
217	0.781 0.439

^a Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

COMPONENTS:

1. Sulfur dioxide; SO₂; [7446-09-5]

 1,2-Ethanediol (dihydroxyethane, ethylene glycol, glycol); C₂H₆O₂; [107-21-1]

ORIGINAL MEASUREMENTS:

Foote, H.W.; Fleisher, J.

J. Am. Chem. Soc. 1934, 56,870-873

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	P _{SO2} mmHg	Mole fraction $x_{\rm SO_2}$	
273.15	1055 1028 951 857 758 571 427 291 168 99.1 66.7	0.707 0.673 0.575 0.499 0.436 0.340 0.272 0.206 0.138 0.093 0.068	

NOTE: A mole fraction of 0.707 is equivalent to a mole ratio of 2.413 moles of SO_2 per mole of 1,2-ethanedio1.

760 mmHg = 1 atm = 101.325 kPa. Observed pressure was taken to be p_{SO_2} .

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

The apparatus and method had been Previously described (1). A glass bulb of 29.3 cm³ capacity was connected via a tap to an open manometer, a Vacuum flask of 2 dm³ capacity, and a source of sulfur dioxide. Component (2) was weighed in the bulb. Sulfur dioxide was condensed in it at 253 K. Equilibrium was attained at 273.15K and at the observed pressure p Total' assumed to be equal to p_{SO}.

SOURCE AND PURITY OF MATERIALS:

- (1) Sulfur dioxide was dried by sulfuric acid.
- (2) The glycol was of Eastman C.P. grade, or purified by customary method.

ESTIMATED ERROR:

- 1. Foote, H.W.; Fleischer, J.
 - J. Am. Chem. Soc. 1931,53,1752.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 2. Diols and glycerol 1968, 89, 369-373. **VARIABLES:** PREPARED BY: C. L. Young EXPERIMENTAL VALUES: T/K = 303 $T/^{\circ}C = 30$ Mole Mole Absorption Bunsen Bunsen coefficient, c,f lc,d ${\tt fraction}^{\tt e}$ coefficient, ratio sa,b 1,2-Ethanediol (ethylene glycol); C2H6O2; [107-21-1] 0.135 0.119 51.8 2,2'-Oxybisethanol (diethylene glycol); $C_4H_{10}O_3$; [111-46-6] 0.500 0.333 119 130 119 1,2-Propanediol (propylene glycol); $C_3H_6O_2$; [57-55-6] 61.9 61.7 0.204 0.169 61.7 68.0 1,2,3-Propanetriol (glycerol); $C_3H_8O_3$; [56-81-5] 0.188 0.158 57.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: (a) static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Determined by static absorption method.

^c Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming vapor pressure of solvent to be negligible.

Other organic compounds containing oxygen 205 COMPONENTS: ORIGINAL MEASUREMENTS: Lenoir, J-Y.; Renault, P.; Renon, H. Sulfur dioxide; SO₂[7446-09-5] J. Chem. Eng. Data 1971, 16,340-342. 2. 1,2-Ethanediol (Ethylene glycol) $C_2H_6O_2$; [107-21-1] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa.T/K Henry's constant *Mole fraction at 1 atm. H_{SO},/atm 298 3.41 0.293 * Calculated by compiler assuming a linear function of P_{SO} , vs x_{SO_2} , i.e. x_{SO_2} (1 atm = 1/H_{SO2}. The authors gave "Henry's constant" as $f_{SO_2}^{(P,T)}$ $H_{SO_2} = \lim_{x_{SO_2} \to 0} \frac{1}{x_{SO_2}}$ x_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition" of pressure and temperature. H_{SO_2} is related to experimental chromatographic parameters based on the number of moles of solvent in in the column, and the absolute retention time of the solute. Helium was the carrier gas. AUXILIARY INFORMATION '-SOURCE AND PURITY OF MATERIALS: METHOD/APPARATUS/PROCEDURE: A conventional gas-liquid chromatog-Sulfur dioxide was provided by raphic unit was used. The chromatl'Air Liquide, and had a stated purity of 99.9%. It was used as ograph was an IGC 12 M Intersmat provided. model, equipped with a thermal conductivity detector. The temperature control was stated to be within 2. Provided by Touzart & Matignon and ± 0.1°C. The pressure drop in the Serlabo, and stated to have a minimum purity of 99%. Distillation column was measured by a mercury was carried out when necessary, manometer. Helium was the carrier and the refractive index was gas. measured. There is serious uncertainty in the ESTIMATED ERROR: estimation of accuracy.

206 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W. 1,2-Ethanediol, (ethylene glycol); J. Appl. Chem. Biotechnol. $C_2H_6O_2$; [107-21-1] 1972, 22,623-650. VARIABLES: PREPARED BY: Temperature W. Gerrard EXPERIMENTAL VALUES: T/K P/kPa Mole ratio *Mole fraction SO₂ / ROH x so₂

0.83

0.420

0.310

0.255

*	Calculated	bv	compiler.

101.5

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

273.15

283.15

293.15

298.15

SOURCE AND PURITY OF MATERIALS:
1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.

0.448

0.296

0.237

0.203

2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED	ERROR:
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P is the total pressure.

	ius containing oxygen 207
COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Schulze, H.
2. 2-Propanone (acetone, dimethyl ketone); C ₃ H ₆ O; [67-64-1]	J. Prakt. Chem. <u>1881</u> , 24,168-183.
VARIABLES:	PREPARED BY:
	W. Gerrard.
EXPERIMENTAL VALUES: 760 mmHg = 1 atm =	= 101.325 kPa.
T/K Weight of SO_2 *Mol- /1g of Comp. (2). SO_2/C_0	e ratio *Mole fraction omp. (2) *SO ₂
273.15 2.07 1	.88 0.653
* Calculated by compiler.	
Pressure of SO ₂ stated to	be 725 mmHg.
1 Volume of acetone absorb	bed 589 volumes of SO2.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The gas was passed into a weighed amount of acetone in a long thin-walled test-tube carrying a rubber stopper and an inlet tube and an outlet tube. The test-tube was cooled by melting snow. The amount of gas absorbed was determined by	No details given.
weighing.	
	ESTIMATED ERROR:
	REFERENCES:

208		Sulfu	ır Dioxide	e Solubilities		
COMPONENTS	:			ORIGINAL MEAS	SUREMENTS:	
		de; SO_2 ; [7446 (acetone); C_3H_6	-09-5] O;	Sci. Pap	J. o. Inst. Phys. C 1931/32, 17, 12	
	[67-64-]	r]				
VARIABLES	:	· · · · · · · · · · · · · · · · · · ·		PREPARED BY:		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
Tempera	ture, pre	essure			C. L. Young	
EXPERIMENT	TAL VALUES:					
т/к	P [§] /bar	Mole fraction of sulfur dioxide in liquid, "SO ₂	T/K	P [†] ∕bar	Mole fraction of sulfur dioxide in liquid, "SO ₂	Ostwald coefficient, L
298.15	0.3053 0.4053 0.4142 0.5086 0.6016 0.6307 0.7647 0.7682 0.9415 0.9860 1.012 1.141 1.232 1.325	0.000 0.142 0.160 0.237 0.294 0.308 0.368 0.372 0.430 0.445 0.470 0.483 0.506 0.519	283.15 298.15 313.15	0.9531 0.8440 0.6008	0.448	276.4 216.4 171.3
† part:	coeffici	e. ure, total pressent (as $x \rightarrow 0$, tant, dp/dx (as	T/K = 2	298.15) = 3	98.	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus consisted of a gas buret, a solvent reservoir and an absorption Dry gas introduced into degassed solvent. System mixed using a magnetic stirrer until saturation Care was taken to prevent occurred. solvent vapor from mixing with gas in the gas buret. Volume of gas determined from gas buret reading; volume of liquid determined from height of meniscus in absorption pipet.

SOURCE AND PURITY OF MATERIALS:

- 1. Sample obtained from Nippon Sulphuric Acid Manufacturing Co. Dried and fractionated several
- 2. Extra pure sample, recrystallized with sodium sulfite. Dried and fractionated. B. pt. 56.09 °C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/bar = \pm 0.001;$ $\delta x_{SO_2} = \pm 0.001$ (estimated by compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. 1968 2-Propanone, (Acetone); 33, 2598-2607. C_3H_6O ; [67-64-1] VARIABLES: PREPARED BY: C.L. Young. Temperature, pressure. EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide in liquid, T/K P/Torr P/kPa ^xso₂ [∞]so₂ 25.625 0.0374 0.0914 293.2 192.20 0.1450 0.0600 26.691 200.20 27.371 0.0741 0.1790 205.30 227.60 30.344 0.1230 0.3000 0.1390 0.3430 237.00 31.597 0.1660 0.4100 253.90 33.851 37.330 0.2020 0.4980 280.00 0.7200 397.30 52.969 0.3130 294.70 39.290 0.0343 0.0814 303.2 0.1340 40.877 0.0562 306.60 0.0829 0.2030 322.40 42.983 350.10 46.676 0.1217 0.3010 0.4310 52.969 0.1759 397.30 59.248 0.2150 0.5180 444.40 74.487 0.2902 0.6780 558.70 0.0325 0.0776 313.2 440.40 58.715 454.80 60.635 0.0513 0.1240 0.1670 470.00 62.662 0.0693 0.1240 0.3030 527.00 70.261 0.1410 0.3510 548.80 73.167 0.3940 0.1600 572.50 76.327 592.70 79.020 0.2340 0.5570 N.B. Same data given in ref.(2) AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Dried with sulfuric acid and A modified Gillespie still was used. Sulfur dioxide in liquid phosphorus pentoxide. and gaseous phases estimated by iodometric titration. Details 2. Analytical grade, fractionally distilled, $d_{20}^4 = 0.7902$. in source and ref. (1). ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta P/kPa = \pm 0.1$ %; δx_{SO_2} , $\delta y_{SO_2} = \pm 0.5\%$. (estimated by compiler). REFERENCES: 1. Dvorak, K.; Boublik, T. Coll. Czech. Chem. Comm. 1963, 28, 1252. Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. 1968,

33, 2608.

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$C_4H_8O; [78-93-3]$	tone); C ₃ H ₆ O; yl ethyl ketone);] none (methyl iso-	ORIGINAL MEASUREMENTS: Sano, H. Nippon Kagaku Zasshi 1968, 89, 362-368.		
VARIABLES:		PREPARED BY:	Young	
EXPERIMENTAL VALUES:	T/°C = 30	T/K = 303		
Absorption coefficient, Sa	Bunsen coefficient,	Mole α ratio	Mole fraction ^b	
	2-Prop	anone		
182.1	201.2	0.665	0.400	
	2-Buta	none		
161.9	163.2	0.656	0.396	
	4-Methyl-2-	pentanone		
109.3	100.5	0.563	0.360	

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Calculated by compiler.

COMPONENTS: ORIGINAL MEASUREMENTS: l. Sulfur dioxide; SO₂; [7446-09-5] Lorimer, J.W.; Smith, B.C.; Smith, G.H. 2. 2-Propanone, (Acetone); C3H6O; [67-64-1]J.C.S. Faraday I, 1975, 71, 2232-50. VARIABLES: PREPARED BY: Temperature, pressure C.L. Young EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide T/K p/mmHg p/kPa in liquid, in vapor, ^xSO₂ y_{SO₂} 227.6 0.501 0.0000 0.000 3.76 0.532 0.187 0.1088 3.99 0.709 0.2123 0.518 5.32 8.77 0.3132 0.792 1,169 1.439 0.880 10.79 0.3899 24.11 3.214 0.4926 0.969 0.990 39.87 5.316 0.5889 6.259 0.994 46.95 0.6241 9.631 0.7419 0.998 72.24 96.61 12.880 0.8623 1.000 116.72 15.561 1.0000 1.000 237.4 7.53 1.004 0.0000 0.000 0.1090 0.238 8.66 1.155 0.2109 11.93 1.591 0.544 0.778 18.42 2.456 0.3120 0.3861 0.881 26.00 3.466 45.93 6.123 0.4884 0.959 0.985 73.19 9.758 0.5848 84.40 0.990 11.252 0.6166 0.997 0.7364 128.49 17.131 0.999 0.8602 172.24 22.963 1.000 208.81 27.839 1.0000 AUXILIARY INFORMATION --METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static vapor-liquid equilibrium apparatus. Total pressure measured using mercury manometers and No details given. Cathetometer. Temperature measured using a sulfur dioxide vapor pressure thermometer. Some details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.01$ δx_{SO_2} , $\delta y_{SO_2} = \pm 1\%$. REFERENCES:

COMPONENTS:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 2-Propanone, (Acetone); C₃H₆O;
 [67-64-1]

ORIGINAL MEASUREMENTS:

Lorimer, J.W.; Smith, B.C.; Smith, G.H.

J.C.S. Faraday I, <u>1975</u>, 71, 2232-50.

EXPERIMENTAL V	'ALUES:
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т/к	p/mmHg	p/kPa	Mole fraction of in liquid, "SO ₂	sulfur dioxide in vapor, y _{SO₂}
250.0	17.92	2.389	0.0000	0.000
	21.16	2.821	0.1076	0.257
	28.59	3.812	0.2092	0.543
	41.91	5.588	0.3094	0.761
	57.83	7.710	0.3792	0.864
	94.94	12.658	0.4797	0.946
	145.57	19.408	0.5750	0.979
	164.17	21.888	0.6016	0.984
	247.81	33.039	0.7248	0.995
	335.03	44.667	0.8554	0.999
	409.65	54.616	1.0000	1.000

COMPONENTS:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Propanoic acid (propionic acid);
 C₃H₆O₂; [79-09-4]

 Hexanoic acid (caproic acid);
 C₆H₁₂O₂; [142-62-1]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of propanoic acid = 0.004 atm

Absorption coefficient, Sa,b	Bunsen coefficient, b	Bunsen coefficient, c,f	ℓc,d	Mole ratio	Mole fraction ^e
	Р	ropanoic acid			
75.7	69.0	-	-	0.232	0.188
	Н	exanoic acid			
37.0	33.5	33.0	33.0	0.187	0.158

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodo-The vapor metric titration. pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming the vapor pressure of hexanoic acid is negligible.

COMPONENTS	3:			ORIGINAL	MEASUREMENTS:		
1. Sulfur dioxide; SO ₂ ; [7446-09-5] 2. Acetic acid, methyl ester (Methyl acetate); C ₃ H ₆ O ₂ ; [79-20-9]				Horiuti, J. Sci. Pap. Inst. Phys. Chem.Res. (Jpn.), <u>1931/32</u> , 17, 125-256.			
VARIABLES	:			PREPARED	BY:		
Tempera	ture, pre	essure			C. L	Young	ı
EXPERIMENT T/K	TAL VALUES:	Mole fraction of	т/к	₽ [†] /ba	Mole frac of ar sulfur di in liqu ^x SO ₂	oxide	Ostwald coefficient, L
298.15	0.2843 0.4237 0.4322 0.5887 0.6084 0.7659 0.8027 0.9471 1.005 1.123 1.191 1.295 1.384	0.000 0.137 0.143 0.243 0.254 0.322 0.336 0.387 0.406 0.438 0.456 0.478 0.497	283.15 298.15 313.15	0.844	0.408	}	254.9 182.1 133.8
† parti	_	e. ure, total present (as $x \rightarrow 0$,		_		325 × 1	.0 ⁵ Pa.

Henry's law constant, dp/dx (as $x \rightarrow 0$, T/K = 298.15) = 861 mmHg = 1.148 bar.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus consisted of a gas buret, a solvent reservoir and an absorption pipet. Dry gas introduced into degassed solvent. System mixed using a magnetic stirrer until saturation occurred. Care was taken to prevent solvent vapor from mixing with gas in the gas buret. Volume of gas determined from gas buret reading; volume of liquid determined from height of meniscus in absorption pipet.

SOURCE AND PURITY OF MATERIALS:

- Sample obtained from Nippon Sulphufic Acid Manufacturing Co. Dried and fractionated several times.
- Merck, extra pure sample, dried and distilled several times.
 pt. 57.12 °C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta P/bar = \pm 0.001;$ $\delta x_{SO_2} = \pm 0.001$ (estimated by compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Bekarek, V.; Hala, E. Coll. Czech. Chem. Comm. 1968, Acetic acid, methyl ester, 33, 2598-2607. (Methyl acetate); C3H6O2; [79-20-9] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide P/kPa in liquid, T/K P/Torr in gas, ^xSO₂ y_{so} 0.0110 0.0387 293.2 174.50 23.265 26.784 0.0636 0.2110 200.90 0.4920 36.517 0.1660 273.90 360.60 48.076 0.2510 0.6650 0.2840 0.7160 53.796 403.50 0.7200 410.00 54.662 0.2860 553.00 73.727 0.3720 0.8290 303.2 274.60 36.610 0.0169 0.0580 329.60 43.943 0.0841 0.2660 0.3600 362.40 48.316 0.1150 0.1340 0.4010 381.00 50.796 0.4370 397.30 52.969 0.1480 476.00 63.461 0.2070 0.5700 64.741 0.2120 0.5830 485.60 0.7260 646.20 86.153 0.3030 0.0401 313.2 413.20 55.089 0.0120 0.1860 466.00 62.128 0.0587 483.60 0.0737 0.2330 64.475 0.1240 0.3700 554.40 73.914 74.127 0.1260 0.3710 556.00 0.4710 632.90 84.380 0.1710 N.B. Same data given in ref.(2) AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A modified Gillespie still was 1. Dried with sulfuric acid and used. Sulfur dioxide in liquid phosphorus pentoxide. and gaseous phases estimated by 2. Added to 5 per cent acetic iodometric titration. Details in anhydride and fractionally source and ref. (1). distilled. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta P/kPa = \pm 0.1$ % δx_{SO_2} , δy_{SO_2} = ±0.5%. (estimated by compiler). REFERENCES: Dvorak, K.; Boublik, T. Coll. Czech. Chem. Comm. 1963, 28, 1252.

Bekarek, V.; Hala, E.

33, 2608.

Coll. Czech. Chem. Comm. 1968,

COMPONENTS:

- Sulfur dioxide; SO₂; [7446-09-5]
- 2. 2-Propanone, C₃H₆O; [67-64-1]

535.0

506.7

686.5

 Acetic acid, methyl ester, (Methyl acetate); C₃H₆O₂; [79-20-9]

ORIGINAL MEASUREMENTS:

0.459

0.834

0.591

Bekarek, V.; Hala, E.

Coll. Czech. Chem. Comm. 1968, 33, 2598-2607.

VARIABLES:

Pressure

PREPARED BY:

C.L. Young

0.302

0.262

0.529

0.361

0.683

0.360

EXPERIMENTAL	VALUES:		Mole fractions				
		40	in li	in liquid in		gas	
T/K	<i>p/</i> Torr	p/kPa	^x so₂	^ж С ₃ Н ₈ О	y _{SO2}	^у С ₃ Н ₈ О	
313.2	450.3 477.1	60.035 63.608	0.0426 0.0609 0.0736	0.829 0.383 0.847	0.107 0.169 0.183	0.769 0.352 0.738	-
	477.1 494.3 501.5	63.608 65.901 66.861	0.0736 0.0801 0.0864	0.411 0.407	0.183 0.214 0.231	0.738 0.353 0.342	

0.114

0.107

0.222

71.327

67.554

91.526

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A modified Gillespie still was used. Sulfur dioxide in liquid and gaseous phases estimated by iodometric titration. Details in source and ref. (1).

To determine the acetone concentration a bulb containing (0.5 - 1.0g) of mixture was broken in a solution containing iodine just sufficient to convert sulfur dioxide to sulfuric acid. Acetone was then determined by Messinger's method (ref.(2)).

SOURCE AND PURITY OF MATERIALS:

- 1. Dried with sulfuric acid and phosphorus pentoxide
- Analytical grade, fractionally distilled, d₂₀ = 0.7902.
- Added to 5 per cent acetic anhydride and fractionally distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.1$ %. δx_{SO_2} , $\delta x_{C_3H_8O}$, δy_{SO_2} , $\delta y_{C_3H_8O}$ (estimated by compiler).

- Dvorak, K,; Boublik, T.
 Coll. Czech. Chem. Comm. 1963, 28, 1252.
- Goodwin, L.F.; J. Am. Chem. Soc., 1920, 42, 39.

0.329

Other organic compounds containing oxygen COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H.; Nakamoto, Y. 2. Cellosolves Nippon Kagaku Zasshi 1968, 89, 369-373. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Vapor pressure of 2-Methoxyethanol = 0.008 atm Vapor pressure of 2-Butoxyethanol = 0.001 atm Mole Mole Bunsen Absorption Bunsen coefficient, c oc,d fractione coefficient, b coefficient, ratio $s^{a,b}$ 2-Methoxyethanol (methyl cellosolve); C3H8O2; [109-86-4] 185.9 185.1 0.652 0.395 184.2 201 2-Butoxyethanol (butyl cellosolve); C₆H₁4O₂; [111-76-2] 103.2 103.7 103.6 0.605 113.5

2-Phenoxyethanol (phenyl cellosolve); C₈H₁₀O₂; [122-99-6]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

96.1

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

0.491

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5;$ $\delta x_{SO_a} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Determined by static absorption method.

C Determined by flow method.

 $[\]alpha = \ell(1 - p_{\alpha}^{\circ})$ where p_{α}° is the vapor pressure of solvent.

e Calculated by compiler.

COMPONENTS:			ORIGINAL	MEASUREMENTS	:	
1. Sulfur diox	ide; SO ₂ ;	[7446-09-5]	Sano, H.			
2. Esters of a	Nipp	on Kagaku l	Zasshi			
			1968	<u>3</u> , <i>89</i> , 362-	368.	
			1			
{			1			
VARIABLES:			PREPAREI	BY:		
			}	C. L	. Young	
EXPERIMENTAL VALUE	S: T/	°C = 30	T/I	x = 303		
	Vapor pr	essure of e essure of b ssure of isa	utyl ace	etate = 0.03	23 atm	
Absorption coefficient,	Dungan	Bung	^n		Mole ratio	Mole fraction ^e
sa,b	α	α				
_	Methyl 142	acetate; C	3H6O2;	[79-20-9] -	0.509	0.337
118.9	Ethyl 119.7	acetate; C	4H8O2; 0.5		0.531	0.347
92.0		acetate; C 8	₆ H ₁₂ O ₂ ; 4.0	[123-86-4] 82.0	0.500	0.333
3-Methyl-1-b 83.0	outanol acet 75.1	ate (<i>iso-am</i> 7	yl aceto 4.8	75.8	O ₂ ; [12 0.500	23-92-2] 0.333

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

I'wo techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

c Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

Other organic compounds containing oxygen 219 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W. 1,2,3-Propanetriol (glycerol); J. Appl. Chem. Biotechnol. 1972, C₃H₈O₃; [56-81**-**5] 22,623-650. VARIABLES: PREPARED BY: W. Gerrard. Temperature EXPERIMENTAL VALUES: *Mole fraction T/K P/kPa Mole ratio SO / ROH xSO2 101.3 0.39 0.281 273.15 283.15 0.20 0.167 293.15 0.117 0.105 * Calculated by compiler P is the total pressure. AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Sulfur dioxide was bubbled into a
weighed amount of component (2) in a
bubbler tube as described in detail,
diagram given, in the original paper.
The amount of gas absorbed at
equilibrium and at the observed
temperature and pressure was weighed.
By means of a manometer assembly, to
which the bubbler tube was attached,
the weight of gas absorbed at successively lower pressure was measured.
Eventually the pressure was reduced
to that of the component (2). The
refractive index, and the infrared
spectrum of the residue showed it to
be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS: 1. Sulfur dioxide was the best

- grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

220	Sulfur Dioxide Solubilities					
COMPONENTS:		ORIGINAL MEASUREMENTS:				
1. Sulfur d	ioxide; SO ₂ ; [7446-09-5]	Lloyd, S.J.				
2. Acetic a [108-24-	cid, anhydride; C₄H6O3; 7]	J. Phys. Chem. <u>1918</u> ,22,300-302.				
VARIABLES:		PREPARED BY: W. Gerrard.				
EXPERIMENTAL	VALUES:	· L				
T/K	Weight of SO₂ *Specu per dm³ of solution/g. *Mole rat	lative values io, $SO_2/Comp.(2)$ *Mole fraction (as for 1 atm) x_{SO_2}				
268.15 273.15		0.342 0.255 0.247 0.198				

760 mmHg = 1 atm = 101.325 kPa

* Calculated by compiler by assuming that the volume of solution is the same as the volume of the component (2) before absorption of gas.

(0.220)

0.225

0.200

0.187

0.173

0.162

0.147

** Based on the original author's statement that the specific gravity of the "saturated acetic anhydride solution" is 1.22 at 273.15 K.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

278.15

283.15

288.15

293.15

298.15

Gas was bubbled through component (2) in a long graduated tube of small diameter. After equilibrium had been attained at a total pressure of about 1 atm (barometric pressure, 756-760 mmHg), the volume of the solution (about 5 cm³) was measured, and the weight of absorbed sulfur dioxide was determined by an iodometric titration.

136

122

114

106

99

90

SOURCE AND PURITY OF MATERIALS:

(1) Prepared from concentrated sulfuric acid and a saturated aqueous solution of sodium bisulfite. Dried by sulfuric acid and phosphorus pentoxide.

(0.181)**

0.184

0.167

0.157 0.148

0.139

0.128

(2) Distilled, dried by calcium chloride, and redistilled before use.

ESTIMATED ERROR:

Other organic compounds containing oxygen 221 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. Nippon Kagaku Zasshi 2. Acetic acid anhydride; C4H6O3; 1968, 89, 362-368. [108-24-7]VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Vapor pressure of acetic anhydride = 0.006 atm

Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c	_l c,d	Mole ratio	Mole fraction ^e
_S a,b	α	α			
136.8	125.2	120.7	120.1	0.607	0.378

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION .-

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: (a) static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5;$ $\delta x_{SO_3} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

 $^{^{}m d}$ $_{
m \alpha}$ = l(1 - $p_{
m s}^{\circ})$ where $p_{
m s}^{\circ}$ is the vapor pressure of solvent.

e Calculated by compiler.

COMPONENTS:

- 1. Sulfur dioxide; SO₂; [7446-09-5
- Acetic acid, anhydride; C₄H₆O₃; [108-24-7]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. <u>1972</u>, 22,623-650.

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total pressure /mmHg	Mole ratio SO ₂ /Component (2)	*Mole fraction ^x SO₂
273.15	760	3.08	0.753
	747	2.89	0.743
	649	2.33	0.700
	526	1.69	0.628
	448	1.35	0.574
	357	1.03	0.507
	253	0,703	0.413
	149	0.405	0.288
	70	0.183	0.155
283.15	747	1.57	0.611
293.15	747	0.95	0.487
298.15	747	0.76	0.432

NOTE: The plot of pressure vs solubility given in the original paper is based on the above data.

760 mmHg= 1 atm = 101.325 kPa.

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

	ORIGINAL MEASUREMENTS:		
7446-09-5]	Nitta, T.; Kido, O.; Katayama, T.,		
	J. Chem. Engng. Japan, <u>1976</u> ,9,317-8.		
<u> </u>	PREPARED BY:		
	C.L. Young		
P/bar	Mole fraction of sulfur dioxide in liquid, x SO2		
0.0547 0.2004 0.7366 1.213 1.628 2.029 2.572 2.908	0.0411 0.1430 0.3940 0.5378 0.6388 0.7288 0.8350 0.9061		
AILTTI TAD	Z INFORMATION		
AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS.		
ase Y given lar to	SOURCE AND PURITY OF MATERIALS: 1. Seitetsu Chemical Co. sample, purity better than 99.9 mole per cent. 2. Merck analytical grade sample.		
	0.0547 0.2004 0.7366 1.213 1.628 2.029 2.572		

224 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Lenoir, J-Y.; Renault, P.; Renon, H. 1. Sulfur dioxide, SO₂; [7446-09-5] J. Chem. Eng. Data 1971, 16,340-342. 4-Methyl-1,3-dioxolan-2-one, (Propylene carbonate); C4H6O3; [108 - 32 - 7]**VARIABLES:** PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa.*Mole fraction at Henry's Constant T/K 1 atm H_{SO2}/atm 298 1.20 0.833

Calculated by compiler assuming a linear function of p_{SO_2} vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$.

3.17

The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x \to \infty} \frac{f_{SO_2}(P,T)}{x_{SO_2}}$.

 x_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition of pressure and temperature. H_{SO2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

343

A conventional gas-liquid chromatographic unit was used. The chromatograph was an IGC 12 M Intersmat model, equipped with a thermal conductivity detector. The temperature control was stated to be within 2. Provided by Touzart & Matignon ±0.1°C. The pressure drop in the column was measured by a mercury manometer. Helium was the carrier gas.

There is serious uncertainty in the estimation of accuracy.

SOURCE AND PURITY OF MATERIALS:

0.315

- 1. Sulfur dioxide was provided by l'Air Liquide, and had a stated purity of 99.9%. It was used as provided.
- and Serlabo, and stated to have a minimum purity of 99%. Distill-ation was carried out when necessary, and the refractive index was measured.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Benoit, R.L.; Milanova, E. Can. J. Chem., 1979, 57, 1319-1323 4-Methyl-1,3-dioxolan-2-one, (Propylene carbonate); C4H6O3; [108-32-7] VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: Henry's law constant T/K H/atm 1.51 298.15 Defined in the original as H = partial pressure of sulfur dioxide mole fraction of sulfur dioxide AUXILIARY INFORMATION ~ METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Few details given. Pressure measured with quartz spiral gauge. Partial Liquid Air, purity 99.98 mole per pressure calculated assuming Raoult's law. Concentration of sulfur dioxide 2. Dried over 4A molecular sieve determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.2 to 1.0 mol 1 1 ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 4\%$ (estimated by compiler) REFERENCES:

ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. Nippon Kagaku Zasshi 2. Cyclic ethers 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Vapor pressure of 1,4-Dioxane = 0.032 atm Absorption Bunsen Bunsen Mole Mole _ℓc,d

coefficient, c coefficient, b fractione ratio coefficient, $s^{a,b}$ Tetrahydrofuran; C4H8O2; [109-99-9] 0.550 0.355 1,4-Dioxane; C₄H₈O₂; [123-91-1] 248.6 257 238.2 0.95 0.487 264.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_3} = \pm 5\%$ (estimated by compiler).

^a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Determined by static absorption method.

Determined by flow method.

 $[\]alpha = \ell(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Benoit, R.L.; Milanova, E. 2. Can. J. Chem., 1979, 57, 1319-1323 Tetrahydrofuran; C4H8O; [109-99-9] VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: Henry's law constant T/K H/atm 298.15 0.392 + Defined in the original as partial pressure of sulfur dioxide mole fraction of sulfur dioxide AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Few details given. Pressure measured with quartz spiral gauge. Partial 1. Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per pressure calculated assuming Raoult's cent. law. Concentration of sulfur dioxide 2. Dried over 4A molecular sieve determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.1 to 0.9 mol 1.1 from 0.1 to 0.9 mol 1 ESTIMATED ERROR: $\delta T/K = +0.1$; $\delta H/atm = +4$ % (estimated by compiler) REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W. 2. 1,4-Dioxane; C₄H₈O₂; [123-91-1] J. Appl. Chem. Biotechnol. 1972, 22, 623-650. **VARIABLES:** PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: T/K Mole ratio *Mole fraction Pressure, total SO₂/dioxane x_{SO_2} mmHg 1.75 0.636 760 288.15 760 mmHg = 1 atm = 101.325 kPa.* Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide was bubbled into a Sulfur dioxide was the best weighed amount of component (2) in a grade contained in a small bubbler tube as described in detail, cylinder. Its high purity was diagram given, in the original paper. attested by the measurement of The amount of gas absorbed at vapor pressure from 258 to 268 K. equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to The best obtainable specimen was carefully purified and rigorwhich the bubbler tube was attached, ously attested. the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The ESTIMATED ERROR: refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2). REFERENCES:

		0.90	
COMPONENTS:			ORIGINAL MEASUREMENTS:
l. Sulfur d	lioxide, SO ₂ ; [7446-09-5]	Nitta, T.; Kido, O.; Katayama, T.;
2. 1,4-Diox	ane; C ₄ H ₈ O ₂ ; [123-91-1]	J. Chem. Engng. Japan. <u>1976</u> ,9,317-8
VARIABLES:		•	PREPARED BY:
Pr	essure		C.L. Young
EXPERIMENTAL V	ALUES:		
	т/к	P/bar	Mole fraction of sulfur dioxide in liquid, $x_{\rm SO_2}$
	293.15	0.0720 0.1108 0.1477 0.2329 0.3976 0.6514 1.139 1.624 2.220 2.824	0.0920 0.1645 0.2162 0.2996 0.3988 0.4960 0.6102 0.6928 0.7829 0.8789
		AUYTITADV	INFORMATION
METHOD			
Static me ion estima details q	thod liquid pha ated by iodomet iven in source o that used in	try. Few method	SOURCE AND PURITY OF MATERIALS: 1. Seitetsu Chemical Co. sample, purity better than 99.9 mole per cent. 2. Nakarai Chemicals Ltd. sample,
			ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta P/bar = \pm 0.001$ (up to 1.3 bar), ± 0.005 (above 1.3 bar); $\delta x_{SO_2} = \pm 1.5\%$ REFERENCES: Quitzich K.; Ulbrecht, H.; Geiseler, G. Z. Physik Chem. 1967,234,33.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Benoit, R.L.; Milanova, E.
 Acetic acid, ethyl ester (ethyl acetate); C₄H₈O₂; [141-78-6] 	Can. J. Chem., <u>1979</u> , 57, 1319-1323
VARIABLES:	PREPARED BY: C.L. Young
EXPERIMENTAL VALUES:	
T/K	Henry's law constant ⁺ H/atm
298.15	1.09
H = <u>partial pressure of su</u> mole fraction of sul	lfur dioxide fur dioxide
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Few details given. Pressure measured with quartz spiral gauge. Partial pressure calculated assuming Raoult's law. Concentration of sulfur dioxide determined by iodometric titration.	Liquid Air, purity 99.98 mole per cent.
Concentration of sulfur dioxide range from 0.1 to 0.5 mol 1 ⁻¹	

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide, SO_2 ; [7446-09-5] Yuferev, R.F.; Maluigin, P.V. 2. 1,1'-Oxybisethane, (Diethylether); C4H10O; [60-29-7] Z. Chim. Prom. 1930, 7, 553-555 VARIABLES: PREPARED BY: W. Gerrard Temperature EXPERIMENTAL VALUES: Volume of SO₂ *Mole ratio T/K Weight of SO₂ per *Mole per cm3 of cm3 of solvent g SO2/diethyl fraction solvent cm3 ether. x_{SO_2} 1.090 381.51 1.712 0.631 273.15 0.457 291.65 0.2828 98.98 0.314 Ether saturated with water; 288.33 273.15 0.8238 291.65 0.3252 113.82 * Calculated by compiler. AUXILIARY INFORMATION ~ METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Sulfur dioxide was dried by Sulfur dioxide was passed into 5 cm³ of ether until saturated. The sulfuric acid. Whole solution was then transferred to a stoppered flask containing an aqueous solution of I_2 + KI. The The ether was dried over "calcined potash," and then over sodium, distilled, and sulfuric acid formed was determined stored over sodium. gravimetrically. The total pressure Was presumably 1 atm; but this was not stated. ESTIMATED ERROR: REFERENCES:

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] 2. 1,1'-Oxybisethane, (Diethyl ether); C₄H₁₀O; [60-29-7] VARIABLES: Pressure ORIGINAL MEASUREMENTS: Nitta, T.; Itami, J.; Katayama, T., J. Chem. Engng. Japan, 1973, 6, 303-9. PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	p/mmHg+	p/kPa+	Mole fraction of sulfur dioxide in liquid,
			^x so₂
293.15	635.9 761.3 887.0 1049 1269 1551 1804 2209	84.78 101.5 118.3 139.9 169.2 206.8 240.5 294.5	0.2209 0.3058 0.3696 0.4542 0.5496 0.6490 0.7342 0.8960

⁺ Total pressure

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with magnetic stirrer. After equilibrium established, pressure measured with Bourdon gauge and approximately 2 cm³ of liquid analysed by iodometric titration.

- SOURCE AND PURITY OF MATERIALS:
- Seitetsu Chemical Co. sample purity better than 99.9 mole per cent.
- 2. Merck Uvasol spectral grade.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$; $\delta p/kPa = \pm 0.5$; $\delta x_{SO_2} = \pm 1\%$ (estimated by compiler)

COMPONENTS:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 2-Furanmethanol (furfuryl alcohol);
 C5H6O2; [98-00-0]
 Tetrahydro-2-furanmethanol

Tetrahydro-2-furanmethanol (tetrahydrofurfuryl alcohol); C₅H₁₀O₂; [97-99-4]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of 2-Furanmethanol = 0.001 atm Vapor pressure of Tetrahydro-2-furanmethanol = 0.001 atm

Absorption coefficient, $s^{a,b}$	Bunsen b coefficient, α	Bunsen coefficient, c	_l c,d	Mole ratio	Mole fraction ^e		
		2-Furanmethanol					
96	86			0.335	0.251		
Tetrahydro-2-furanmethanol							
184	167	160.0	165.8	0.724	0.420		

- a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.
- b Determined by static absorption method.
- C Determined by flow method.
- d α = l(1 p_s°) where p_s° is the vapor pressure of solvent.
- e Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodo-The vapor metric titration. pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

234 Sulfur Dioxide Solubilities ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. Nippon Kagaku Zasshi 2. Ethers 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Vapor pressure of diisopropyl ether = 0.202 atm Vapor pressure of 1,2-dimethoxyethane = 0.056 atm Mole Absorption Bunsen Bunsen Mole coefficient, b coefficient, c & c,d fractione coefficient, $s^{a,b}$ [60-29-7] 1,1'-Oxybisethane (diethyl ether); C4H10O;

Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

38.9

1,2-Dimethoxyethane (ethylene glycol dimethyl ether); $C_4H_{10}O_2$; [110-71-4] 226.0

2,2'-Oxybispropane (isopropyl ether);

Dimethoxymethane (methylal); C₃H₈O₂;

37.4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

32.85

230.4

Two techniques were used: (a) static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

C6H14O;

[109-87-5]

31.0

215.0

1. Purity 99.0-99.8 mole per cent.

0.407

0.190

0.550

0.507

[108-20-3]

0.235

1.22

1.03

ESTIMATED ERROR:

 $\delta x_{SO_3} = \pm 5\%$ $\delta T/K = \pm 0.5;$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

 $[\]alpha = \ell(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

Other organic compounds containing oxygen COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7746-09-5] Lenoir, J-Y.; Renault, P.; Renon, H. J. Chem. Eng. Data. 1971, 16, 340-342 Phenol; C₆H₆O; [108-95-2] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: T/K Mole fraction " Henry's constant H_{SO},/atm at 1 atm 7.07 0.141 323 Calculated by compiler assuming a linear function of p_{SO_2} vs x_{SO_2} i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$. The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x \to \infty} \frac{f_{SO_2}(P,T)}{x}$ x_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition" of pressure and temperature. H_{SO_2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit was used. The chromatograph was an IGC 12 M Intersmat model, equipped with a thermal conductivity detector. The temperature control was stated to be within The temperat-±0.1° C. The pressure drop in the column was measured by a mercury manometer. Helium was the carrier gas.

There is serious uncertainty in the estimation of accuracy.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was provided by l'Air Liquide, and had a stated purity of 99.9%. It was used as provided.
- 2. Provided by Touzart & Matignon and Serlabo, and stated to have a minimum purity of 99%. Distillation was carried out when necessary, and the refractive index was measured.

1	Ξ	ST	IM	ATE	D ER	ROR:

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H.; Nakamoto, Y. 2. Phenol; C₆H₆O; [108-95-2] Nippon Kagaku Zasshi 1,2-Benzenediol (1,2-Cresol); C₆H₆O₂; [120-80-9] 2-Methoxyphenol (Guaiácol); C₇H₈O₂; [90-05-1] VARIABLES: PREPARED BY: C. L. Young

EXPERIMENTAL VALUI	ES: T/°C =	= 30 T/K	< = 303		
Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c, f	¿c,d	Mole ratio	Mole fraction ^e
s ^a ,b	α	α			
		Phenol			
75.1	68.6	68.1	68.1	0.273	0.214
	1,2	2-Benzenediol			
75.0	68.3	68.0	68.0	0.315	0.240
	2-M	Methoxyphenol			
108	98.4	-	-	0.489	0.328

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

 $^{^{\}rm d}$ α = $\ell(1 - p_{\rm S}^{\circ})$ where $p_{\rm S}^{\circ}$ is the vapor pressure of solvent.

^e Calculated by compiler.

f Assuming the vapor pressure of phenol and 1,2-benzenediol to be negligible.

Other organic compounds containing oxygen COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. Nippon Kagaku Zasshi 2. Esters 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: T/K = 303 $T/^{\circ}C = 30$ Bunsen Mole Mole Absorption coefficient, c,f &c,d Bunsen coefficient, b fractione ratio coefficient, sa,b Dimethyl maleate (z)-2-Butenedioic acid, dimethyl ester;

 $C_6H_8O_4$; [624-48-6]

99.1

90.1

0.508

0.337

Dimethyl phthalate 1,2-Benzenecarboxylic acid, dimethyl ester; $C_{10}H_{10}O_4$; [131-11-3]

96.5

87.9

88.0

88.0 0.643 0.391

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used; static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when Calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5; \quad \delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Determined by static absorption method.

^C Determined by flow method.

 $[\]alpha = \ell(1 - p_s^{\circ})$ where p_s° is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming vapor pressure of dimethyl phthalate to be negligible.

COMPONENTS:	ORIGINAL MEASUREMENTS:				
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Weissenberger, G.; Hadwiger, H.				
2. Cyclohexanone; C ₆ H ₁₀ O; [108-94-1] or	Z. angew. Chem. <u>1927</u> , 40, 734-736.				
3-Methylcyclohexanone; C ₇ H ₁₄ O; [591-23-1]					
	PREPARED BY:				
	W. Gerrard				
THE PARTY OF THE P					
EXPERIMENTAL VALUES:					
T/K Volume of Volume of SO ₂ Comp.(2)/cm ³ absorbed/cm ³	*Mole ratio				
	(pressure assumed to be barometric)				
cyclo	hexanone				
293.15 103.24 2353.87	0.10 0.0911				
3-methylcyclohexanone					
293.15 124.6 2082.82	0.089 0.0817				
* Calculated by	compiler				
AUXILIARY	INFORMATION				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:				
Used an absorption vessel of 200 cm ³ capacity, and a vessel with a two-way tap. Simply stated that the absorptiometer was like that used by Manchot, but the reference was not cited; probably ref. (1).	No details given.				
	ESTIMATED ERROR:				
	DEPENDING				
	REFERENCES:				
	1. Manchot, W. Z. anorg. Chem.				
	<u>1924</u> , <i>141</i> , 38.				

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Cyclohexanone; C₆H₁₀O;
 [108-94-1]

1-Phenylethanone (Acetophenone); C₈H₈O; [98-86-2]

ORIGINAL MEASUREMENTS:

Sano, H. *Nippon Kagaku Zasshi*1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of cyclohexanone = 0.005 atm Vapor pressure of acetophenone = 0.001 atm

Absorption coefficient, Sa	Bunsen coefficient, α	Mole ratio	Mole fraction ^b
	Cyclohexanone		
133.4	122.1	0.567	0.362
	l-Phenylethanone		
96.4	87.9	0.460	0.315

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5; \quad \delta x_{SO_2} = \pm 5\%$

(estimated by compiler).

b Calculated by compiler.

240 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂ [7446-09-5] Gerrard, W.; "Solubility of Gases and Liquids,: Plenum Press, New York, 1976, p. 239. Cyclohexanone; C6H10O; [108-94-1] or 2-Methylcyclohexanone; C7H12O; [583-60-8] VARIABLES: PREPARED BY: Temperature W. Gerrard. EXPERIMENTAL VALUES: Weight of SO₂ Mole ratio SO₂ /Comp.(2) Mole fraction T/K Weight of component(2) x_{SO_2} Cyclohexanone (Total pressure = 1 atm) 2.0601 2.1639 0.617 283,15 1.611 293.15 2.0601 1.4730 1.100 0.521 Methyl cyclohexanone (Total pressure = 1 atm) 2.5852 1.9010 1.290 0.563 283.15 293.15 2.5852 1.3808 0.937 0.484 760 mmHg = 1 atm = 101.325 kPa.

AUXILIARY INFORMATION

METHOD:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube. The amount of gas absorbed was determined by reweighing the tube. The total pressure was barometric, very nearly l atm. See ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high degree of purity was attested by the measurement of vapor pressure from 258-268 K.
- 2. The best commercial specimen was purified and attested.

ESTIMATED ERROR:

REFERENCES:

Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22,623.

- Sulfur dioxide; SO₂; [7446-09-5]
 1,2-Ethanediol diacetate (Ethylene
- 2. 1,2-Ethanedioi diacetate (Ethytena glycol diacetate); C₆H₁₀O₂; [111-55-7] 2-Ethoxyethanol acetate (Ethylene

2-Ethoxyethanol acetate (Ethylene glycol monoethyl monoacetate); C₆H₁₂O₃; [111-15-9]

ORIGINAL MEASUREMENTS:

Sano, H. Nippon Kagaku Zasshi 1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of ethylene glycol diacetate = 0.001 atm
Vapor pressure of ethylene glycol monoethyl monoacetate = 0.002 atm

Absorption coefficient, Sa	Bunsen coefficient, α	Mole ratio	Mole fraction ^b
	Ethylene glycol dia	cetate	
150.4	137.0	0.808	0.447
	Ethylene glycol monoethyl	monoacetate	
141.7	129.4	0.786	0.440

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Calculated by compiler.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. 2. 3-Oxobutanoic acid, ethyl ester (Ethyl acetoacetate); $C_6H_{10}O_3$; [141-97-9] Nippon Kagaku Zasshi 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Mole Mole Absorption Bunsen fractionb coefficient, s^a coefficient, α ratio 0.407 0.687 133.3 120.7 a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere. b Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static absorption method consisted 1. Purity 99.0-99.8 mole per cent. of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The vapor pressure of the solvents were measured roughly and were assumed to be equal to the ESTIMATED ERROR: partial pressure of the solvent by $^{\delta x}$ so₂ $\delta T/K = \pm 0.5$; the authors when calculating the (estimated by compiler). Bunsen coefficient. REFERENCES:

- Sulfur dioxide; SO₂; [7446-09-5]
- Hexanoic acid; C6H12O2; 2. [142-62-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972, 22,

623-650

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

RIMENT	TAL VALUES:P: T/K	ressure,total /mmHg	Mole ratio SO₂/Comp.(2)	*Mole fraction ^x SO ₂
	273.15	755	0.86	0.462
	ž	** 712 660 566 206 124 45	0.824 0.690 0.521 0.143 0.076 0.028	0.452 0.408 0.343 0.125 0.0706 0.0272
	283.15	755 ***756 700 620 510 370 244 158 42	0.440 0.442 0.417 0.353 0.277 0.182 0.113 0.070 0.017	0.306 0.307 0.294 0.261 0.217 0.154 0.102 0.065 0.017
	293.15 298.15	755 755	0.276 0.25	0.216 0.200
ŧ		= 1 atm = 101.32 ed by compiler	5 kPa.	
· ·*			oility given in Ref.	(1) is based

- on these data.
- Plot of pressure vs solubility given in original paper is based on these data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268K.
- 2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

REFERENCES:

Gerrard, W. Solubility of Gases and Liquids, Plenum Press, New York, 1976.

- 1. Sulfur dioxide, SO₂; [7446-09-5]
- 2. Benzenemethanol (Benzyl alcohol); J. Chem. Eng. Data 1971, 16,340-342. C7H8O; [100-51-6]

ORIGINAL MEASUREMENTS:

Lenoir, J-Y.; Renault, P.; Renon, H.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

760 mmHg = 1 atm = 101.325 kPa.

T/K

Henry's Constant H_{SO2}/atm

*Mole fraction at 1 atm

298

2.08

0.481

* Calculated by compiler assuming a linear function of p_{SO_2} vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$.

The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x_{SO_2} \to 0} \frac{f_{SO_2}(P,T)}{x_{SO_2}}$

 H_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition" of pressure and temperature. H_{SO_2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit was used. The chromatograph was an IGC 12 M Intersmat model, equipped with a thermal conductivity detector. The temperature control was stated to be within ±0.1°C. The pressure drop in the column was measured by a mercury manometer. Helium was the carrier gas. There is serious uncertainty in the estimation of accuracy..

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was provided by 1'Air Liquide, and had a stated purity of 99.9%. It was used as provided.
- 2. Provided by Touzart & Matignon and Serlabo, and stated to have a minimum purity of 99%. Distillation was carried out when necessary and the refractive index was measured.

ESTIMATED ERROR:

0.267

Other organic compounds containing oxygen 245 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. Benzoic acid, methyl ester (methyl benzoate); C₈H₈O₂; Nippon Kagaku Zasshi 1968, 89, 362-368. [93-58-3] VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Vapor pressure of methyl benzoate = 0.001 atm Absorption Bunsen Mole Mole fractionb coefficient, Sa coefficient, α ratio

65.5 *

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

72.1

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The vapor pressure of the cally. solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

0.365

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta x_{SO_2} = \pm 5\%$ $\delta T/K = \pm 0.5;$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Calculated by compiler.

246 Sulfur Dioxide Solubilities ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 2. 2-Hydroxybenzoic acid, methyl ester (methyl salicylate); 1968, 89, 369-373. C₈H₈O₃; [119-36-8] VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Mole Mole Absorption Bunsen fractionb coefficient, Sa ratio coefficient, α 0.306 76.7 0.441 84.3 a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere. b Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Purity 99.0-99.8 mole per Static absorption method consisted of equilibrating solvent and sulfur cent. dioxide in a 50 ml flask and measuring the absorption volumetri-

The vapor pressure of the cally. solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

- Sulfur dioxide; SO₂; [7446-09-5]
- 2-Hydroxybenzoic acid, methyl ester; (methyl salicylate) C₈H₈O₃; [119-36-8]

ORIGINAL MEASUREMENTS:

Gerrard, W. J. Appl. Chem.

Biotechnol. 1972, 22,623-650.

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure, total /mmHg	Mole ratio SO ₂ /Component (2)	*Mole fraction ^x SO ₂	
273.15	761	2.21	0.688	
	** 616 477 289 146	1.43 0.949 0.477 0.222	0.588 0.487 0.323 0.182	
283.15	761	1.03	0.507	

760 mmHg'= 1 atm = 101.325 kPa.

- Calculated by compiler
- The plot of pressure and solubility given in the original paper, and that in Ref. (1) are based on these data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- 2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

REFERENCES:

1. Gerrard, W. Solubility of Gases and Liquids, Plenum Press, New York, 1976.

Sulfur Dioxide Solubilities 248 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. 2. Aromatic ethers Nippon Kagaku Zasshi 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young **EXPERIMENTAL VALUES:** $T/^{\circ}C = 30$ T/K = 303Vapor pressure of methoxybenzene = 0.004 atm Absorption Bunsen Mole Mole Bunsen coefficient, b coefficient, c,f &c,d fractione ratio coefficient, sa,b 1,1'-(Methoxymethylene)bisbenzene (benzyl ether); C14H14O; [1016-09-7] 63.3 63.3 0.549 0.354 Methoxybenzene (anisole); C7H8O; [100-66-3] 87.8 87.5 0.424 0.298 86.8 94.9 a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: (a) static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

^C Determined by flow method.

 $[\]alpha = \ell(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming vapor pressure of benzyl ether is negligible.

- Sulfur dioxide; SO₂; [7446-09-5]
- Ethoxybenzene , (phenetole); $C_8H_{10}O;$ [103-73-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972, 22, 623-650.

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Pressure, total /mmHg	Mole ratio SO ₂ /Comp.(2)	*Mole fraction ^x SO ₂	
 273.15	760	2.10	0.677	
	** 715 665 600 480 390 252 148	1.81 1.57 1.27 0.874 0.664 0.375 0.213	0.644 0.611 0.559 0.466 0.399 0.273 0.176	
283.15	760	0.93	0.482	

760 mmHg = 1 atm = 101.325 kPa.

- * Calculated by compiler
- ** Data on which the graph in the original paper is based.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

- SOURCE AND PURITY OF MATERIALS:
- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was 2. carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS:		ORIGINAL MEASUREMENTS:		
1. Sulfur dioxide; SO ₂ ;	[7446-09-5]	Albright, L.F.; Shannon, P.T.;		
2. 2-Octanone; C ₈ H ₁₆ O; [111-13-7]	Yu, SN.; Chueh, P.L.		
		Chem. Engng. Prog. Symp. Ser. 1963.		
		59, (44), 66-74.		
VARIABLES:		PREPARED BY:		
Temperature, pressure		C.L. Young.		
EXPERIMENTAL VALUES:				
т/к	P/bar	Mole fraction of sulfur dioxide in liquid, so ₂		
298.14	1.14 2.03 3.45	0.402 0.609 0.854		
310.93	1.63 2.98 5.01	0.400 0.604 0.854		
338.71	3.41 6.04 6.10 10.67	0.389 0.587 0.594 0.845		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURL:

Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).

SOURCE AND PURITY OF MATERIALS:

 and 2. Commercial grade samples, no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta P/bar = \pm 0.3$; $\delta x_{SO_2} = \pm 1$ %.

- 1. Albright, L. F.; Shannon, P. T.;
 Terrier, F.; Chueh, P. L.
 Am. Inst. Chem. Engrs. J.
 1962, 8, 668.
- 2. Albright, L. F.; Buclez, P. C.; Pluche, C. R.; Doody, T.C. ASHRAE Trans. 1960, 66, 423.

Other organic compounds containing oxygen 251 COMPONENTS: ORIGINAL MEASUREMENTS: Hill, A.E.; Fitzgerald, T.B. 1. Sulfur dioxide; SO₂; [7446-09-5] J. Am. Chem. Soc. 1935, 57,250-254. 2. 1,1'-Oxybisbutane, (dibutyl ether); C₈H₁₈O; [142-96-1] VARIABLES: PREPARED BY: W. Gerrard **EXPERIMENTAL VALUES:** "Const.of *Mole Ratio T/K Weight of SO₂ Total pressure, Mole Henry" K P, mmHg SO₂/ ether fraction absorbed by 5 cm3 of ether, (Note) x_{SO_2} 11.0 293.15 0.0 87.5 1.00 0.040 0.0389 0.0764 170.5 1.04 0.082 0.0755 0.1541 0.121 1.05 0.108 0.2291 250.1 0.3128 332.4 1.03 0.166 0.142 0.3960 413.5 1.02 0.210 0.173 483.5 0.252 0.201 0.99 0.4762

760 mmHg = 1 atm = 101.325 kPa

* Calculated by compiler.

NOTE: p_{SO_2} is taken to be p_{total} - 11.0 mmHg throughout. This

cannot be strictly correct.

NOTE: "Constant of Henry's Law", $K = p_{SO_2}/W$

W = Milligrams SO₂ absorbed by 5 cm³ of the ether.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

The apparatus had been previously described (1).

A weighed amount of liquid was treated with a measured volume of sulfur dioxide at a constant temperature and at a measured total pressure. A gas buret and a mercury manometer were used.

SOURCE AND PURITY OF MATERIALS:

- (1) Not stated.
- (2) Purified by distillation.

ESTIMATED ERROR:

- 1. Hill, A.E.
 - J. Am. Chem. Soc. 1931, 53,2598.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 1,4-Dimethoxybenzene (hydroquinone
 dimethy1 ether); C₈H₁₀O₂;
 [150-78-7]
 - 1,3-Dimethoxybenzene (recordinol dimethyl ether); C₈H₁₀O₂; [151-10-0]
 - 1,1'-Oxybis(2-methoxyethane)

VARIABLES:

 $(diglyme); C_6H_1 + O_3; [111-96-6]$

ORIGINAL MEASUREMENTS:

Sano, H. Nippon Kagaku Zasshi 1968, 89, 362-368.

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of 1,1'-Oxybis(2-methoxyethane) = 0.002 atm

Absorption coefficient, S ^a	Bunsen coefficient, α	Mole ratio	Mole b fraction
	1,4-Dimethoxybe	enzene	
116.2	105.5	0.625	0.385
	1,3-Dimethoxybe	enzene	
102.6	96.3	1.02	0.505
	1,1'-Oxybis(2-metho	oxyethane)	
177.6	96.3	0.345	0.257

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Calculated by compiler.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Acetic acid, phenylmethyl ester,
 (benzyl acetate); C₉H₁₀O₂;
 [140-11-4] or Benzoic acid,
 phenylmethyl ester, (benzyl
 benzoate); C₁₄H₁₂O₂; [120-51-4]

ORIGINAL MEASUREMENTS:

Gerrard, W.; "Solubility of Gases and Liquids," Plenum Press, New York, 1976, p. 239.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Weight of Component(2) g	Weight of absorbed,	g $SO_2 / Comp(2)$	
		Acetic a	acid, phenylmethyl	ester
293.15	6.1630	2.4370	0.928	0.481
		Benzoic	acid, phenylmethyl	ester
293.15	7.2841	1.5875	0.723	0.420

760 mmHg = 1 atm = 101.325 kPa

AUXILIARY INFORMATION

METHOD:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube. The amount of gas absorbed was determined by reweighing the tube. The total pressure was barometric, very nearly 1 atm. See ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high degree of purity was attested by the measurement of vapor pressure from 258-268 K.
- 2. The best commercial specimen was purified and attested.

ESTIMATED ERROR:

REFERENCES:

 Gerrard, W. J. Appl. Chem. Biotechnol. <u>1972</u>, 22,623.

254	Sulfur Dioxide Solubilities					
COMPON	ENTS:			ORIGINAL MEASUREMEN	TS:	
1.	Sulf	ur dioxide;	SO ₂ ; [7446-09-5]			
2.	hepta		bicyclo [2.2.1] (Camphor); 9-3]	Ann. Chim. Phys Information rej J. Prakt. Chem	peated in :	
				e. Hako. onem	1045, 10,25	0 301.
VARIA	RLES:			PREPARED BY:		
\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \						
i				W. G.	errard.	
EXPERI	MENTAL	VALUES:	760 mmHg = 1 atm	= 101.325 kPa.	······	
	T/K	Pressure,	Weight of SO ₂ /	*Mole fraction	* ^x so ₂	* [#] SO ₂
		total /mmHg.	100 g camphor	^x SO ₂	(700 mmHg)	(760mmHg)
	297	524 650	25.5 30.8	0.377 0.423		
1		745	35.4	0.423	(0.440)	(0.46)
	294	670	34.7	0.452	(0 472)	
	293 288.6	730 355	39.7 28.0	0.485 0.399	(0.472)	
		744	47.6	0.531	(0.513)	(0.536)
	287	611 738	40.4 48.6	0.490 0.536	(0.526)	(0.543)
ļ	285.6		37.3	0.470	(0,320)	(0.543)
		703	49.1	0.538	(0.505)	(0.555)
	283	727 320	50.5 31.7	0.545 0.429	(0.537)	(0.555)
	203	560	42.6	0.503		
		720	55.8	0.570	(0.562)	(0.582)
	281	304 503	33.0 42.0	0.439 0.499		
		682	57.4	0.577	(0.582)	(0.605)
	277	490	46.0	0.522	(0.000)	(0.5-5)
	275	720 469	73.6 48.4	0.636 0.535	(0.626)	(0.656)
		650	72.0	0.631	-	(0.690)
	* Calc weight column gray	umn for x_{50}	compiler. The co f Bineau estimate (760 mmHg) show	lumn x_{SO_2} (700 m) d for x_{SO_2} 700 m) s a value read f	mHg) is based Hg. The corr rom the compi	on the responding ler's
			AUXILIARY	INFORMATION		
METHO	D/APPAF	RATUS/PROCEDUR	Ε:	SOURCE AND PURITY	OF MATERIALS:	
	No	o informatio	on	No infor	mation.	
				ESTIMATED ERROR:		
				DEPENDENCES.	· · · · · · · · · · · · · · · · · · ·	
				REFERENCES:		

COMPONENTS: ORIGINAL MEASUREMENTS: Schulze, H. 1. Sulfur dioxide; SO₂; [7446-09-5] 2. 1,7,7-Trimethylbicyclo [2.2.1] J. Prakt. Chem. 1881, 24, 168-183. heptan-2-one, (Camphor); C10H16O; [464-49-3] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa.*Mole fraction *Mole ratio T/K Weight of SO2 / 1 g of Comp. (2) $SO_2/Comp.(2)$ ^xso₂ 0.880 2.090 0.676 273.15 * Calculated by compiler. Pressure of SO₂ stated to be 725 mmHg. 1 Volume of camphor absorbed 308 volumes of SO2. Schulze quoted three values by Bineau; but one NOTE: reference was wrong, and the other did not appear to apply. Bineau's data have been compiled. Markham and Kobe (1) cited only the Bineau group; but attributed it to Schulze. Bineau's name was not mentioned. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD/APPARATUS/PROCEDURE: The gas was passed into a weighed amount of liquid camphor in a thin-No details given. walled test-tube fitted with a rubber stopper carrying an inlet tube and an out-let tube. The testtube was cooled in melting snow. The amount of gas absorbed was determined by weighing. ESTIMATED ERROR: REFERENCES: 1. Markham, A.E.; Kobe, K.A. Chem. Rev. 1941, 28, 519.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. 2. 1,7,7-Trimethylbicyclo[2.2.1]heptan-2-one (camphor); C₁₀H₁₆O; [76-22-2] or [464-49-3] Nippon Kagaku Zasshi 1968, 89, 362-368. **VARIABLES:** PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Mole fractiona Bunsen coefficient, α Mole ratio 99.0 0.670 0.401 a Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static absorption method consisted 1. Purity 99.0-99.8 mole per of equilibrating solvent and sulfur cent. dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the ESTIMATED ERROR: partial pressure of the solvent by $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ the authors when calculating the (estimated by compiler). Bunsen coefficient. REFERENCES:

EXPERIMENTAL VALUES:

	T/K	=	29:	3.	15
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	1/11 450145		
"Percent solution of camphor"	Solvent	Vol. of 1 mole of mixture /cm³	Vol. SO ₂ absorbed /cm ³ mol ⁻¹ (soln)
10	*Tetrahydro- naphthalene C ₁₀ H ₁₂ ; [119-64-2]	141.1	1001.81
10	Cyclohexanone C ₆ H ₁₀ O; [108-94-1]	111.67	1697.38
20	Cyclohexanone	120.09	1765
10	1,3-Methylcyclo- hexanol $C_8H_{16}O$;	- 130.9	2264.57
20	1,3-Methylcyclo- hexanol	- 137.18	1508.98

Tetrahydronaphthalene itself was stated to absorb no measurable volume of gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Used an absorption vessel of 200 cm³ capacity, and a vessel with a two-way tap. Simply stated that the absorptiometer was like that used by Manchot, but the reference was not cited; probably ref. (1).

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

- 1. Manchot, W.
 - Z. anorg. Chem. 1924, 141, 38:

ORIGINAL MEASUREMENTS: COMPONENTS: Albright, L.F.; Shannon, P.T., Sulfur dioxide; SO₂; [7446-09-5] Yu, S.-N.; Chueh, P.L. 2,5,8,11,14-Pentaoxapentadecane, Chem. Engng. Prog. Symp. Ser. 1963, (Tetraethylene glycol dimethyl ether); $C_{10}H_{22}O_5$; [143-24-8] 59, (44), 66-74. VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of T/K P/bar Mole fraction of T/K P/bar sulfur dioxide sulfur dioxide in liquid, x_{SO2} in liquid, x_{SO2} 298.15 0.042 0.157 310.93 5.03 0.925 0.157 0.086 0.253 338.71 0.245 0.448 0.159 0.361 0.252 0.358 0.484 0.830 0.283 1.52 0.484 0.834 0.671 3.65 0.672 2.36 0.841 0.844 0.676 2.45 3.76 3.31 0.926 7.91 0.833 0.921 310.93 0.085 0.157 10.9 366.48 0.597 0.155 0.253 0.157 0.283 0.359 1.091 0.251 0.483 1.98 0.355 0.508 1.52 0.683 2.35 0.476 0.658 0.687 7.36 1.55 0.838 14.55 0.830 3.59 0.915 20.31 0.841 3.69

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).

SOURCE AND PURITY OF MATERIALS:

1. and 2. Commercial grade samples, no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta P/bar = \pm 0.3$; $\delta x_{SO_2} = \pm 1$ %.

- Albright, L. F.; Shannon, P. T.;
 Terrier, F.; Chueh, P. L.
 Am. Inst. Chem. Engrs. J. 1962, 8, 668.
- 2. Albright, L. F.; Buclez, P. C.; Pluche, C. R.; Doody, T. C. ASHRAE Trans. 1960, 66, 423.

Other organic compounds containing oxygen				
COMPONENTS:	ONENTS: ORIGINAL MEASUREMENTS:			
 Sulfur dioxide, SO₂; 	[7446-09-5]	Albright, L.F.; Shannon, P.T.;		
<pre>2. Dodecanoic acid, eth (Ethyl laurate); C₁₄ [106-33-2]</pre>		Yu, SN.; Chueh, P.L. Chem. Engng. Prog. Symp. Ser. 1963, 59, (44) 66-74.		
VARIABLES:		PREPARED BY:		
Temperature, pr	essure	C.L. Young.		
EXPERIMENTAL VALUES:				
T/K	P/bar	Mole fraction of sulfur dioxide in liquid $^x\mathtt{SO}_2$		
298.15	1.45 2.48 3.45 3.51	0.453 0.638 0.839 0.846		
310.93	2.14 3.69 5.07 5.21	0.448 0.626 0.839 0.844		
338.71	4.30 7.10 10.78 10.87	0.432 0.615 0.828 0.841		
366.48	7.31 11.85 19.55	0.412 0.591 0.824		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).

SOURCE AND PURITY OF MATERIALS:

l and 2. Commercial grade samples, no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \ \delta P/bar = \pm 0.3; \\ \delta x_{SO_2} = \pm 18.$

- Albright, L. F.; Shannon, P. T.; Terrier, F.; Chueh, P. L. Am. Inst. Chem. Engrs. J. 1962, 8, 668.
 Albright, L.F.; Buclez, P. C.; Pluche, C. R.; Doody, T. C. ASHRAE Trans. 1960, 66, 423.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. 2. Polyethylene glycol (α -hydro- ω hydroxy-poly(oxy-1,2-ethanediyl)); (C₂H₄O)_nH₂O; [25322-68-3] Nippon Kagaku Zasshi 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Mole fractiona Mole ratio Bunsen coefficient, a 140.8 0.295 0.228 a Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static absorption method consisted 1. Purity 99.0-99.8 mole per of equilibrating solvent and sulfur cent. dioxide in a 50 ml flask and measuring the absorption volumetri-2. Molecular weight 400. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the ESTIMATED ERROR: partial pressure of the solvent by $\delta T/K = \pm 0.5; \quad \delta x_{SO_2} = \pm 5\%$ the authors when calculating the Bunsen coefficient. (estimated by compiler). REFERENCES:

- 1. Sulfur dioxide; SO₂;
 [7446-09-5]
- 2. Compounds containing nitrogen

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

December 1982

CRITICAL EVALUATION:

N, N-Dimethylformamide; C₂H₇NO; [68-12-2]

Measurements on this system have been reported by five groups of workers. The data of Gerrard (1) and Albright, Shannon, Yu and Church (2) are consistent with each other and broadly consistent with the isolated value from DuPont (3). Values of mole fraction of sulfur dioxide for smooth values of temperatures estimated from the data of refs. (1) and (2) are as follows:

T/K	273	283	293	298	303	
x_{SO_2} (total pressure = 1 atm)	0.787	0.706	0.636	0.600	0.564	
T/K	313	323	333	343	353	363
x_{SO_2} (total pressure = 1 atm)	0.494	0.425	0.363	0.307	0.259	0.218

The data of Pfeifer (4) deviate considerably from these values at low temperatures but agree at 333 K. The isolated data of Sano (5) agrees with that of Pfeifer at 303 K.

The isolated value of Benoit and Milanova (6) was determined at a low partial pressure and is not considered further as extrapolation on the basis of Henry's law to 1 atmosphere total pressure would not be valid.

Pyridine; C_5H_5N ; [110-86-1]

This system has been investigated by three groups of workers. The isolated value of Benoit and Milanova (6) was determined at a low partial pressure and is not considered further as extrapolation on the basis of Henry's law to 1 atmosphere pressure would not be valid. Gerrard's (1) data extrapolated to a partial pressure of 1 atmosphere and 303 K is broadly consistent with the value found by Sano and Nakamoto (7).

Nitrobenzene; C₆H₅NO₂; [98-95-3]

This system has been investigated by six groups of workers (1,2,5,6,8,9). The data of Lenoir $et\ al.$ (8) was determined using gas chromatography and corresponds to a very low partial pressure of sulfur dioxide. It is considerably larger than the data of Lloyd (9), Albright $et\ al.$ (2), and Gerrard (1) and is classified as doubtful. Similarly the data of Benoit and Milanova correspond to a low partial pressure of sulfur dioxide.

There is moderate agreement between the data of Gerrard (1), Albright et al. (2), and Lloyd (9). Because of the different ranges of pressure and temperature involved and the fact that considerable approximation was incurred in calculating mole fraction solubility from Lloyd's data (9), precise comparison is not possible and the data are classified as tentative. The value of Sano (5) is considerably larger than the value of Lloyd at the same temperature.

N, N-Dimethylbenzenamine; C₈H₁₁N; [121-69-7]

Hill and Fitzgerald (10) gave data for this compound as mole ratio $SO_2/Dimethylaniline$ for several pressures up to above 75 kPa at 298.15 K. Balej and Regner (11) used mixtures of nitrogen and sulfur dioxide to achieve different partial pressures of sulfur dioxide below about 35 kPa for temperatures 288 K, 293 K, 298 K and 313 K. There is qualitative agreement between the two sets of results where they overlap and both are classified as tentative. The isolated value of Sano and Nakamoto (7) is broadly consistent with the two sets of data but no precise comparison is possible.

(cont.)

- 1. Sulfur dioxide; SO₂;
 [7446-09-5]
- 2. Compounds containing nitrogen

EVALUATOR:

Colin L. Young, School of Chemistry, University of Meloburne, Parkville, Victoria 3052, Australia.

December 1982

CRITICAL EVALUATION:

References

- 1. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
- 2. Albright, L. F.; Shannon, P. T.; Yu, S.-N.; Cheuh, P. L. Chem. Engng. Prog. Symp. Ser. 1963, 59, 66.
- 3. DuPont de Nemours and Co. Chem. Eng. New 1955, 33, 2366.
- 4. Pfeifer, G. Magy. Kem. Folyoirat. 1963, 69, No. 3, 138.
- 5. Sano, H. Nippon Kagaku Zasshi 1968, 89, 362.
- 6. Benoit, R. L.; Milanova, E. Can. J. Chem. 1979, 57, 1319.
- 7. Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369.
- 8. Lenoir, J.-Y.; Renault, P.; Renon, H.J. Chem. Engng. Data 1971, 16, 340.
- 9. Lloyd, S. J. J. Phys. Chem. 1918, 22, 300.
- 10. Hill, A. E.; Fitzgerald, T. B. J. Am. Chem. Soc. 1935, 57, 250.
- 11. Balej, J.; Regner, A. Chem. Listy 1956, 50, 1374.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 2. Formamide; CH₃NO; [75-12-7] 1968, 89, 369-373. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Vapor pressure of formamide = 0.001 atm Bunsen Mole Mole Absorption Bunsen coefficient, c _ℓc,d coefficient, b fractione ratio coefficient, sa,b 160.0 159.2 158.0 0.286 0.222 175.2

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Two techniques were used: (a) static absorption method and (b) Static method conflow method. sisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodo-The vapor metric titration. pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5; \quad \delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Determined by static absorption method.

C Determined by flow method.

 $^{^{\}rm d}$ α = ℓ (1 - $p_{\rm s}^{\circ}$) where $p_{\rm s}^{\circ}$ is the vapor pressure of solvent.

e Calculated by compiler.

COMPONENTS:		01	RIGINAL MEASUREME	NTS:	
1. Sulfur dio	kide; SO ₂ ; [744	6-09-5]	Sano, H.		
2. Nitromethane; CH ₃ NO ₂ ; [75-52-5]			Nippon Kagak	u Zasshi	
Nitrobenze	ne; C ₆ H ₅ NO ₂ ; [9	98-95 - 3]	<u>1968</u> , 89, 36	2-368.	
VARIABLES:		P	REPARED BY:		-
			c.	L. Young	
EXPERIMENTAL VALUE	ES: T/°C =	 = 30	T/K = 303		-
	Vapor pressure	e of nitro	omethane = 0.04	12 atm	
Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficie	ent, c,f lc,d	Mole ratio	Mole fraction ^e
s ^{a,b}	α	α			
	Nitromethane;	CH ₃ NO ₂ ,	[75-52-5]		
150.5	142.0	149.3	3 143.5	0.531	0.347
	Nitrobenzene;	C ₆ H ₅ NO ₂ ;	[98-95-3]		
70.4	64.1	65.0	65.0	0.500	0.333

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR: $\delta x/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

 $^{^{}m d}$ $_{
m \alpha}$ = $l(1-p_{
m S}^{
m o})$ where $p_{
m S}^{
m o}$ is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming the vapor pressure of nitrobenzene is negligible.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Benoit, R.L.; Milanova, E.
 Nitromethane; CH₃NO₂; [75-52-5] 	Can. J. Chem., 1979, 59, 1319-1323
VARIABLES:	PREPARED BY:
	C.L. Young
EXPERIMENTAL VALUES:	
т/к	Henry's law constant ⁺ #/atm
298.15	2.33
AUXILIARY	1-4
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Few details given. Pressure measured with quartz spiral gauge. Partial pressure calculated assuming Raoult's law. Concentration of sulfur dioxide determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.1 to 0.8 mol 1 1	SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per cent. 2. Dried over 4A molecular sieve

	<u></u>
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] Nitriles 	Sano, H. Nippon Kagaku Zasshi 1968, 89, 362-368.
VARIABLES:	PREPARED BY:
	C. L. Young
EXPERIMENTAL VALUES:	T/K = 303
	•
Vapor pressure of be	nzonitrile = 0.001 atm
Absorption Bunsen Buns coefficient, coefficient, coeffi	en cient, c,f lc,d Mole Mole cient, fraction e
s ^{a,b} α	
Acetonitrile;	C ₂ H ₃ N; [75-05-8]
	5.7 - 0.920 0.479
Benzonitrile;	C_7H_5N ; [100-47-0]
82.9 75.3	5.8 75.7 0.509 0.337
Benzyl cyanide (Benzenead	etonitrile); C ₈ H ₇ N; [140-29-4]
98.3 89.3	0.2 90.2 0.781 0.439

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR: $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Nitriles

ORIGINAL MEASUREMENTS:

Sano, H.

Nippon Kagaku Zasshi

1968, 89, 362-368.

- a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.
- b Determined by static absorption method.
- c Determined by flow method.
- d $\alpha = l(1 p_S^{\circ})$ where p_S° is the vapor pressure of solvent.
- e Calculated by compiler.
- f Assuming the vapor pressure of benzyl cyanide is negligible.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Benoit, R.L.; Milanova, E.
2. Acetonitrile; C ₂ H ₃ N; [75-05-8]	Can. J. Chem., 1979, 57, 1319-1323
2. 100001201110, 0211311, [75 05 0]	<u> </u>
VARIABLES:	PREPARED BY:
	C.L. Young
EXPERIMENTAL VALUES:	
m /1/	Henry's law constant +
T/K	H/atm
· · · · · · · · · · · · · · · · · · ·	
298.15	1.91
250.15	1.071
+	
⁺ Defined in the original as	
H = partial pressure of sul	fur dioxide
mole fraction of sulf	ur dioxide
ΔΙΙΥΤΙΤΔΡΥ	INFORMATION
METHOD/AFFARATUS/FROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Few details given. Pressure measured	1. Anhydrous sample from Canadian
with quartz spiral gauge. Partial pressure calculated assuming Raoult's	Liquid Air, purity 99.98 mole per cent.
law. Concentration of sulfur dioxide determined by iodometric titration.	2. Dried over 4A molecular sieve
Concentration of sulfur dioxide ranged	
from 0.2 to 1.4 mol 1 ⁻¹	
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1$; $\delta H/atm = \pm 4\%$ (estimated by compiler)
	(cs cimated by compiler)
	REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:			
1. Sulfur d	dioxide; SO ₂ ; [7446-09-5]	DuPont de Nemours and Co.			
2. N,N-Dime C ₃ H ₇ NO;	ethylformamide; [68-12-2]	Chem. Eng. New. <u>1955</u> , 33, 2366.			
VARIABLES:		PREPARED BY: W. Gerrard			
EXPERIMENTAL VA	ALUES:	101.325 kPa			
2° by	olume of SO_2 (adjusted to 73.15 K and 1 atm) absorbed y 1 volume of N,N-dimethylormamide at 298.15 K and SO_2	d *Mole ratio *Mole fraction			
298.15	405	1.432 0.589			
		d_4^{25} taken to be 0.9445 g cm ⁻³			
	* Calculated by compi	ler.			
	Molar volume SO_2 at 273.15 K and 1 atm taken to be 21885 cm 3 , based on the published density.				
	AUXILIARY	INFORMATION			
METHOD/APPARATI	US/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
No stated.		Not stated.			
		ESTIMATED ERROR:			
		REFERENCES:			

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. N,N-Dimethylformamide; C₃H₇NO; [68-12-2]

ORIGINAL MEASUREMENTS:

Pfeifer, Gyula,

Magy. Kem. Folyoirat. 1963, 69, No. 3. 138-141.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

1 atm = 760 mmHg = 101.325 kPa

T/K	ml SO ₂ /g DMF	$p_{SO_2}/mmHg$	*M.R.	$*M.F.x_{SO_2}$
293.15	159	135	0.531	0.347
	177	155	0.591	0.372
	195	179	0.651	0.394
	231	225	0.772	0.435
	258	270	0.862	0.463
	284	314	0.949	0.487
	307	357	1.025	0.506
	332	401	1.109	0.526
	350	431	1.169	0.539
	382	512	1.276	0.561
	402	582	1.343	0.573
	414	660	1.383	0.580
	424	758	1.416	0.586
	428	842	1.430	0.588
	(424)	(760)	(1.416)	(0.586)
303.15	125	177	0.4175	0.295
	141	207	0.471	0.320
	160	235	0.534	0.348
	180	270	0.601	0.376
	216	334	0.721	0.419
	240	384	0.802	0.445
	262	425	0.875	0.467
	281	475	0.939	0.484
	308	641	1.029	0.507
	313	745	1.045	0.511

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known volume of gas was added to the evacuated absorption vessel containing a known amount of component (2). After equilibrium, pressure and decrease in volume of gas were measured. The vapor pressure was measured by Smith-Menzies isoteniscopic method.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was probably of acceptable purity.
- 2. Dried and distilled; $d^{20} = 0.950$ g ml⁻¹

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. N,N-Dimethylformamide; C3H7NO; [68-12-2]

ORIGINAL MEASUREMENTS:

Pfeifer, Gyula,

Magy. Kem. Folyoirat, 1963, 69, No. 3, 138-141.

EXPERIMENTAL VALUES:

1 atm = 760 mmHg = 101.325 kPa

		, , , , , , , , , , , , , , , , , , , ,	101.020 a	
T/K	ml SO ₂ /g DMF	$p_{SO_2}/mmHg$	*M.R.	*M.F. *xSO2
303.15	314	845	1.049	0.512
	(313)	(760)	(1.045)	(0.511)
313.15	124	210	0.414	0.293
	134	230	0.448	0.309
	164	292	0.548	0.354
	188	363	0.628	0.386
	214	423	0.715	0.417
	230	489	0.768	0.435
	237	511	0.792	0.442
	248	594	0.828	0.453
	254	715	0.848	0.459
	258	793	0.862	0.463
	(257)	(760)	(0.858)	(0.462)
323.15	86	225	0.287	0.223
	106	278	0.354	0.261
	117	315	0.391	0.281
	154	432	0.514	0.340
	157	454	0.524	0.344
	174	521	0.581	0.368
	192	610	0.641	0.391
	203	722	0.678	0.404
	208	795	0.695	0.410
	(205)	(760)	(0.685)	(0.406)
333.15	79 94 99 116 136 149 158 164	286 343 363 444 533 612 677 719 (760)	0.264 0.314 0.331 0.387 0.454 - 0.498 0.528 0.548 (0.558)	0.209 0.239 0.249 0.279 0.312 0.332 0.345 0.354 (0.358)

Vapor pressure, p_{DMF} , stated to be as follows:

 $\frac{T/K:}{mmHg:}$ 283.15 288.15 293.15 298.15 303.15 308.15 313.15 318.15 323.15 333.15

*M.R. Mole ratio SO₂/DMF, calculated by compiler.

*M.F. Mole fraction, x_{SO_2} , calculated by compiler.

COMPONENTS:		ORIGINAL MEASUREMENTS:	
 Sulfur dioxide; SO₂; [7446-09-5] N,N-Dimethylformamide; C₃H₇NO; [68-12-2] 		Albright, L.F.; Shannon, P.T.; Yu, SN.; Chueh, P.L. Chem. Engng. Prog. Symp. Ser. 1963, 59, (44), 66-74.	
VARIABLES:		PREPARED BY:	
Temperature, pressure		C.L. Young	
EXPERIMENTAL VALUES:	<u> </u>		
т/к	P/bar	Mole fraction of sulfur dioxide in liquid, x_{SO_2}	
298.15	0.096 0.317 1.331 2.661	0.180 0.407 0.626 0.799	
310.93	3.089 0.129 0.517 1.999 4.033	0.851 0.180 0.407 0.625 0.798	
338.71	4.654 4.585 0.328 1.489 4.420 8.494	0.850 0.851 0.180 0.406 0.620 0.793	
366.48	9.956 0.845 3.296 8.722 15.975 18.733	0.847 0.180 0.401 0.609 0.787 0.841	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).

SOURCE AND PURITY OF MATERIALS:

1. and 2. Commercial grade samples, no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta P/bar = \pm 0.3$; $\delta x_{SO_2} = \pm 1$ %.

- Albright, L. F.; Shannon, P. T.; Terrier, F.; Chueh, P. L. Am. Inst. Chem. Engrs. J. 1962, 8, 668.
- 2. Albright, L. F.; Buclez, P. C.; Pluche, C. R.; Doody, T. C. ASHRAE Trans. 1960, 66, 423.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. N, N-Dimethylformamide; C_3H_7NO ; [68-12-2]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. <u>1972</u>,22, 623-650.

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

NTAL VALUES:							
Total pressure /mmHg	Mole ratio SO ₂ /amide	Mole * fraction ^x SO ₂	T/K	Total pressure /mmHg	Mole ratio SO ₂ /amide	Mole * fraction *SO2	
760 709 611 527 330 167 100 32 22	3.70 3.47 2.89 2.48 1.69 1.13 0.844 0.504 0.417	0.787 0.776 0.742 0.712 0.627 0.531 0.458 0.335 0.294 0.187	293.15 283.15	127 760 733 670 614 530 479 368 275	0.758 0.590 2.40 2.30 2.12 1.97 1.78 1.60 1.36	0.431 0.371 0.706 0.697 0.679 0.663 0.640 0.615 0.576	
760 695 581 491 404 300	1.75 1.66 1.55 1.37 1.21 0.990	0.636 0.624 0.608 0.578 0.548 0.497	298.15	87 65 35 26	0.728 0.549 0.367 0.300 0.275	0.421 0.354 0.268 0.231 0.216	
	Total pressure /mmHg 760 709 611 527 330 167 100 32 22 7 760 695 581 491 404	Total Mole ratio SO2/amide 760 3.70 709 3.47 611 2.89 527 2.48 330 1.69 167 1.13 100 0.844 32 0.504 22 0.417 7 0.230 760 1.75 695 1.66 581 1.55 491 1.37 404 1.21	Total Mole ratio fraction SO2/amide ratio raction SO2/amide raction raction SO2/amide raction	Total Mole ratio fraction	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Total pressure ratio fraction x_{SO_2} Total pressure ratio

1 atm = 760 mmHg = 101.325 kPa.

* Calculated by compiler

 ${\hbox{{\tt NOTE}}\over\hbox{\tt given}}$ The pressure/solubility values are the basis of the plots

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component The refractive index, and (2). the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. Nippon Kagaku Zasshi Dimethylformamide; C₃H₇NO; 1968, 89, 362-368. [68-12-2] VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Mole fractiona Mole ratio Bunsen coefficient, α 0.512 1.05 303 a Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static absorption method consisted 1. Purity 99.0-99.8 mole per cent. of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the ESTIMATED ERROR: partial pressure of the solvent by $\delta T/K = \pm 0.5; \quad \delta x_{SO_2} = \pm 5\%$ the authors when calculating the (estimated by compiler). Bunsen coefficient. REFERENCES:

ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Benoit, R.L.; Milanova, E. N, N-Dimethylformamide; C₃H₇NO; [68-12-2] Can. J. Chem., 1979, 57, 1319-23 VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: T/K Henry's law constant + H/atm 0.172 298.15 ⁺ Defined in the original as H = partial pressure of sulfur dioxide mole fraction of sulfur dioxide AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Pressure measured Few details given. Liquid Air, purity 99.98 mole per with quartz spiral gauge. Partial pressure calculated assuming Raoult's cent. law. Concentration of sulfur dioxide 2. Dried over 4A molecular sieve determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.4 to 1.7 mol 1 ESTIMATED ERROR: $\delta T/K = +0.1$; $\delta H/atm = +4$ % (estimated by compiler) REFERENCES:

270			
COMPONENTS:		ORIGINAL MEASUREMENTS:	
1. Sulfur dioxide, SO ₂ ; [7446-09-5]		Albright, L.F.; Shannon, P.T.; Yu, SN. Chueh, P.L.	
2. N,N-Dimethylacetamide; C ₄ H ₉ NO; [127-19-5]		Chem. Engng. Prog. Symp. Ser. 1963, 59, (44), 66-74.	
VARIABLES:		PREPARED BY:	
Temperature, pres	sure	C.L. Young	
EXPERIMENTAL VALUES:			
т/к	P/bar	Mole fraction of sulfur dioxide in liquid, x_{SO_2}	
298.15	0.021 0.061 0.127 0.248 1.207	0.105 0.166 0.297 0.391 0.625	
310.93	2.413 0.041 0.094 0.228 0.417 1.875	0.771 0.105 0.166 0.297 0.391 0.624	
338.71	3.65 0.137 0.254 0.614 1.155 4.247	0.769 0.105 0.166 0.294 0.389 0.619	
366.48	7.708 0.399 0.665 1.517 1.551 2.613 8.239	0.763 0.105 0.166 0.291 0.293 0.383 0.611	
	14.445	0.756	
	INFORMATION		
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:	
Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).		1. and 2. Commercial grade samples, no other details given.	
		ESTIMATED ERROR: $\delta T/K = \pm 0.2; \ \delta P/bar = \pm 0.3;$ $\delta x_{SO_2} = \pm 1\%.$	
·		REFERENCES: 1. Albright, L. F.; Shannon, P. T.; Terrier, F.; Chueh, P. L. Am. Inst. Chem. Engrs. J. 1962, 8, 668. 2. Albright, L. F.; Buclez, P. C.; Pluche, C. R.; Doody, T. C. ASHRAE Trans. 1960, 66, 423.	

Organic compounds containing nitrogen			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Sano, H.; Nakamoto, Y.		
2. Amines	Nippon Kagaku Zasshi		
	<u>1968</u> , <i>89</i> , 369-373.		
	,		
VARIABLES:	PREPARED BY:		
	C. L. Young		
EXPERIMENTAL VALUES: T/°C = 30	T/K = 303		
Absorption Bunsen coefficient, Sa coefficient,	Mole Mole α ratio fraction		
1-Butanamine (butylamine); C ₄ H ₁₁ N; [109-73-9]		
_ 350	1.6 0.615		
N,N-Dibutylbutanamine (<i>tributy</i>	lamine); C ₁₂ H ₂₇ N; [102-82-9]		
206.1 187.5	2.02 0.669		
2-Aminoethanol (monoethanola)	mine); C ₂ H ₇ NO; [141-43-5]		
_ 380	1.1 0.52		
a Volume of sulfur dioxide absorberimental temperature and	orbed by unit volume of solvent at a total pressure of 1 atmosphere.		

b Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5; \delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Pyridine; C₅H₅N; [110-86-1]
 Methylpyridine (Picoline); C₆H₇N;
 [1333-41-1]
 Quinoline; C₉H₇N; [91-22-5]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Bunsen coefficient, α	Mole ratio	Mole fraction ^a
	Pyridine	
424	1.54	0.606
	Methylpyridine	
335.5	1.47	0.595
	Quinoline	
229.5	1.21	0.549

a Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted or equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Pyridine; C₅H₅N; [110-86-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972,22,

623-650.

VARIABLES:

Temperature, pressure

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

EAFERIPENIAL VALUES:				
т/к	Total pressure /mmHg	Mole ratio SO ₂ / C ₅ H ₅ N	*Mole fraction ^x SO ₂	
273.15	** 760 735 658	3.40 3.35 3.02	0.773 0.770 0.751	
	580 520 312 261	2.62 2.37 1.70 1.56	0.724 0.703 0.630 0.609	
	102	1.13	0.531	
283.15 293.15 298.15	757 757 757	2.26 1.70 1.56	0.693 0.630 0.609	,

** The plot of pressure vs solubility in the original paper is based on these data.

760 mmHg = 1 atm = 101.325 kPa.

* Calculated by compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

de Colubilities		
ORIGINAL MEASUREMENTS:		
Benoit, R.L.; Milanova, E.		
Can. J. Chem., <u>1979</u> , 57, 1319-23		
PREPARED BY: C.L. Young		
<u></u>		
Henry's law constant ⁺ H/atm		
0.088		
ulfur dioxide lfur dioxide		
INFORMATION		
SOURCE AND PURITY OF MATERIALS:		
 Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per cent. Dried over 4A molecular sieve 		
ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta H/atm = \pm 4\%$ (estimated by compiler)		

ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Sano, H. 2. 1-Methyl-2-pyrrolidinone (N-Methylpyrrolidone); C₅H₉NO; [872-50-4] Nippon Kagaku Zasshi 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Absorption Bunsen Mole Mole fractionb coefficient, Sa ratio coefficient, α 309.6 1.52 0.603 340.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The vapor pressure of the cally. solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR: $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Calculated by compiler.

282 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Lloyd, S.J. 1. J. Phys. Chem. 1918,22,300-302 2. Nitrobenzene; C6H5NO2; 198-95-31 VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: Weight of SO₂ per dm³ of T/K *Speculative values *Mole fraction (as solution /g. *Mole ratio, SO₂/Comp. (2) for 1 atm) x_{SO_2} 0.400 288.15 311.4 0.668 0.355 0.549 293.15 267.4 0.451 0.311 298.15 227.9 0.364 0.267 303.15 190.0 132.0 0.194 0.241 313.15 0.150 323.15 98.7 0.177 78.6 0.139 0.122 333.15 760 mmHg = 1 atm = 101.325 kPa* Calculated by compiler by assuming that the volume of solution is the same as the volume of the component (2) before absorption of gas.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

Gas was bubbled through component (2) in a long graduated tube of small diameter. After equilibrium had been attained at a total pressure of about 1 atm (barometric pressure, 756-760 mmHg), the volume of the solution (about 5cm³) was measured, and the weight of absorbed sulfur dioxide was determined by an iodometric titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Prepared from concentrated sulfuric acid and a saturated aqueous solution of sodium bisulfite. Dried by sulfuric acid and phosphorus pentoxide.
- (2) Distilled, dried by calcium chloride, and redistilled before use.

ESTIMATED	ERROR:
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COMPONENTS: 1. Sulfur dioxide; SO ₂ ; [7446-09-5]	ORIGINAL MEASUREMENTS: Albright, L.F.; Shannon, P.T.;	
2. Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]	Yu, SN.; Chueh, P.L. Chem. Engng. Prog. Symp. Ser. 1963, 59, (44), 66-74.	
VARIABLES: Temperature, pressure	PREPARED BY: C.L. Young	

DAT BELLEVIATE ANTOR	٠.

T/K	P/bar	Mole fraction of sulfur dioxide in liquid, x_{so_2}
298.15	1.32 2.16 3.30 3.39	0.371 0.569 0.842 0.843
310.93	1.97 3.25 5.05	0.367 0.565 0.841
338.71	4.03 6.65 10.65	0.355 0.549 0.837
366.48	7.12 11.68 19.87	0.340 0.515 0.828

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with Bourdon pressure gauge. Temperature measured with mercury in glass thermometer. The equipment used in this investigation was stated to be similar to that used in previous studies, (1), (2).

SOURCE AND PURITY OF MATERIALS:

 and 2. Commercial grade samples, no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta P/bar = \pm 0.3$; $\delta x_{SO_2} = \pm 1$ %.

- Albright, L. F.; Shannon, P. T.; Terrier, F.; Chueh, P. L. Am. Inst. Chem. Engrs. J. 1962, 8, 668.
- 2. Albright, L. F.; Buclez, P. C.; Pluche, C. R.; Doody, T. C. ASHRAE Trans. 1960, 66, 423.

ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide, SO_2 ; [7446-09-5] Lenoir, J-Y.; Renault, P.; Renon, H. Nitrobenzene; C₆H₅NO₂; J. Chem. Eng. Data. 1971, 16, 340-342 [98-95-3] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: Henry's constant Mole fraction T/K H_{SO},/atm at 1 atm 298 1.64 0.610 Calculated by compiler assuming a linear function of p_{SO_2} vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$. The authors gave "Henry's constant" as $H_{SO_2} = \lim_{n \to \infty} \frac{1}{n}$ $x_{\mathrm{SO_2}}$ is the mole fraction. $f_{\mathrm{SO_2}}$ is the fugacity of $\mathrm{SO_2}$ "in the equilibrium condition" of pressure and temperature. ${\rm H}_{\rm SO_2}$ is related to experimental chromatographic parameters based on number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A conventional gas-liquid chromato-1. Sulfur dioxide was provided by graphic unit was used. The l'Air Liquide, and had a stated chromatograph was an IGC 12 M purity of 99.9%. It was used as Intersmat model, equipped with a provided. thermal conductivity detector. The 2. Provided by Touzart & Matignon temperature control was stated to be within $\pm 0.1^{\circ}$ C. The pressure drop and Serlabo, and stated to have a minimum purity of 99%. in the column was measured by a Distillation was carried out when mercury manometer. Helium was the necessary, and the refractive carrier gas. index was measured. There is serious uncertainty in the estimation of accuracy. ESTIMATED ERROR: REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Nitrobenzene; C₆H₅NO₂;
 [98-95-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972, 22,623-650.

VARIABLES:

PREPARED BY:

Temperature, pressure

W. Gerrard

EXPERIMENTAL VALUES:

T	Y/K Pre	essure,total /mmHg	Mole ratio SO ₂ /Comp.(2)	*Mole fraction ^x SO ₂
	.15	772 772	2.0 0.878	0.667 0.468
280	.15 **	760 733 670 593 427 285 186 51	1.105 1.040 0.901 0.745 0.487 0.291 0.177	0.525 0.510 0.474 0.427 0.328 0.225 0.150 0.040
	.15 .15	772 772	0.545 0.45	0.353 0.310

** The plot of pressure vs solubility given in the original paper is based on these data.

760 mmHg = 1 atm = 101.325 kPa.

Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Benoit, R.L.; Milanova, E.
2. Nitrobenzene; C ₆ H ₅ NO ₂ ; [98-95-3]	Can. J. Chem., <u>1979</u> , 57, 1319-1323
VARIABLES:	PREPARED BY:
	C.L. Young
EXPERIMENTAL VALUES:	
т/к	Henry's law constant ⁺ H/atm
298.15	3.18
<pre>H = partial pressure of sulf mole fraction of sulf</pre>	fur dioxide ur dioxide
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Few details given. Pressure measured with quartz spiral gauge. Partial pressure calculated assuming Raoult's law. Concentration of sulfur dioxide determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.1 to 0.5 mol 1 ⁻¹	1. Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per cent. 2. Dried over 4A molecular sieve
	ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 4\%$ (estimated by compiler)
	REFERENCES:

Organic compound	is containing nitrogen	287
COMPONENTS: 1. Sulfur dioxide; SO ₂ ; [7446-09-5] 2. Benzenamine (aniline); C ₆ H ₇ N; [62-53-3] ar-Methylbenzenamine (toluidine (mixed)); C ₇ H ₉ N; [26915-12-8] ar, ar-Dimethylbenzenamine (xylidine (mixed)); C ₈ H ₁₁ N; [1300-73-8]	ORIGINAL MEASUREMENTS: Sano, H.; Nakamoto, Y. Nippon Kagaku Zasshi 1968, 89, 369-373.	
VARIABLES:	PREPARED BY:	
	C. L. Young	
EXPERIMENTAL VALUES: T/°C = 30	T/K = 303	
Bunsen coefficient, α Mole	ratio Mole fraction ^a	
Benzene	amine	
274	.14 0.534	
ar-Methylbenzenamine	(mixture of isomers)	
241		
	() ()	
ar , ar - Dimethylbenzenamin	e (mixture of isomers)	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the	1. Purity 99.0-99.8 mole per cent.	
partial pressure of the solvent by		
the authors when calculating the	ESTIMATED ERROR:	
Bunsen coefficient.	$\delta T/K = \pm 0.5; \delta x_{SO_2} = \pm 5\%$	
	(estimated by compiler).	
	REFERENCES:	

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 2. Benzonitrile; C₇H₅N; [100-47-0] 22, 623-650. VARIABLES: PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

Temperature, pressure

T/K	Pressure, /mmH		Mole ratio SO ₂ /Comp.(2)	*Mole fraction ^x SO ₂
273.15	754		2.19	0.687
	** 736		2.07	0.674
	712		1.93	0.659
	660		1.64	0.621
	577		1.30	0.565
	469		0.951	0.487
	343		0.633	0.388
	176		0.288	0.224
	71		0.0972	0.0886
283.15	754		1.01	0.502
293.15	754		0.629	0.386
298.15	754		0.50	0.333
	760	= 1 atm =	101.325 kPa.	
	* Calc	ulated by	compiler	

AUXILIARY INFORMATION

paper is based.

** Data on which the graph in the original

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibirium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- 2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED	ERROR
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ORIGINAL MEASUREMENTS:
Lloyd, S.J.
J. Phys. Chem. <u>1918</u> , 22,300-302
PREPARED BY: W. Gerrard

T/K	Weight of SO ₂ per dm ³ of	*Speculative values	
	solution /g.	*Mole ratio, SO ₂ / Comp.(2)	*Mole fraction (as for 1 atm) $x_{\rm SO_2}$
288.15	290.8	0.711	0.415
293.15	236.0	0.545	0.353
298.15	192.2	0.426	0.299
303.15	160.7	0.347	0.258
313.15	118.5	0.248	0.199
323.15	87.0	0.178	0.151
333.15	68.8	0.140	0.123

760 mmHg = 1 atm = 101.325 kPa

* Calculated by compiler by assuming that the volume of solution is the same as the volume of the component (2) before absorption of gas.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

Gas was bubbled through component (2) in a long graduated tube of small diameter. After equilibrium had been attained at a total pressure of about 1 atm (barometric pressure, 756-760 mmHg), the volume of the solution (about 5 cm 3) was measured, and the weight of absorbed sulfur dioxide was determined by an iodometric titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Prepared from concentrated sulfuric acid and a saturated aqueous solution of sodium bisulfite. Dried by sulfuric acid and phosphorus pentoxide.
- (2) Distilled, dried by calcium chloride, and redistilled before use.

ESTIMATED	ERRO	DR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. N-Methylbenzenamine,
 (methylaniline); C₇H₉N; [100-61-8]

ORIGINAL MEASUREMENTS:

Hill, A.E.; Fitzgerald, T.B.

J. Am. Chem. Soc. 1935, 57,250-254.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure, total, mmHg	Mole ratio SO ₂ / component (2)	*Mole frac	tion,
298.15	2.0 19.5 42.0 72.5 114.4 166.1 237.0 329.0 436.0 552.5 (760.0)	0.00 0.124 0.258 0.396 0.525 0.652 0.772 0.896 1.010	0.110 0.205 0.284 0.344 0.395 0.436 0.473 0.502 0.527 (0.560)	Extrapolated by compiler.

760 mmHg = 1 atm = 101.325 kPa

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

The apparatus had been previously described (1).

A weighed amount of liquid was treated with a measured volume of sulfur dioxide at a constant temperature and at a measured total pressure. A gas buret and a mercury manometer were used.

SOURCE AND PURITY OF MATERIALS:

- (1) Not specified.
- (2) Purified by distillation.

ESTIMATED ERROR:

- 1. Hill, A.E.
 - J. Am. Chem. Soc. 1931, 53,2598.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. N,N-Dimethylbenzenamine,
 (N,N-dimethylaniline); C₈H₁₁N;
 [121-69-7]

ORIGINAL MEASUREMENTS:

Hill, A.E.; Fitzgerald, T.B.

J. Am. Chem. Soc. 1935,57,250-254.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure, total mmHg	Mole ratio SO ₂ / component (2)	*Mole fraction, xSO2	
298.15	2.0 14.6 30.0 56.5 106.0 189.1 290.2 449.5 575.0 (760.0)	0.00 0.185 0.362 0.564 0.770 0.950 1.090 1.271 1.400	0.156 0.266 0.361 0.435 0.487 0.522 0.560 0.583 (0.610) Extrapolated by compiler.	·

760 mmHg = 1 atm = 101.325 kPa

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

The apparatus had been previously described (1).

A weighed amount of liquid was treated with a measured volume of sulfur dioxide at a constant temperature and at a measured total pressure. A gas buret and a mercury manometer were used.

SOURCE AND PURITY OF MATERIALS:

- (1) Not specified.
- (2) Purified by distillation.

ESTIMATED ERROR:

- 1. Hill, A.E.
 - J. Am. Chem. Soc. 1931, 53,2598.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. N, N-Dimethylbenzenamine, (N, N-dimethylaniline); C_BH₁₁N; [121-69-7]

ORIGINAL MEASUREMENTS:

Balej, J.; Regner, A. Chem. Listy, 1956, 50, 1374-1380

Collection Czech. Chem. Communs. 1956 21, 1545-1552.

VARIABLES:

PREPARED BY:

W. Gerrard

		•					
EXPERIMENT	TAL VALUES:	760		101.325	kPa.		*
T/K	^p so₂ /mmHg	Mole ratio SO /comp.(2)	* [∞] so₂	T/K	p _{SO2} /mmHg	Mole ratio SO /Comp.(2)	[*] ≈so₂
288.15	13.25 21.23 28.08 39.90 42.20 89.0 137.3 150.0 235.5	0.2238 0.3913 0.4171 0.5320 0.6225 0.7610 0.8550 0.8980 0.9150 0.9575 1.029 1.150 1.243 0.3031 0.3122 0.4240 0.5075 0.5838 0.5975 0.829 0.954 0.983 1.145 le fraction o	0.1829 0.2812 0.2943 0.3473 0.3837 0.4321 0.4609 0.4731 0.4731 0.4735 0.554 0.2379 0.2379 0.2379 0.2379 0.3666 0.3740 0.453 0.488 0.496 0.534 f SO ₂ .	298.15 313.15 * Cal	13.78 25.72 48.0 49.7 56.0 89.2 119.5 162.0 232.5 8.98 13.30 25.80 36.30 39.10 43.00 58.5 93.5 103.95 154.9 158.0 246.0	0.225 0.230 0.363 0.520 0.524 0.562 0.707 0.792 0.896 1.028 0.0703 0.0910 0.1595 0.2219 0.2346 0.2460 0.3302 0.4420 0.4606 0.5850 0.5972 0.7212 by compiler.	0.184 0.187 0.266 0.342 0.344 0.360 0.414 0.442 0.473 0.507 0.0657 0.0834 0.1376 0.1816 0.1974 0.2482 0.3017 0.3153 0.3691 0.3739 0.4190
1	5U2						

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Diagram given. See Hill and Fitzgerald (1). Separate streams of purified nitrogen and sulfur dioxide were mixed in a vessel containing glass wool covered with phosphorus pentoxide. The gaseous mixture was then passed into the absorption vessel and then to a sampling tap to enable the SO₂ content of the gas phase to be determined by an iodometric titration. The SO2 content of the solution was likewise determined. The method was described as a dynamic ESTIMATED ERROR: one.

SOURCE AND PURITY OF MATERIALS:

- Probably of satisfactory purity.
- 2. B.p. 192-193.5°C, probably at atmospheric pressure.

REFERENCES:

1. Hill, A.E.; Fitzgerald, T.B. J. Am. Chem. Soc. 1935, 57, 250.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H.; Nakamoto, Y. 2. N,N-Dimethylbenzenamine (N, N-dimethylaniline); $C_8H_{11}N;$ Nippon Kagaku Zasshi [121-69-7]1968, 89, 369-373. Benzenemethanamine (Benzylamine); C_7H_9N ; [100-46-9] VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Bunsen Mole Mole Absorption fractionb coefficient, sa coefficient, α ratio N, N-Dimethylbenzenamine 0.591 254 1.44 280

Benzylamine

288

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The vapor pressure of the cally. solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1.40

1. Purity 99.0-99.8 mole per cent.

0.583

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5; \quad \delta x_{SO_3} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Calculated by compiler.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- N-Ethylbenzenamine, (ethylaniline); C₈H₁₁N; [103-69-5]

ORIGINAL MEASUREMENTS:

Hill, A.E.; Fitzgerald, T.B.

J. Am. Chem. Soc. 1935, 57,250-254.

VARIABLES:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure, mmHg	total,	Mole ratio SO₂ / component (2	*Mole fraction, 2) **SO ₂
298.15	1.5 46.5 101.0 172.5 264.5 378.0 510.0 655.0 (760.0)	,	0.00 0.182 0.361 0.536 0.706 0.870 1.027 1.183	0.154 0.265 0.349 0.414 0.465 0.507 0.542 (0.560) Extrapolated by compiler.

760 mmHg = 1 atm = 101.325 kPa.

*Calculated by compiler.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

The apparatus had been previously described (1).

A weighed amount of liquid was treated with a measured volume of sulfur dioxide at a constant temperature and at a measured total pressure. A gas buret and a mercury manometer were used.

SOURCE AND PURITY OF MATERIALS:

- (1) Not specified.
- (2) Purified by distillation.

ESTIMATED ERROR:

- 1. Hill, A.E.
 - J. Am. Chem. Soc. 1931, 53,2598.

Organic compounds containing nitrogen COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Foote, H.W.; Fleischer, J. J. Am. Chem. Soc. 1934, 56,870-873. 2. N, N-Diethylbenzenamine, [diethylaniline); C₁₀H₁₅N; [91-66-7] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: $\mathsf{p}_{\mathsf{SO_2}}^{\mathrm{mmHg}}$ Mole fraction T/K ^xso₂ 273 1008 0.891 946 0.862 845 0.817 0.793 784

733 0.774 673 0.751 584 0.716 472 0.671 359 0.618 276 0.570 225 0.532 149 0.459 0.347 81 44 0.252 13 0.092

NOTE: A mole fraction of 0.891 is equivalent to a mole ratio of 8.17 moles of SO2 to 1 of N, N-diethyl aniline.

> 760 mmHg = 1 atm = 101.325 kPa. Observed pressure was taken to be p_{SO2}.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

The apparatus and method had been previously described (1).

A glass bulb of 29.3 cm³capacity was connected via a tap to an open manometer, a vacuum flask of 2 dm³ capacity, and a source of sulfur dioxide. Component (2) was weighed in the bulb. Sulfur dioxide was condensed in the bulb and 253 K. Equilibrium at 273.15 K and at the observed pressure, total, but assumed to be equal to p_{SO_2} , was attained.

SOURCE AND PURITY OF MATERIALS:

- Sulfur dioxide: Dried by sulfuric acid.
- (2) "The compounds used were either of Eastman C.P. grade or were purified by customary methods."

ESTIMATED ERROR:

REFERENCES:

Foote, H.W.; Fleischer, J. J. Am. Chem. Soc. 1931,53,1752

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Sulfur dioxide; SO₂; [7446-09-5] N,N-Diethylbenzenamine, (diethylaniline); C₁₀H₁₅N; [91-66-7] 	Hill, A.E.; Fitzgerald, T.B. J. Am. Chem. Soc. <u>1935</u> , 57,250-254.
VARIABLES:	PREPARED BY: W. Gerrard

EXPERIMENTAL	VALUES:			
T/K	Pressure, total, mmHg	Mole ratio SO ₂ / component (2)	*Mole fraction, x SO $_2$	
298.15	1.5 120.8 249.0 393.1 529.5 679.5	0.000 0.204 0.410 0.617 0.803 1.010	0.169 0.291 0.382 0.445 0.502	

760 mmHg = 1 atm = 101.325 kPa

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD:/APPARATUS/PROCEDURE:

The apparatus had been previously described (1).

A weighed amount of liquid was treated with a measured volume of sulfur dioxide at a constant temperature and at a measured total pressure. A gas buret and a mercury manometer were used.

(760.0)

SOURCE AND PURITY OF MATERIALS:

- (1) Not specified.
- (2) Purified by distillation.

(0.530) Extrapolated by compiler.

ESTIMATED ERROR:

REFERENCES:

1. Hill, A.E.

J. Am. Chem. Soc. 1931,53,2598

COMPONENTS:			
	ORIGINAL MEASU	REMENTS:	
<pre>1. Sulfur dioxide; SO₂; [7446-09-5]</pre>	Bogeatzes,	A. S.; Tassios,	D. P.
• • • • • • • • • • • • • • • • • • • •	Ind. Eng.	Chem. Process Des	. Develo
2. Miscellaneous solvents	<u>1973</u> , 12,	274-278.	
VARIABLES:	PREPARED BY:		
		C. L. Young	
EXPERIMENTAL VALUES:	<u> </u>	Activity	
Solvent	i	coefficient at nfinite dilution,	T/K
N, N-Dimethylaniline (N, N-Dimethylben	zonamino):		
$C_8H_{11}N$; [121-69-7]	zenamine,,	0.027	314.2
N, N-Dimethylformamide; C ₃ H ₇ NO; [68	-12-2]	0.081	313.7
N, N-Dimethylacetamide; C4H9NO; [12	7-19-5]	0.036	314.7
		0.070 0.077	339.2 366.2
W. 1		0.910	298.7
Nitrobenzene; $C_6H_5NO_2$; [98-95-3] Trimethylpyridine; $C_6H_{11}N$; [29611-	84-51	0.123	312.2
Xylidine (ar, ar-dimethylbenzenamine)	; CaH11N;	0.123	31212
[1300-73-8]		0.140	313.2
Benzonitrile; C ₇ H ₅ N; [100-47-0]		0.532	312.2
3-Methylsulfolane (tetrahydro-3-meth	ylthiophene-		
1,1-dioxide); C ₅ H ₁₀ O ₂ S; [8	72-93-5]	0.609	313.2
3-Methoxysulfolane (tetrahydro-3-met 1,1-dioxide); C5H10O3S; [2	noxytniopnene 0627-66-11	1.090	312.2
N-Methylmethanamine (Dimethylamine);	0027-00-1]	1.050	712.2
C_2H_7N ; [124-40-3] N,N'-Bis(2-aminoethyl)-1,2-Ethanedia	mine	1.590	315.2
(Triethylenetetramine); C ₆ H [112-24-3]	18N4;	1.580	314.2
Equimolar mixture of xylidine and N , N -dimethylaniline		0.040	313.2
	100		
	INFORMATION	·	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PUR	ITY OF MATERIALS:	
Gas chromatographic method.			
Activity coefficients determined	į.	ails given except	
from retention volumes of sulfur	purity better than 99 mole		
dioxide on solvents as stationary	per cer	nt.	
_	•		
phases. It is probable that the	}		
activity coefficients are in error	1		
because of the continues the country	1		
because of absorption at the carrier			
gas-solvent interface.			
	ESTIMATED ERRO	OR:	
		$\delta r = \pm 0.05.$	
			- 4.5 s.
	δT/K = ±0.2		

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Organic compounds containing halogens

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

December 1982

CRITICAL EVALUATION:

Trichloromethane; CHCl₃; [67-66-3]

Although this system has been investigated by three groups (1,2,3) the ranges of temperature and pressure of the measurements do not overlap. The measurements are broadly consistent but no precise comparison is possible.

Tetrachloromethane; CCl4; [56-23-5]

This system has been investigated by three groups. The data of Sobolev $et\ al.$ (4) is classified as doubtful, the mole fraction solubilities being considerably smaller than those of Horiuti (5) and Sano (2). The datum of Sano (2) is several per cent higher than the value obtained by interpolation of Horiuti values.

Chlorobenzene; C₆H₅Cl; [108-90-7]

The data of Horiuti (5) and Gerrard (6) for this system are in reasonable agreement. The isolated value of Sano (2) appears to be a few percent low when compared with the values of Gerrard at low temperatures.

References

- Lindner, J. Monatsh. <u>1912</u>, 33, 613.
- 2. Sano, H. Nippon Kagaku Zasshi 1968, 89, 362.
- 3. Lorimer, J. W.; Smith, B. C.; Smith, G. H. J.C.S. Faraday I <u>1975</u>, 71, 2232.
- Sobolev, I. A.; Kukarin, V. A.; Dzhagatspanyan, R. V.; Kosorotov,
 V. I.; Zogarets, P. A.; Popov, A. I. Khim. Prom. 1970, 46, 668.
- 5. Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn.) 1931/32, 17, 125.
- 6. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.

ORIGINAL MEASUREMENTS: COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Lindner, J. Trichloromethane, (chloroform); Monatsh. 1912, 33, 613-672. $CHCl_3$; [67-66-3] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa.*Mole ratio *Mole fraction Pressure. T/K Weight Weight of SO₂/mmHg $SO_2/Comp.(2)$. ^xso₂ of SO₂ solution g (sp.gr.) 160.7 (1.526) 160.3 (1.526) (2.7?)0.000857 273.15 0.0738 5.6 0.00218 0.1879 0.00858 198.1 (1.525) 22.0 0.9068 0.0373 0.0387 3.4395 169.1 (1.523) 90.2 133.0 (1.514) 219.6 0.107 0.0967 7.222 *Rational extrapolation (760) (0.540)(1.174)0.000844 160.7 (1.480) 5.7 298.15 0.0727 0.00216 0.00215 160.3 (1.480) 12.9 0.1853 0.00845 0.9008 48.0 0.00852 198.1 (1.479) 0.0382 0.0368 169.1 (1.472?) 200.2 3.3943 133.0 (1.472) 488.8 0.105 0.0950 7.0866 (0.202)(0.168)*Rational extrapolation(760) *By compiler's plot of x_{SO} , vs p_{SO} on the reference line diagram of Gerrard (1) *Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Somewhat complex arrangement of six glass vessels containing the liquid. A small sealed tube containing a weighed amount of sulfur dioxide was fitted onto each tube assembly by a flexible joint. The previously scratched tip of the tube was broken to release sulfur dioxide, and the absorption of this was encouraged by a twirling motion of the apparatus The pressure was measured manometrically. To obtain the amount absorbed, an allowance was made for the amount in the gas phase. The description of the procedure for deciding the partial pressure of the sulfur dioxide is somewhat involved, and cannot be briefly reported. One of the bulbs contained pure chloroform so that its vapor pressure at the operational temperature could be indicated.

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide may be taken as pure.
- May be taken as pure, density compared with the literature value.

ESTIMATED ERROR:

REFERENCES:

Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1976.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Trichloromethane (chloroform);
 CHCl₃; [67-66-3]

Tetrachloromethane (carbon tetrachloride); CCl4; [56-23-5]

ORIGINAL MEASUREMENTS:

Sano, H. Nippon Kagaku Zasshi

1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

$$T/^{\circ}C = 30$$

$$T/K = 303$$

Vapor pressure of trichloromethane, $p_{CHCl_3}^{\circ} = 0.272$ atm

Vapor pressure of tetrachloromethane, $p_{CC1}^{\circ} = 0.200$ atm

Absorption coefficient, Sa,b	Bunsen coefficient, b	Bunsen coefficient, α	_l c,d	Mole ratio	Mole fraction ^e
***************************************	Trich	loromethane	<u>-</u>	•••••••••••••••••••••••••••••••••••••••	
30.1	37.6	-	-	0.134	0.118
	Tetra	chloromethane			
12.3	14.0	12.2	9.8	0.061	0.0575

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of passing sulfur dioxide through a micro gas absorption tube and . estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

C Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

ORIGINAL MEASUREMENTS: COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] Lorimer, J.W.; Smith, B.C.; Smith, G.H. Trichloromethane, (chloroform); $CHCl_3$; [67-66-3] J.C.S. Faraday I, 1975, 71, 2232-50. VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of sulfur dioxide in liquid, p/mmHg in vapor, p/kPa T/K xso2 y_{SO₂} 3.44 0.459 0.000 0.0000 227.6 30.58 4.077 0.0920 0.897 0.2091 0.946 52.83 7.043 67.28 8.970 0.3154 0.961 0.3812 0.966 73.73 9.830 82.05 10.939 0.4878 0.972 0.977 0.5928 89.25 11.899 91.65 12.219 0.6335 0.979 0.984 98.81 13.174 0.7674 106.48 14.196 0.8885 0.990 1.000 116.49 15.531 1.0000 237.4 7.20 0.960 0.0000 0.000 51.50 0.0824 0.871 6.866 0.932 11.912 89.35 0.1922 116.32 15.508 0.3018 0.952 0.958 126.75 16.899 0.3590 0.966 142.74 19.030 0.4701 0.972 157.11 20.946 0.5803 162.44 0.974 21.657 0.6120 176.86 23.579 0.7577 0.981 0.8861 0.989 25.487 191.17 208.74 27.830 1.0000 1.000 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static vapor-liquid equilibrium apparatus. Total pressure measured using mercury manometers and No details given. cathetometer. Temperature measured using a sulfur dioxide vapor pressure thermometer. Some details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta p/kPa = \pm 0.01$; δx_{SO_2} , $\delta y_{SO_2} = \pm 1$ %. REFERENCES:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Trichloromethane, (chloroform);
 CHCl₃; [67-66-3]

ORIGINAL MEASUREMENTS:

Lorimer, J.W.; Smith, B.C.; Smith, G.H.

J.C.S. Faraday I, <u>1975</u>, 71, 2232-50.

T/K	p/mmHg	p/kPa	Mole fraction o in liquid,	f sulfur dioxide in vapor,
1/10	p/ natarg	p/ KI d	^x SO ₂	y _{SO₂}
249.8	16.31	2.174	0.0000	0.000
	88.56 156.27	11.807	0.0650	0.827
	211.30	20.834 28.171	0.1656 0.3019	0.909 0.940
	226.36	30.179	0.3093	0.944
	266.04	35.469	0.4274	0.957
	296.86	39.578	0.5493	0.966
	303.07	40.406	0.5708	0.968
	338.45	45.123	0.7395	0.977
	372.26	49.631	0.8816	0.987
	405.40	54.049	1.0000	1.000

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] 2. Tetrachloromethane, (Carbon tetrachloride); CCl4; [56-23-5] VARIABLES: Temperature, pressure

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn.), 1931/32, 17, 125-256.

PREPARED BY:

C. L. Young

EXPERIMENT	AL VALUES:					
т/к	P [§] /bar	Mole fraction of sulfur dioxide in liquid, "SO ₂	T/K	P [†] /bar	Mole fraction of sulfur dioxide in liquid, "SO ₂	Ostwald coefficient, L
298.15	0.1497 0.3537 0.4765 0.6776 0.7090 0.8610 0.9611 1.085 1.172 1.260 1.321	0.0000 0.0126 0.0208 0.0348 0.0371 0.0490 0.0567 0.0673 0.0748 0.0827 0.0880	283.15 298.15 313.15	0.9338 0.8585 0.7285	0.1111 0.0604 0.0342	30.96 18.45 12.52

total pressure.

Ostwald coefficient (as $x \rightarrow 0$, T/K = 298.15) = 15.1.

Henry's law constant, dp/dx (as $x \rightarrow 0$, T/K = 298.15) = 12700 mmHg = 16.93 bar

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus consisted of a gas buret, a solvent reservoir and an absorption pipet. Dry gas introduced into degassed solvent. System mixed using a magnetic stirrer until saturation Care was taken to prevent occurred. solvent vapor from mixing with gas in the gas buret. Volume of gas determined from gas buret reading; of liquid determined from height of meniscus in absorption pipet.

SOURCE AND PURITY OF MATERIALS:

- 1. Sample obtained from Nippon Sulphuric Acid Manufacturing Co. Dried and fractionated several times.
- 2. Kahlbaum sample, dried and distilled. B. pt. 76.74 °C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta P/bar = \pm 0.001$; $\delta x_{\rm SO_2} = \pm 0.001$ (estimated by compiler).

partial pressure, total pressure = 1 atmosphere = 1.01325×10^5 Pa.

304	Sulfur Dioxid	de Solubilities		
COMPONENTS: 1. Sulfur dioxide; SO ₂ ; [74 2. Tetrachloromethane, (Car tetrachloride); CCl ₄ ; [5	bon	ORIGINAL MEASUREMENTS: Sobolev, I.A.; Kukarin, V.A.; Dzhagatspanyan, R.V.; Kosorotov, V.I.; Zogorets, P.A.; Popov, A.I. Khim. Prom. 1970, 46, 668-70.		
VARIABLES: Temperature		PREPARED BY: C.L. Young		
EXPERIMENTAL VALUES:		<u> </u>		
т/к	Solubility /mol 1-1	*,S Mole fraction of sulfur dioxide in liquid, *SO ₂		
283.15 288.15 293.15 298.15 303.15 + calculated by * at atmospher: In S = 1528/(T/Mof mol 15	ic pressure			
	AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: Bubbler method. Samples of saturated liquid taken and added to sodium hydroxide solution and then excess alkali back titrated.		SOURCE AND PURITY OF MATERIALS: 1. Purity at least 95 mole per cent. 2. Chemically pure. Dried.		

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; δ (Solubility) = $\pm 2\%$; $\delta x_{SO_2} = \pm 0.001$; (estimated by compiler).

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] 2. 2,2,2-Trichloroethanol; C₂H₃Cl₃O; [115-20-8] VARIABLES:

Temperature

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972,

22, 623-650.

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

T/K	P/kPa	Mole ratio SO₂ /ROH	*Mole fraction x SO $_2$	
273.15 283.15 293.15 298.15	99.1	0.70 0.377 0.240 0.200	0.412 0.274 0.194 0.167	

- * Calculated by compiler.
- P is the total pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Sulfur dioxide was bubbled into a
Weighed amount of component (2) in a
bubbler tube as described in detail,
diagram given, in the original paper.
The amount of gas absorbed at
equilibrium and at the observed
temperature and pressure was weighed.
By means of a manometer assembly, to
which the bubbler tube was attached,
the weight of gas absorbed at successively lower pressure was measured.
Eventually the pressure was reduced
to that of the component (2). The
refractive index, and the infrared
spectrum of the residue showed it to
be essentially pure component (2).

- SOURCE AND PURITY OF MATERIALS:
 - 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
 - The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 1,2-Dichloroethane; C₂H₄Cl₂; [107-06-2] 1,2-Dichloropropane; C₃H₆Cl₂; [78-87-5]

Trichloroethene (trichloroethylene); C₂HCl₃; [79-01-6] ORIGINAL MEASUREMENTS:

Sano, H.
Nippon Kagaku Zasshi
1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of 1,2-dichloroethane, $p_{\rm S}^{\,\circ}=0.110$ atm Vapor pressure of 1,2-dichloropropane, $p_{\rm S}^{\,\circ}=0.065$ atm Vapor pressure of trichloroethene, $p_{\rm S}^{\,\circ}=0.120$ atm

Absorption coefficient,	Bunsen coefficient, b	Bunsen coefficient, c	_l c,d	Mole ratio	Mole fraction ^e
s ^a ,b	α	α			
	1,	2-Dichloroethane			
67.0	68.4	72.9	62.0	0.296	0.228
	1,	2-Dichloropropa	ne		
47.6	46.0	47.0	43.5	0.200	0.167
		Trichloroethene			
22.0	22.5	22.9	20.1	0.091	0.0834

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1wo techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Determined by static absorption method.

^C Determined by flow method.

 $[\]alpha = \ell(1 - p_s^{\circ})$ where p_s° is the vapor pressure of solvent.

e Calculated by compiler.

Organic compounds containing halogen 307 COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Benoit, R.L.; Milanova, E. 1,2-Dichloroethane; C2H4Cl2; Can. J. Chem., 1979, 59, 1319-1323 [107-06-2] VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: Henry's law constant T/K H/atm 4.23 298.15 + Defined in the original as $H = \frac{\text{partial pressure of sulfur dioxide}}{\text{mole fraction of sulfur dioxide}}$ AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Few details given. Pressure measured Liquid Air, purity 99.98 mole per With quartz spiral gauge. Partial pressure calculated assuming Raoult's cent. law. Concentration of sulfur dioxide determined by iodometric titration. Concentration of sulfur dioxide ranged 2. Dried over 4A molecular sieve from 0.05 to 0.2 mol 1

ESTIMATED ERROR:

REFERENCES:

 $\delta T/K = \pm 0.1$; $\delta H/atm = \pm 4\%$ (estimated by compiler)

1. Sulfur dioxide; SO_2 ; [7446-09-5]

2. Chlorobenzene; C_6H_5C1 ; [108-90-7]

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res.

(Jpn.), 1931/32, 17, 125-256.

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMEN	TAL VALUES:	Mole fraction of sulfur dioxide in liquid,	T/K	P [†] /bar	Mole fraction of sulfur dioxide in liquid,	Ostwald coefficient, L
298.15	0.0155 0.3662 0.4058 0.6745 0.7626 0.9318 1.0369 1.193 1.229 1.373 1.397	0.000 0.0602 0.0660 0.1163 0.1328 0.1666 0.1876 0.2202 0.2271 0.2590 0.2635	273.15 283.15 293.15 303.15 313.15 323.15 333.15 343.15 353.15	1.008 1.003 0.9950 0.9816 0.9612	0.5310 0.3415 0.2181 0.1532 0.1102 0.0821 0.0614 0.0466 0.0365	169.3 97.4 59.14 41.17 29.92 22.88 17.83 14.33 12.23

total pressure.

Ostwald coefficient (as $x \rightarrow 0$, T/K = 298.15) = 40.4.

Henry's law constant, dp/dx (as $x \rightarrow 0$, T/K = 298.15) = 4502 mmHg = 6.002 bar

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus consisted of a bas buret, a solvent reservoir and an absorption pipet. Dry gas introduced into degassed solvent. System mixed using a magnetic stirrer until saturation occurred. Care was taken to prevent solvent vapor from mixing with gas in the gas buret. Volume of gas determined from gas buret reading; volume of liquid determined from height of meniscus in absorption pipet.

SOURCE AND PURITY OF MATERIALS:

- 1. Sample obtained from Nippon Sulphuric Acid Manufacturing Co. Dried and fractionated several times.
- Sample from Kahlbaum, dried and distilled. Boiling point at atmospheric pressure, 131.96 °C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/\text{bar} = \pm 0.001;$ $\delta x_{\text{SO}_2} = \pm 0.001 \text{ (estimated by compiler)}.$

 $^{^{\}dagger}$ partial pressure, total pressure = 1 atmosphere = 1.01325 \times 10 5 Pa.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Chlorobenzene; C₆H₅Cl;
 [108-90-7]

1,2-Dichlorobenzene; C₆H₄Cl₂; [95-50-1]

ORIGINAL MEASUREMENTS:

Sano, H.
Nippon Kagaku Zasshi
1968, 89, 362-368.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of chlorobenzene, $p_c^{\circ} = 0.020$ atm

Absorption coefficient, Sa,b	Bunsen b coefficient,	Bunsen coefficient, c,f	_l c,d	Mole ratio	Mole fraction ^e
		Chlorobenzene			
40.1	37.2	38.0	37.1	0.170	0.145
	1	,2-Dichlorobenzer	ne		
25.7	23.6	24.1	24.1	0.117	0.105

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetri-The flow method consists of cally. passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodo-The vapor metric titration. pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when Calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5$? (estimated by compiler).

b Determined by static absorption method.

c Determined by flow method.

 $d_{\alpha} = \ell(1 - p_s^{\circ})$ where p_s° is the vapor pressure of solvent.

e Calculated by compiler.

f Assuming vapor pressure of 1,2-dichlorobenzene to be negligible.

- 1. Sulfur dioxide; SO₂; [7446-09.5]
- 2. Chlorobenzene; C₆H₅Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. <u>1972</u>, 22,623-650.

VARIABLES:

PREPARED BY:

Temperature, pressure

W. Gerrard.

EXPERIMENTAL VALUES:

T/K	Pressure, total /mmHg	Mole ratio SO ₂ /Comp.(2)	*Mole fraction \$\frac{x}{50_2}\$
273 .15	760	1.20	0.545
	** 715 694 636 530	1.06 0.962 0.783 0.546	0.516 0.490 0.439 0.353
283.15 293.15 298.15	760 760 760	0.510 0.28 0.23	0.338 0.219 0.187

760 mmHg = 1 atm = 101.325 kPa.

- * Calculated by compiler
- ** The plot of pressure vs solubility given in the original paper is based on these data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

- SOURCE AND PURITY OF MATERIALS:
- Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
 - The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS: Sulfur dioxide; SO₂; [7446-09-5] 2. Bromobenzene; CaHsBr; [108-86-1] VARIABLES: Temperature EXPERIMENTAL VALUES:

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972,

22, 623-650

PREPARED BY:

W. Gerrard

T/K	Pressure, total /mmHg	Mole ratio SO ₂ /Comp.(2)	*Mole fraction *SO2
273.15	760	0.91	0.476
283.15	760	0.41	0.291
293.15	760	0.245	0.197
298.15	760	0.21	0.174

760 = mmHg = 1 atm = 101.325 kPa

Calculated by compiler.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to Which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

- SOURCE AND PURITY OF MATERIALS: 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS: Sulfur dioxide; SO_2 ; [7446-09-5] Iodobenzene; C₆H₅I; [591-50-4]

ORIGINAL MEASUREMENTS:

Gerrard, W.

J. Appl. Chem. Biotechnol. 1972, 22, 623-650

VARIABLES:

PREPARED BY:

Temperature,

W. Gerrard.

EXPERIMENTAL VALUES:

Pressure, total /mmHg	Mole ratio SO /Comp.(2)	*Mole fraction x SO $_2$	
760	0.81	0.448	-
760 760	0.21	0.174	
	/mmHg 760 760 760	760 0.81 760 0.335	760 0.81 0.448 760 0.335 0.251 760 0.21 0.174

760 mmHg = 1 atm = 101.325 kPa.

* calculated by compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Sulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

- SOURCE AND PURITY OF MATERIALS:
 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
 - 2. The best obtainable specimen was carefully purified and rigorously attested.

ESTIMATED ERROR:

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. 2-Chlorophenol; C₆H₅ClO;
 [95-57-8]

ORIGINAL MEASUREMENTS:

Sano, H.; Nakamoto, Y.
Nippon Kagaku Zasshi
1968, 89, 369-373.

VARIABLES:

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Absorption coefficient, Sa	Bunsen coefficient, $\boldsymbol{\alpha}$	Mole ratio	Mole fraction ^b
76.2	69.4	0.323	0.244

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Calculated by compiler.

- Sulfur dioxide; SO₂; [7446-09-5]
- 1-Chloro-octane; (octyl chloride); Biotechnol. 1972, 22,623-650. 2. $C_8H_{17}C1;$ [111-85-3]

ORIGINAL MEASUREMENTS:

Gerrard, W. J. Appl. Chem.

VARIABLES:

PREPARED BY:

Temperature

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure, total /mmHg	Mole ratio SO ₂ /Comp.(2)	*Mole fraction x SO ₂	
273.15	748	0.75	0.429	
283.15	748	0.40	0.286	
293.15	748	0.25	0.200	
298.15	748	0.21	0.174	

760 mmHg = 1 atm = 101.325 kPa.

* Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

bulfur dioxide was bubbled into a weighed amount of component (2) in a bubbler tube as described in detail, diagram given, in the original paper. The amount of gas absorbed at equilibrium and at the observed temperature and pressure was weighed. 2. The best obtainable specimen was By means of a manometer assembly, to which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared spectrum of the residue showed it to be essentially pure component (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Sulfur dioxide was the best grade contained in a small cylinder. Its high purity was attested by the measurement of vapor pressure from 258 to 268 K.
- carefully purified and rigorously attested.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] Gerrard. W. 1. J. Appl. Chem. Biotechnol. 1972, 1-Bromooctane, (octyl bromide); C₈H₁₇Br; [111-83-1] 22, 623-650. VARIABLES: PREPARED BY: Temperature W. Gerrard EXPERIMENTAL VALUES: *Mole fraction Mole ratio T/K Pressure, total $SO_2/Comp.(2)$ x_{SO_2} /mmHq 0.398 0.66 273.15 757 0.267 757 0.365 283.15 0.235 0.190 293.15 757 0.163 757 0.195 298.15 760 mmHg = 1 atm = 101.325 kPa.* Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Sulfur dioxide was the best Sulfur dioxide was bubbled into a weighed amount of component (2) in a grade contained in a small bubbler tube as described in detail, cylinder. Its high purity was diagram given, in the original paper. The amount of gas absorbed at attested by the measurement of vapor pressure from 258 to 268 K. equilibrium and at the observed The best obtainable specimen was temperature and pressure was weighed. carefully purified and rigor-By means of a manometer assembly, to ously attested. which the bubbler tube was attached, the weight of gas absorbed at successively lower pressure was measured. Eventually the pressure was reduced to that of the component (2). The refractive index, and the infrared ESTIMATED ERROR: spectrum of the residue showed it to be essentially pure component (2). REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO2; Sobolev, I. A.; Kurkarin, V. A.; [7446-09-5] Dzhogatspanyan, R. V.; Kosorotov, 2. Heptadecane; C₁₇H₃₆; [629-78-7] V. I.; Zogorets, P. A.; Popov, 3. Tetrachloromethane, (Carbon A. I. Khim. Prom. 1970, 46, 668-70. tetrachloride); CCl₄; [56-23-5] VARIABLES: PREPARED BY: Temperature, concentration C. L. Young

EXPERIMENTAL VALUES:

T/K	Percentage of heptadecane by volume	Solubility*, S /mol ℓ^{-1}
283.15	25	0.530
288.15		0.440
293.15		0.350
298.15		0.299
303.15		0.248
283.15	50	0.421
288.15		0.350
293.15		0.292
298.15		0.248
303.15		0.211
283.15	75	0.313
288.15		0.266
293.15		0.226
298.15		0.196
303.15		0.172
303.15		0.1/2

^{*} at atmospheric pressure

Authors claim solubility is given by

 $\ln S = -((967x - 1582)/(T/K) + 8.47 - 2.71x)$

where x is the mole fraction of heptadecane and S is in units of mol 1⁻¹ atm⁻¹.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Bubbler method. Samples of saturated liquid taken and added to excess sodium hydroxide solution and back titrated.	SOURCE AND PURITY OF MATERIALS: 1. Purity at least 95 mole per cent. 2 and 3. Chemically pure, dried.
	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \delta \text{(Solubility)} = \pm 2\%$ (estimated by compiler). REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide; SO₂; [7446-09-5] 1. Sobolev, I.A.; Kukarin, V.A.; Dzhagatspanyan, R.V.; Kosorotov, V.I.; Zogorets, P.A; Popov, A.I. 2. Soft paraffin (see note). З. Tetrachloromethane, Khim. Prom. 1970, 46, 668-70. (carbon tetrachloride); CCl4; [56-23-5]VARIABLES: PREPARED BY: Temperature, composition C.L. Young

EXPERIMENTAL VALUES:		at.	
т/к	Percentage of soft paraffin (by volume)	Solubility, S /mol 1-1	
283.15 288.15 293.15 298.15 303.15 283.15	25 50	0.533 0.419 0.344 0.294 0.246 0.412	
288.15 293.15 298.15 303.15 283.15	75	0.343 0.283 0.238 0.208 0.317	
288.15 293.15 298.15 303.15		0.265 0.221 0.195 0.167	
288.15 293.15 298.15 303.15	90	0.227 0.204 0.180 0.157	
* at atm	mospheric pressure.		
-((838 x - x is the to be bas	aim solubility is given 1582)/(T/K) + 8.27 - 2. mole fraction of hydroged on assuming a molecut) and S is in units of	49x) where arbon (appears lar weight of	
		•	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Bubbler method. Sample of saturated liquid taken and added to excess sodium hydroxide solution and back titrated.

NOTE: Mixture of C_{12} - C_{22} hydrocarbons (86.7% normal paraffins, 11.3% branched paraffins, 0.4% aromatic and 1.6% naphthenic hydrocarbons).

SOURCE AND PURITY OF MATERIALS:

- 1. Purity at least 95 mole per cent.
- 2. See note.
- 3. Chemically pure. Dried.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta (\text{Solubility}) = \pm 2\$; \\ \delta x_{\text{SO}_2} = \pm 0.001; \ (\text{estimated by compiler.}$

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Sulfinylbismethane; C_2H_6OS ; [67-68-5]

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.

December 1982

CRITICAL EVALUATION:

The isolated value of Sano (1) is in fair agreement with the data of Smedslund (2). Both the value of Lenoir et al. (3) and Benoit and Milanova (4) were determined at low partial pressures of sulfur dioxide and extrapolation to 1 atmosphere partial pressure assuming Henry's law, is not valid. However, the two values, one obtained using chemical analysis and the other using gas chromatographic retention datum, are in fair agreement, which suggests the values are essentially correct but refer to very low partial pressures of sulfur dioxide.

References

- 1. Sano, H. Nippon Kagaku Zasshi 1968, 89, 362.
- 2. Smedslund, T. H. Finska Kemisteamfundets Medd. 1950, 59, 40.
- 3. Lenoir, J.-Y.; Renault, P.; Renon, H. J. Chem. Engng. Data 1971, 16, 340.
- 4. Benoit, R. L.; Milanova, E. Can. J. Chem. 1979, 57, 1319.

COMPONENTS: ORIGINAL MEASUREMENTS: Smedslund, T.H. Sulfur dioxide; SO₂; [7446-09-5] Finska Kemistsamfundets Medd. 1950, 59, 40-43. 2. Sulfinylbismethane (Dimethylsulfoxide); C_2H_6OS ; [67-68-5]VARIABLES: PREPARED BY: W. Gerrard Temperature EXPERIMENTAL VALUES: *Mole fraction SO2, Weight % *Mole ratio T/K $SO_2/(CH_3)_2$ SO x so₂ 291 60.13 1.839 0.648 59.12 1.763 0.638 293 373 17.9 0.266 0.210 3.2 0.0403 434 0.039 T/K SO2, Weight % Partial Pressure * Mole ratio Mole fraction * SO2, mmHg $SO_2/(CH_3)_2SO$ [∞]so₂ "293" 0.0590 4.9 5.2 0.0628 21 0.208 0.172 Probably 14.6 27.6 71 0.465 0.317 See also general statement (data not given) in U.S. Patent No. 2,539,871, 1951. * Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Information not available. The first set of data are for 2. Dimethylsulfoxide was prepared "the saturation of dimethylsulfoxide at a pressure of 1 atm." Details by the catalytic oxidation of dimethyl sulfide in the vapor are not available for the second set. state. The purified product had b.p. 63°C/6 mmHg. (1). ESTIMATED ERROR: REFERENCES: Smedslund, T.H. U.S. Patent, 2,581,050, 1952.

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- Sulfinylbismethane (dimethyl-sulfoxide); C₂H₆OS; [67-68-5]
 Sulfuric acid, dimethyl ester (dimethyl sulfate); C₂H₆O₄S; [77-78-1]

Tetramethylene sulfone (tetrahydro thiophene, 1,1-dioxide);

VARIABLES:

C4H8O2S; [126-33-0]

ORIGINAL MEASUREMENTS:

Sano, H.

Nippon Kagaku Zasshi 1968, 89, 362-368.

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

 $T/^{\circ}C = 30$

T/K = 303

Vapor pressure of dimethyl sulfate = 0.001 atm

	•		
Absorption coefficient, Sa	Bunsen coefficient, α	Mole ratio	Mole fraction ^b
	Sulfinylbismethane		
-	447	1.42	0.587
	Dimethyl sulfate		
124.2	113.3	0.482	0.325
	Tetrahydrothiophene 1,1-d	ioxide	
186.4	169.6	0.929	0.482

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

b Calculated by compiler.

COMPONENTS: ORIGINAL MEASUREMENTS: Sulfur dioxide, SO₂; [7446-09-5] Lenoir, J-Y.; Renault, P.; Renon, H. 1. J. Chem. Eng. Data 1971, 16,340-342. 2. Sulfinylbismethane, (dimethylsulfoxide); C2H6OS; [67-68-5] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa.Henry's constant *Mole fraction at T/K H_{SO},/atm l atm. 0.117 8.55 (An impossible condition) 298 * Calculated by compiler assuming a linear function of $\mathbf{p}_{\mathrm{SO}_2}$ vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$. The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x_{SO_2} \to 0} \frac{f_{SO_2}(P,T)}{x_{SO_2}}$ $x_{\mathrm{SO_2}}$ is the mole fraction. $f_{\mathrm{SO_2}}$ is the fugacity of $\mathrm{SO_2}$ "in the equilibrium condition of pressure and temperature. H_{SO_2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A conventional gas-liquid chromato-1. Sulfur dioxide was provided by l'Air Liquide, and had a stated graphic unit was used. The chromatograph was an IGC 12 M Intersmat model, purity of 99.9%. It was used as equipped with a thermal conductivity detector. The temperature control provided. was stated to be within ±0.1 °C. The 2. Provided by Touzart & Matignon and Serlabo, and stated to have a pressure drop in the column was measured by a mercury manometer. Helium was the carrier gas. minimum purity of 99%. Distillation was carried out when necessary and the refractive index was There is serious uncertainty in the measured. estimation of accuracy. ESTIMATED ERROR: REFERENCES:

Sulfur Dioxide Solubilities			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Sulfur dioxide; SO ₂ ; [7446-09-5]	Benoit, R.L.; Milanova, E.		
 Sulfinylbismethane (Dimethylsulfoxide); C₂H₆OS; [67-68-5] 	Can. J. Chem., <u>1979</u> , 57, 1319-1323		
VARIABLES:	PREPARED BY:		
	C.L. Young		
EXPERIMENTAL VALUES:			
T/K	Henry's law constant + H/atm		
298.15	0.109		
H = partial pressure of some mole fraction of such	lfur dioxide		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: Few details given. Pressure measured with quartz spiral gauge. Partial pressure calculated assuming Raoult's law. Concentration of sulfur dioxide determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.3 to 1.5 mol 1 ⁻¹	SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Liquid Air, purity 99.98 mole per cent. 2. Dried over 4A molecular sieve.		
	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \; \delta H/atm = \pm 4\%$ (estimated by compiler) REFERENCES:		

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Benoit, R.L.; Milanova, E. Can. J. Chem., 1979, 57, 1319-1323 Tetrahydrothiophene, 1,1dioxide, (sulfolane); C4H8O2S; [126-33-0] VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: Henry's law constant T/K H/atm 1.01 303.15 [†] Defined in the original as H = partial pressure of sulfur dioxide mole fraction of sulfur dioxide AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Anhydrous sample from Canadian Few details given. Pressure measured with quartz spiral gauge. Partial Liquid Air, purity 99.98 mole per pressure calculated assuming Raoult's cent. law. Concentration of sulfur dioxide determined by iodometric titration. Concentration of sulfur dioxide ranged from 0.1 to 1.0 mol 1.7 2. Dried over 4A molecular sieve from 0.1 to 1.0 mol 1 ESTIMATED ERROR: $\delta T/K = +0.1; \delta H/atm = +4%$ (estimated by compiler) REFERENCES:

324 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: [7446-09-5] Sulfur dioxide; SO2; Sano, H. Nippon Kagaku Zasshi 2. Esters of phosphoric acid 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Absorption Bunsen Mole Mole Bunsen coefficient, c,f &c,d coefficient, b fractione ratio coefficient, sa,b Phosphoric acid, tributyl ester (Tributyl phosphate); C12H27PO4; [126-73-8] 77.3 75.5 75.5 0.942 0.485 84.9 Phosphoric acid, tris(methylphenyl) ester(Tritolyl phosphate); C21H21PO4; [1330-78-5]

56.0

55.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

61.2

Two techniques were used: static absorption method and (b) flow method. Static method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The flow method consists of passing sulfur dioxide through a micro gas absorption tube and estimating sulfur dioxide by iodometric titration. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

56.0

1. Purity 99.0-99.8 mole per cent.

0.790

0.441

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

a Volume of sulfur dioxide absorbed by unit volume of solvent at experimental temperature and a total pressure of 1 atmosphere.

b Determined by static absorption method.

Determined by flow method.

d $\alpha = l(1 - p_s^o)$ where p_s^o is the vapor pressure of solvent.

e Calculated by compiler.

Assuming vapor pressure of solvent to be negligible.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7746-09-5] Lenoir, J-Y,; Renault, P.; Renon, H. J. Chem. Eng. Data. 1971, 16, 340-342 2. Esters of phosphoric acid. VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: Mole fraction Henry's constant T/K H_{SO},/atm at 1 atm Phosphoric acid, triethyl ester; C₆H₁₅O₄P; [78-40-0] 1.41 Phosphoric acid, tripropyl ester; C₉H₂₁O₄P; [513-08-6] 323 0.621 343 Phosphoric acid, tris (2-methyl propyl) ester; C, H, O, P; [126-71-6] 0.695 Calculated by compiler assuming a linear function p_{SO_2} vs x_{SO_2} , i.e. x_{SO_2} (1 atm) = $1/H_{SO_2}$. The authors gave "Henry's constant" as $H_{SO_2} = \lim_{x \to 0} \frac{\sqrt{SO_2}}{x}$ x_{SO_2} is the mole fraction. f_{SO_2} is the fugacity of SO_2 "in the equilibrium condition" of pressure and temperature. H_{SO2} is related to experimental chromatographic parameters based on the number of moles of solvent in the column, and the absolute retention time of the solute. Helium was the carrier gas. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD /APPARATUS / PROCEDURE: 1. Sulfur dioxide was provided by A conventional gas-liquid chromatol'Air Liquide, and had a stated graphic unit was used. The chromatograph was an IGC 12 M Intersmat purity of 99.9%. It was used as provided. model, equipped with a thermal conductivity detector. The temperature control was stated to be within 2. Provided by Touzart & Matignon and Serlabo, and stated to have ±0.1° C. The pressure drop in the a minimum purity of 99%. column was measured by a mercury manometer. Helium was the carrier Distillation was carried out when gas. necessary, and the refractive index was measured. There is serious uncertainty in the estimation of accuracy. ESTIMATED ERROR: REFERENCES:

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Cooper, D.F.; Smith, J.W. 2. Tributylphosphate, (Phosphoric acid, tributyl ester); C₁₂H₂₇O₄P; [126-73-8] VARIABLES: PREPARED BY: C. L. Young

EXPERIMENTAL	VALUES:			*
т/к	p _{SO₂} /mmHg +	p _{SO₂} /kPa +	Wt ratio SO ₂ /C ₁₂ H ₂₇ O ₄ P	Mole fraction of sulfur dioxide in liquid, **SO2
279.2	6.9 8.7 12.4 19.3 30.4 43.7 64.0 72.8 105 162	0.92 1.16 1.65 2.57 4.05 5.83 8.53 9.71 14.0 21.6	0.0239 0.0291 0.0389 0.0584 0.0807 0.1045 0.1315 0.1426 0.1731 0.2156	0.0904 0.1079 0.1392 0.1954 0.2512 0.3029 0.3535 0.3722 0.4185 0.4727
290.2	219 299 394 492 33.8 44.9 57.8 73.9 94.6	29.2 39.9 52.5 65.6 4.51 5.99 7.71 9.85	0.2538 0.3116 0.3771 0.4256 0.0608 0.0730 0.0871 0.1016 0.1192	0.5134 0.5644 0.6106 0.6389 0.2018 0.2328 0.2658 0.2970
	130 179 267	17.3 23.9 35.6	0.1458 0.1764 0.2203	0.3774 0.4231 0.4780

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell. After equilibrium established samples of liquid removed and analysed by GC. Partial pressure of sulfur dioxide obtained by mixing with air to a total pressure of atmospheric pressure (757 ± 3 mmHg)

SOURCE AND PURITY OF MATERIALS:

- 1. Matheson sample, purity 99.9 mole per cent.
- 2. BDH sample containing 0.099 weight per cent water.

ESTIMATED ERROR:

 $\begin{array}{lll} \delta T/K &=& \pm 0.1; & \delta p/k Pa &= \pm 2 \% \\ \delta x_{SO_2} &=& \pm 2 \% & \text{(estimated by compiler)} \end{array}$

- 1. Sulfur dioxide; SO₂; [7446-09-5]
- 2. Tributylphosphate (Phosphoric
 acid, tributyl ester);
 C₁₂H₂₇O₄P; [126-73-8]

ORIGINAL MEASUREMENTS:

Cooper, D. F.; Smith, J. W.

J. Chem. Eng. Data

1974, 19, 133-6.

т/к	$p_{SO_2}/mmHg^+$	p _{SO2} /kPa ⁺	Wt ratio SO ₂ /C ₁₂ H ₂₇ O ₄ P	Mole fraction of sulfur dioxide in liquid,
290.2	362	48.3	0.2663	0.5254
	534	71.2	0.3279	0.5768
	661	88.1	0.3809	0.6129
307.0	7.4	0.99	0.0073	0.0295
	11.0	1.47	0.0106	0.0422
	17.6	2.35	0.0167	0.0649
	31.6	4.21	0.0288	0.1069
	38.8	5.17	0.0345	0.1254
	44.4	5.92	0.0388	0.1389
	55.1	7.35	0.0467	0.1626
	70.8	9.44	0.0575	0.1929
	105	14.0	0.0785	0.2461
	177	23.6	0.1131	0.3198
	269	35.9	0.1478	0.3806
	326	43.5	0.1655	0.4076
	458	61.1	0.2009	0.4551
	486	64.8	0.2078	0.4635
	570	76.0	0.2279	0.4865
327.3	13.6	1.81	0.0062	0.0251
	23.7	3.16	0.0106	0.0422
	37.2	4.96	0.0155	0.0605
	54.4	7.25	0.0222	0.0845
	69.6	9.28	0.0285	0.1059
	115 115 139 176 226 320 405 429 449 480 511 590	15.3 15.3 18.5 23.5 30.1 42.7 54.0 57.2 59.9 64.0 68.1 78.7 90.3	0.0427 0.0429 0.0486 0.0611 0.0733 0.0995 0.1160 0.1192 0.1220 0.1320 0.1367 0.1458 0.1610	0.1508 0.1514 0.1681 0.2026 0.2336 0.2926 0.3254 0.3314 0.3365 0.3543 0.3624 0.3774 0.4010
342.7	21.7	2.89	0.0056	0.0228
	58.7	7.83	0.0137	0.0539
	142	18.9	0.0315	0.1158
	200	26.7	0.0449	0.1573
	262	34.9	0.0548	0.1856
	331	44.1	0.0630	0.2076
	365	48.7	0.0710	0.2279
	430	57.3	0.0850	0.2611
	587	78.3	0.1028	0.2994
	663	88.4	0.1148	0.3231

⁺p_{SO₂} = partial pressure of SO₂

^{*} Calculated by compiler

328 Sulfur Dioxide Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Sano, H. 2. Carbon disulfide; CS₂; [75-15-0] Nippon Kagaku Zasshi 1968, 89, 362-368. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: $T/^{\circ}C = 30$ T/K = 303Mole fractiona Mole ratio Bunsen coefficient, α 10.1 0.027 0.0263 a Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static absorption method consisted of equilibrating solvent and sulfur dioxide in a 50 ml flask and measuring the absorption volumetrically. The vapor pressure of the solvents were measured roughly and were assumed to be equal to the partial pressure of the solvent by the authors when calculating the Bunsen coefficient.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.0-99.8 mole per cent.

ESTIMATED ERROR: $\delta T/K = \pm 0.5$; $\delta x_{SO_2} = \pm 5\%$ (estimated by compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Schulze, H. Sulfuryl chloride; O₂Cl₂S; J. Prakt. Chem. <u>1881</u>, 24, 168-183 [7791-25-5] VARIABLES: PREPARED BY: W. Gerrard. EXPERIMENTAL VALUES: 760 mmHg = 1 atm = 101.325 kPa. T/K Weight of SO₂ *Mole ratio *Mole fraction /1 g of comp.(2) $SO_2/Comp.(2)$ [∞]so₂ 0.681 0.405 273.15 0.323 *Calculated by compiler. Pressure of SO2 stated to be 725 mmHg. 1 Volume of sulfuryl chloride absorbed 187 volumes of SO2 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The gas was passed into a weighed amount of sulfuryl chloride in a 1. Probably of satisfactory purity. thin-walled test-tube fitted with Probably of satisfactory purity. The paper gave details on the preparation of sulfuryl chloride. a rubber stopper carrying an inlet, and an outlet tube. The test tube was cooled in melting snow. The amount of gas absorbed was determined by weighing. ESTIMATED ERROR: REFERENCES:

- (1) Sulfur dioxide; SO₂; [7446-09-5]
- (2) Lithium tetrachloro aluminate(1-); AlCl₄.Li; [14024-11-4]
- (3) Thionyl chloride; SOCl₂; [7719-09-7]

ORIGINAL MEASUREMENTS:

Domeniconi, M.; Klinedinst, K.; Marincic, N.; Schlaikjer, C.; Staniewicz, R.; Swette, L.

ONR Contract # N00014~76-C-0524 Interim Report Jan. 1976 - Oct. 1977.

VARIABLES:

T/K: 273 - 333P: Atmospheric

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Fifteen measurements of the solubility of sulfur dioxide, SO_2 , in a 1.8 mole LiAlCl $_4$ dm $^{-3}$ solution in thionyl chloride were made between 273 and 333 K. The mole fraction solubility values are shown on a graph (Figure 10 of the report). The data are not tabulated, but they were fitted to the following equation by the authors.

$$\ln x_{SO_2} = [(2.417 \pm 0.184) \times 10^3]/T - (9.863 \pm 0.613)$$

The equation can be used to calculate the mole fraction solubility of sulfur dioxide at a partial pressure of 1 atm between temperatures of 273 and 333 K in 1.8 molar LiAlCl₄ in SOCl₂.

The authors imply that they also measured the solubility of sulfur dioxide in pure thionyl chloride. However, they give neither data nor an equation. They do show what may be a smoothed curve for the sulfur dioxide solubility in thionyl chloride. (Figure 10 of report).

Figure 10 of the report compares the ln mole fraction solubility vs. 1/T and Figure 11 compares the molar solubility vs. temperature in pure thionyl chloride and in the 1.8 M LiAlCl $_4$ solution. In both solubility units the solubility appears to be equal at a temperature near 288 K. At lower temperatures sulfur dioxide is more soluble in pure thionyl chloride than in the 1.8 M LiAlCl $_4$ solution, above 288K the sulfur dioxide is more soluble in the solution than in the pure solvent.

In the original report the equation intercept is given erroneously as 0.863 instead of 9.863.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The sulfur dioxide was determined gravimetrically. A special Erlenmeyer flask fitted with a side arm bubbler was dried and weighed. The solvent was added and the flask weighed again The flask was placed in either an oil or a water bath. A glass wool-packed water-jacketed condenser was attached to the flask. The sulfur dioxide was bubbled in until saturation. The flask was weighed. Dry argon was bubb bubbled through the solution as it was heated to reflux, thus driving off ESTIMATED ERROR: the previously dissolved SO2. The flask was again weighed.

The authors do not explain their reason for weighing the SO₂ gain on saturation, and the weight loss on degassing. It is not clear whether this is a check on the measurement, or the degassing procedure for the next determination at another temperature.

SOURCE AND PURITY OF MATERIALS:

- (1) Sulfur dioxide.
- (2) Lithium tetrachloroaluminate(1-).
- (3) Thionyl chloride. Source not given. Distilled twice before

 $\delta X_1/X_1 = 0.20$ (Compiler)

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Sulfur dioxide; SO₂;[7446-09-5] Driscoll, J. R.; Brummer, S. B.; Gudrais, P.; Holleck, G. L.; (2) Lithium tetrachloro aluminate(1-); Toland, D. E.; Turchan, M. J. AlCl₄.Li; [14024-11-4] Report ECOM-74-0030-F (3) Thionyl chloride; SOCl2; March 1978 [7719-09-7] VARIABLES: PREPARED BY: T/K: 273 , H. L. Clever Р: atmosphere

EXPERIMENTAL VALUES:

Т/К	Mol Fraction X ₁	Molarity mol SO ₂ dm ⁻³ solution ^a	
Thionyl o	chloride; SOCl ₂ ;	7719-09-7	
273	0.465	8.0	
298	0.160	2.3	
Lithium to 1.5 mol 1	tetrachloro alumi LiAlCl ₄ dm ⁻³ solu	nate(l-) + thionyl chlo tion	ride;
273	>0.498	8.4	
298	0.512 0.192 0.187	8.7 2.7 2.6	

The mole fraction values were calculated directly from the weights of the components in the saturated solutions. The molarities were calculated assuming a solution density of 1.60 g cm⁻³. The solution densities were calculated from $\rho(\text{solution}) = \rho(\text{SO}_2) \cdot x(\text{SO}_2) + \rho(\text{solvent}) \cdot x(\text{solvent})$. All of the calculated densities were within ± 0.03 of 1.60 g cm⁻³. The 1.60 value was chosen to calculate all of the molarity values.

The present values confirm the authors earlier values by gas chromatography. They are much greater than values reported by Spandau and Brunneck (1). The present results are in substantial agreement of those of Domeniccui et at. (2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined gravimetrically. The sufur dioxide gas cylinder was connected to three gas bubblers joined in series. The first bubbler contained glass wool, the second bubbler contained a weighed portion of the solvent, and the third bubbler contained concentrated H₂SO₄. The third bubbler both isolated the system from the atmosphere, and acted as a flow monitor. The flow of SO₂ was set to minimize thionyl chloride loss by allowing little or no exit bubbling. Bubbling was continued until there was no more weight gain.

The sample bubbler was maintained at 25 $^{\circ}\text{C}$ in air or at 0 $^{\circ}\text{C}$ in a ice bath

SOURCE AND PURITY OF MATERIALS:

- (1) Sulfur dioxide. Matheson Co., Inc. Anhydrous, minimum purity 99.98 per cent.
- (2) Lithium tetrachloro aluminate(1-). Source and purity not given.
- (3) Thionyl chloride. Eastman Co. Number 246, used as received.

ESTIMATED ERROR:

$$\delta X_1/X_1 = 0.03 - 0.05$$
 (Compiler)

- Spandau, H.; Brunneck, E. Z. Anorg. Allgem. Chem. 1952, 270, 201.
- Domeniccui, M.; Kliaedinst, K.; Marin-cic, N.; Schlaikjer, C.; Staniewicz, R.; Swette, L.
 Interim Report, Jan. 1976-Oct. 1977, ONR Contract # N00014-76-C-0524.

COMPONENTS: 1. Sulfur dioxide; SO₂; [7446-09-5] Venable, C.S.; Fuwa, T. Ind. Eng. Chem. 1922, 14, 139-142. VARIABLES: PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

The data were expressed as quantity of gas measured as $S = cm^3$ gas (273.15K, 1 atm) absorbed by 100 cm³ of rubber.

At 293-295 K, S=1950. The pressure appears to be the prevailing barometric one.

The compiler assumes that the isoprene unit, C_5H_8 , may be taken to calculate an equivalent mole ratio (and hence mole fraction) as follows:

Equivalent mole ratio $SO_2/C_5H_8 = (19.50/21868) \times (68/0.75) = 0.0808; x_{SO_2} = 0.075.$

The gram mole volume of sulfur dioxide is taken to be 21868 cm^3 at 273.15 K and 1 atm.); 0.75 is the assumed density of the rubber.

The x_{SO_2} value of 0.075 obtained in this way fits the value for the pure hydrocarbons, C_5 onwards, obtained by Makranczy *et al.*(1).

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The rubber was held under high vacuum for 48 hours. A weighed amount of the degassed rubber, as thin strips, was left in contact with the gas until equilibrium had been attained, as indicated by the constancy of pressure in the bulb. The gas was removed by a pump and measured over mercury. Temperature control was by a large bath of water.

SOURCE AND PURITY OF MATERIALS:

 Dried over phosphorus pentoxide. From a cylinder.

ESTIMATED ERROR:

REFERENCES:

 Makranczy, J.; Magyery-Balog, K.; Rusz, L.; Patyi, L.

Hung. J. Ind. Chem. 1976, 4, 269.

Water 333

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] 2. Water; H₂O; [7732-18-5] EVALUATOR: Rubin Battino, Department of Chemistry, Wright State University, Dayton, Ohio 45435, U.S.A.

July 1981

CRITICAL EVALUATION:

The solubility of chlorine in pure water is complicated by two factors: (a) it reacts chemically with the water hydrolyzing to form Cl and HClO; and (b) at relatively low pressures (near atmospheric) it forms a hydrate (Cl₂.8H₂O) which separates out. The hydrolysis has been studied in great detail by Yakovkin (1) whose work was analyzed by Arkadiev (2). Unfortunately, neither of these papers was available to the Evaluator at the time of writing this critical evaluation. However, a summary of both of these papers was provided by Adams and Edmonds (3). Formation of the hydrate was specifically studied by Bakhuis Roozeboom (4) and Stackelberg and Müller (5).

There were a number of papers reporting on the solubility of chlorine in water. We take these solubilities to be bulk solubilities, i.e., we assume that all of the chlorine containing species present are present as Cl₂(aq). The work reported by Bunsen (6) and cited in other places was apparently carried out by Schönfeld (7) using a chemical method for determining the amount of dissolved chlorine. Roscoe (8) repeated Schönfeld's work at one temperature while studying gaseous mixtures of chlorine and hydrogen in aqueous solutions. Bakhuis Roozeboom (4) determined the solubility of chlorine in water at three temperatures (and extrapolated to two lower temperatures). Mellor (9) measured the solubility of chlorine in water at one temperature by chemical means while studying hydrogen and chlorine reactions. Winkler's results (10) are reported in the International Critical Tables for a wide range of temperature (283-383 K). Finally, Whitney and Vivian (11) reported on solubilities they determined while studying the hydrolysis constants of chlorine in water.

The solubility results fall into two main groups with that of Bakhuis Roozeboom falling roughly in the middle. Roscoe, Mellor, and Bunsen/Schönfeld's values are in quite good agreement with each other. Winkler, Whitney and Vivian, and Yakovkin's results (the latter as analyzed by Arkadiev and by Adams and Edmonds) are in good agreement with each other, but higher than the other group. The recommended values below were calculated from Table 1 in Adams and Edmonds' paper (3). They should be reliable to about ±2 per cent. The mole fractions are calculated for 101.325 kPa partial pressure of the gas.

T/K	10 ³ x ₁	T/K	10 ³ x ₁
283.15	2.48	343.15	0.849
293.15	1.88	353.15	0.784
303.15	1.50	363.15	0.737
313.15	1.23	373.15	0.697
323.15	1.06	383.15	0.668
333.15	0.939		

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]

EVALUATOR:

Rubin Battino, Department of Chemistry, Wright State University, Dayton, Ohio 45435, U.S.A.

July 1981

CRITICAL EVALUATION:

References:

- 1. Yakovkin, A. J. Russ. Phys.-Chem. 1900, 32, 673.
- 2. Arkadiev, V. J. Russ. Phys.-Chem. 1918, 50, 205.
- 3. Adams, F. W.; Edmonds, R. G. Ind. Eng. Chem. 1937, 29, 447-50.
- 4. Bakhuis Roozeboom, H. W. Recl. Trav. Chim. Pays-Bas 1884, 3, 59-72.
- 5. Stackelberg, von M.; Müller, H. R. Z. Elektrochem. 1954, 58, 25-39.
- 6. Bunsen, R. Phil. Mag. 1855, 9, 181-201.
- 7. Schönfeld, M. Ann. 1855, 93, 26.
- 8. Roscoe, H. E. J. Chem. Soc. 1856, 8, 14-26.
- 9. Mellor, W. J. Chem. Soc. 1901, 79, 216-38.
- 10. Winkler, L. W. Mathematikai es Termeszettudomanyi Ertesitö

 Budapest 1907, 25, 86.
- 11. Whitney, R. P.; Vivian, J. E. Ind. Eng. Chem. 1941, 33, 741-4;
 Tech. Assoc. Papers 1941, 24, 435-6; Paper Trade J. 1941,
 113, 31-2. (Note that the last two papers are essentially identical.)

						
COMPONENTS	,		ORIGINAL	MEASUREMENTS:		
1. Chlor	ine; Cl ₂ ; [7782	2-50-5]	Bunsen, R.			
ļ			Phil.	Mag.		
2. Water	; H ₂ O; [7732-18	8-51	1855.	9, 181-201.		
	,207 [7,702 2.			.,		
VARIABLES:		·				
VARIABLES:	T/K = 283-313	,	PREPARED	R. Battino		
	1/1 = 203-313	•		R. Battino		
	· · · · · · · · · · · · · · · · · · ·		<u> </u>			
EXPERIMENT	AL VALUES:					
	_a ,	a,b	_a.c	α ^d /cm³ (STP) cm ⁻³ atm ⁻¹		
t/°C	T ^a /K	$10^{\circ}x_1$	L.,,	α /cm (STP) cm atm		
7.0				0.5050		
10 11	283 284	2.074 2.039	2.680 2.644	2.5852 2.5413		
12	285	2.005	2.607	2.4977		
13	286	1.970	2.571	2.5453		
14	287	1.936	2.535	2.4111		
15	288	1.901	2.498	2.3681		
16 17	289 290	1.867 1.834	2.462 2.425	2.3253 2.2828		
18	290 291	1.800	2.425	2.2405		
19	292	1.767	2.351	2.1984		
20	293	1.733	2.314	2.1565		
21	294	1.700	2.277	2.1148		
22 23	295 296	1.667	2.240	2.0734		
23 24	296 297	1.635 1.602	2.203 2.166	2.0322 1.9912		
25	298	1.570	2.129	1.9504		
26	299	1.538	2.092	1.9099		
27	300	1.506	2.054	1.8695		
28	301	1.474	2.017	1.8295		
29 30	302 303	1.442 1.411	1.979 1.942	1.7895 1.7499		
31	304	1.379	1.905	1.7104		
32	305	1.348	1.867	1.6712		
33	306	1.317	1.829	1.6322		
				(cont.)		
		AUXILIARY	INFORMATIO	И		
METHOD/APP	ARATUS/PROCEDURE:		SOURCE AN	D PURITY OF MATERIALS:		
Thomas day						
	a are values rep			N = 3-1-21		
=	olaces as having			No details given.		
mined by	a chemical metho	d by	1			
M. Schönf	eld (1) of Dusse	ldorf.				
			ESTIMATED			
			δα/α =	±0.02 (compiler's estimate	e).	
			REFERENCE	S:		
			1. Sch	önfeld, M.		
				alen		
			F			
			185	<u>5</u> , 93, 26.		
1						

1. Chlorine; Cl₂; [7782-50-5]

2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bunsen, R.

Phil. Mag.

1855, 9, 181-201.

EXPERIMENTAL VALUES:

t/°C	T ^a /K	10^3x_1 a,b	L ^{a,c}	$\alpha^{\rm d}/{\rm cm}^3$ (STP) cm ⁻³ atm ⁻¹
34	307	1.286	1.792	1.5934
35	308	1.256	1.754	1.5550
36	309	1.225	1.716	1.5166
37	310	1.195	1.679	1.4785
38 39	311	1.165	1.641	1.4406
39	312	1.135	1.603	1.4029
40	313	1.105	1.566	1.3655
1				

a Calculated by compiler.

b Mole fraction solubility at 101.325 kPa partial pressure of gas.

^C Ostwald coefficient.

d Bunsen coefficient.

Roscoe, H. E. J. Chem. Soc.
<u>1856</u> , 8, 14-26.
PREPARED BY:
R. Battino

t/°C	T ^a /K	10 ³ x ₁ ^a ,b	L ^{a,c}	$\alpha^{\rm d}/{\rm cm}^3$ (STP) cm ⁻³ atm ⁻¹	/cm³ (STP) cm ⁻³ at	:m-1
14.0	287.2	1.920	2.514	2.3911	2.3911	

a Calculated by compiler.

METHOD/APPARATUS/PROCEDURE: The amount of chlorine dissolved appears to have been determined chemically using Schönfeld's method. ESTIMATED ERROR: $\delta \alpha / \alpha = \pm 0.02 \text{ (compiler's estimate)}.$ REFERENCES: 1. Schönfeld, M. Annalen

1855, 93, 26.

b Mole fraction solubility at 101.325 kPa partial pressure of gas.

^C Ostwald coefficient.

d Bunsen coefficient.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Bakhuis Roozeboom, H. W.,
2. Water; H ₂ O; [7732-18-5]	Recl. Trav. Chim. Pays-Bas
	<u>1884</u> , 3, 59-72.
VARIABLES:	PREPARED BY:
T/K = 273-285	R. Battino
EXPERIMENTAL VALUES:	
a a.b	_a.c a.d _e

t/°C	T ^a /K	$10^3 x_1^{a,b}$	L ^{a,c}	_α a,d	β ^e
0 3	273 276	3.72 3.17	4.64 4.00	4.64	4.61 ^f 3.93 ^f
6	279	2.77	3.53	3.45	3.42
9	282	2.46	3.17	3.07	3.03
12	285	2.26	2.93	2.81	2.77

a Calculated by compiler.

METHOD/APPARATUS/PROCEDURE:

AUXILIARY INFORMATION

The author was investigating the						
hydrate formed between chlorine						
and water and incidentally deter-						
mined the solubility of chlorine						
in water at 6, 9 and 12 °C at a total						
pressure of 1 atm. The β values						
given above are those appearing in						
the International Critical Tables						
(1).						

SOURCE AND PURITY OF MATERIALS:

ESTIMATED ERROR:

REFERENCES:

1. International Critical Tables, Vol. III, p.256.

b Mole fraction solubility at 101.325 kPa partial pressure of gas.

^C Ostwald coefficient.

d Bunsen coefficient. Units of cm3 (STP) cm-3 atm-1.

^e Solubility coefficient similar to Bunsen coefficient but at 1 atm total pressure. $\alpha = \beta \times 760/(760 - P_{\rm H_2O})$.

 $^{^{\}rm f}$ Points interpolated by author. The original values are presented as 1.07% Cl $_2$ (6 °C), 0.95% Cl $_2$ (9 °C), and 0.87% Cl $_2$ (12 °C) at a total pressure of 1 atm.

		ter				339	
COMPONENTS:			ORIGINAL MEASU	REMENTS:			
1. Chlorine; Cl ₂ ; [7782-50-5]			Mellor, W.				
2. Water; H ₂ O; [7732-18-5]			J. Chem. Soc. 1901, 79, 216-38.				
VARIABLES:			PREPARED BY:				
T/K =	294.2			R. Bat	tino		
EXPERIMENTAL	VALUES:					-	
t/°C	т ^а /к	10 ³ x ₁ ^a	,b _L a,c	α ^d /cm³	(STP)	cm ⁻³	atm ⁻¹
21.0	294.2	1.701	2.278		2.115	57	

- ^a Calculated by compiler.
- b Mole fraction solubility at 101.325 kPa partial pressure of gas.
- ^C Ostwald coefficient.
- d Bunsen coefficient.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine bubbled through solution. Amount determined by reaction with Potassium iodide and titration of iodine with sodium thiosulfate soln.

SOURCE AND PURITY OF MATERIALS:

1. Prepared by reaction of hydrochloric acid with chromic acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$; $\delta \alpha/\alpha = \pm 0.02$ (compiler's estimate).

COMPONENTS: 1. Chlorine; Cl ₂ ; [7782-50-5]			ORIGINAL MEASUREMENTS:			
			Winkler, L. W.			
2. Water; H ₂ O; [7732-18-5]			Mathematikai es Termeszettudomanyi			
2. Water	; H ₂ O; [7/32-18-5]		Budapest		
				86. (Inte		
			Critical	Tables, Vol.	III, p.256)	
VARIABLES:			PREPARED BY:	PREPARED BY:		
T/K = 283-373			R. Battino			
EXPERIMENT	AL VALUES:	-				
t/°C	т ^а /К	10 ³ x ₁ a,b	L ^{a,c}	_α a,d	β ^e	
10	283	2.556	3.304	3.187	3.148	
11 12	284	2.476	3.211	3.087 2.991	3.047 2.950	
13	285 286	2.399 2.326	3.112 3.037	2.899	2.856	
14	287	2.256	2.955	2.811	2.767	
15	288	2.188	2.876	2.726	2.680	
16	289	2.123	2.799	2.644	2.597	
17	290	2.061	2.726	2.566	2.517 2.440	
18 19	291 292	2.009 1.944	2.655 2.588	2.491 2.420	2.368	
20	293	1.891	2.525	2.353	2.299	
21	294	1.844	2.470	2.294	2.238	
22	295	1.800	2.418	2.238	2.180	
23	296	1.757	2.368	2.184	2.123	
24 25	297 298	1.716 1.677	2.320 2.275	2.133 2.084	2.070 2.019	
26	299	1.641	2.273	2.034	1.970	
27	300	1.605	2.190	1.993	1.923	
28	301	1.573	2.153	1.953	1.880	
29	302	1.543	2.118	1.915	1.839	
30 35	303 308	1.514 1.374	2.084 1.920	1.878 1.702	1.799 1.608	
		2.27.5			nt.)	
		AUVITA	ARY INFORMATION			
METUOD /ADD	ADATHS /DDOCED		<u> </u>	UDITAL OF MARCH	ATC.	
METHOD/APP	ARATUS/PROCED	UKE:	SOURCE AND P	URITY OF MATERI	ALS:	

SOURCE AND FORTH OF MATERIALS,
,
ESTIMATED ERROR:
REFERENCES:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Winkler, L. W.

Mathematikai es Termeszettudomanyi Ertesitö, Budapest

1907, 25, 86. (International Critical Tables, Vol. III, p.256)

t/°C	T ^a /L	10 ³ x ₁ a,b	La,c	αa,d	β ^e
40	313	1.265	1.793	1.564	1.450
45	318	1.182	1.698	1.458	1.320
50	323	1.125	1.639	1.385	1.216
60	333	1.042	1.556	1.276	1.025
70	343	1.022	1.564	1.245	0.862
80	353	1.059f	1.657f	1.282f	0.683 ^f
90	363	1.052f	1.682f	1.265f	0.39 ^f

a Calculated by compiler.

b Mole fraction solubility at 101.325 kPa partial pressure of gas.

c Ostwald coefficient.

d Bunsen coefficient in units of cm3 (STP) cm-3 atm-1.

e Solubility coefficient similar to the Bunsen coefficient but at 1 atm total pressure. $\alpha = \beta \times 760/(760 - P_{\rm H_2O})$.

f Doubtful points due to very high vapor pressure of water at these temperatures.

Components: 1. Chlorine; Cl₂; [7782-50-5] Whitney, R.P.; Vivian, J.E. 2. Water; H₂O; [7732-18-5] Ind. Eng. Chem. 1941, 33,741-4 VARIABLES: Temperature, pressure EXPERIMENTAL VALUES: T/K Partial Pressure Solubility + Mole fraction of pCl₂/atm pCl₂/kPa g/10²g H₂O chlorine, xCl₂ 283.2 0.0601 6.09 0.124 0.000315

T/K	Partial P $p_{\mathtt{Cl_2}}$ /atm	Pressure PCl ₂ /kPa	Solubility ⁺ g/10 ² g H ₂ O	Mole fraction of chlorine, x_{Cl_2}
283.2	0.0601	6.09	0.124	0.000315
	0.0660	6.69	0.131	0.000333
	0.155	15.7	0.228	0.000579
	0.157	15.9	0.237	0.000602
	0.292	29.6	0.368	0.000934
	0.293	29.7	0.366	0.000929
	0.498	50.5	0.541	0.001373
	0.498	50.5	0.555	0.001408
288.2	0.0581	5.89	0.111	0.000282
	0.0611	6.19	0.115	0.000292
	0.140	14.2	0.195	0.000495
	0.145	14.7	0.201	0.000510
	0.291	29.5	0.330	0.000838
	0.297	30.1	0.330	0.000838
	0.488	49.4	0.477	0.00121
	0.490	49.6	0.480	0.00128
	0.951	96.4	0.825	0.00209
	0.951	96.4	0.825	0.00209
293.2	0.0665	6.74	0.112	0.000284
	0.1195	12.11	0.160	0.000406
	0.260	26.3	0.262	0.000665
	0.260	26.3	0.265	0.000673
	0.487	49.3	0.415	0.00105

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Single pass flow apparatus. Chlorine and nitrogen at a total pressure of atmospheric pressure was bubbled through water in an "equilibrium" cell. After one hour samples of saturated liquid analysed by adding to excess potassium iodide and titrating the liberated iodine with sodium thiosulfate. Partial pressure of chlorine varied by adjusting proportion in nitrogen chlorine mixture. Also see references (1) and (2) (which are identical) for additional calculations on this system.

SOURCE AND PURITY OF MATERIALS;

- 1. Purity 98.5 mole per cent.
- 2. Distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$; $\delta x_{\text{Cl}_2}/x_{\text{Cl}_2} = \pm 0.02$ (estimated by compiler)

- Whitney, R. P.; Vivian, J. E. Tech. Assoc. Papers 1941, 24, 435-6.
- Whitney, R. P.; Vivian, J. E. Paper Trade J. <u>1941</u>, 113, 31-2.

- Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Whitney, R.P.; Vivian, J.E.

Ind. Eng. Chem. 1941,33, 741-4.

EXPERIMENTAL VALUES:

T/K	Partial F	pressure PCl ₂ /kPa	Solubility ⁺ , g/10 ⁵ g H ₂ O	Mole fraction of chlorine, xCl2
293.2	0.490	49.6	0.422	0.00107
2,5012	0.965	97.8	0.725	0.00184
298.2	0.0621	6.29	0.104	0.000264
	0.0655	6.64	0.106	0.000269
	0.104	10.5	0.139	0.000353
	0.109	11.0	0.143	0.000363
	0.174	17.6	0.189	0.000480
	0.270	27.4	0.246	0.000625
	0.551	55.8	0.391	0.000992
	0.589	59.7	0.418	0.00106
	0.961	97.4	0.628	0.00159

T/K	10 ⁴ x ₁ a
283.2	26.25
288.2	22.11
293.2	19.20
298.2	16.19

Extrapolated values at 101.325 kPa partial pressure of gas calculated by compiler from a least squares smoothing of the data at each temperature.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Hydrochloric acid; HCl; [7647-01-0]

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia. March 1982

EVALUATION:

Much of the solubility data for chlorine in aqueous hydrochloric acid solutions has been determined in order to study the various chemical equilibria established in solution. Jakowkin (Yakovkin) (1) found that the solubility of chlorine in water was decreased by small additions of hydrogen chloride, but is increased by larger additions. Other early investigations were those of Roscoe (2), Berthelot (3) and Goodwin (4). None of these workers data are considered accurate enough for inclusion in the compiled tables. The early data of Mellor (5) are compiled but are classified as doubtful. The data of Hine and Inuta (6) are classified as tentative but are considered inferior to the data of Sherrill and Izard (7), (8) but because of the different temperatures employed, the two sets of data are not directly comparable.

References

- Jakowkin, A. A.
 z. physik. Chem., <u>1899</u>, 29, 613.
- 2. Roscoe, H. E. J. Chem. Soc., 1956, 8, 14.
- Berthelot, M.
 Ann. Chim. Phys., 1881, 22, 462 and Compt. rend., 1880, 91, 194.
- Goodwin, W. L.
 Trans. Roy. Soc. Edin., 1882, 30, 597 or Ber., 1882, 15, 3039.
- Mellor, W.
 J. Chem. Soc., <u>1901</u>, 79, 216.
- 6. Hine, F.; Inuta, S. Bull. Chem. Soc. Japan, 1968, 41, 71.
- 7. Sherrill, M. S.; Izard, E. F. J. Am. Chem. Soc., 1928, 50, 1665.
- Sherrill, M. S.; Izard, E. F.
 J. Am. Chem. Soc., <u>1931</u>, 53, 1667.

Water 345

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Mellor, W.
2. Water; H ₂ O; [7732-18-5]	J. Chem. Soc.
3. Hydrochloric acid; HCl; [7647-01-0]	<u>1901</u> , 79, 216.
VARIABLES:	PREPARED BY:
	C. L. Young

EXPERIMENTAL VALUES:

t/°C	т/к	Conc. of HCl /g dm ⁻³	p/mmHg	p/kPa	Conc. of Cl ₂ † /g dm ⁻³	Bunsen Coefficient α	Ostwald Coefficient
21.0	294.2	313.401	761	101.5	12.03	3.5492	3.8224
21.0	294.2	282.060	761 750	101.5	11.87	3.3278	3.5859
21.0	294.2	250.720	759	101.2	10.68	3.1272	3.3677
21.0	294.2	219.380	759	101.2	9.93	2.9243	3.1312
20.2	293.4	188.040	761	101.5	9.23	2.7020	2.9117
20.2	293.4	156.700	761	101.5	8.58	2.5095	2.7043
20.5	293.7	125.360	761	101.5	7.76	2.2711	2.4473
20.5	293.7	94.020	760	101.3	7.19	2.1044	2.2677
20.0	293.2	62.680	760	101.3	6.38	1.8682	2.0131
21.0	294.2	31.340	762	101.6	5.81	1.6736	1.8033
21.0	294.2	15.670	759	101.2	5.10	1.4933	1.6092
21.0	294.2	12.540	759	101.2	4.85	1.4200	1.5292
21.0	294.2	9.402	760	101.3	4.76	1.3942	1.5013
20.0	293.2	6.248	760	101.3	4.94	1.4483	1.5607
21.0	294.2	3.134	760	101.3	5.30	1.5496	1.6698
21.0	294.2	0.00	760	101.3	7.23	2.1157	2.2799
1							

 $^{^{\}dagger}$ volume measured after saturation with chlorine.

AUXILIARY INFORMATION

ETHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Chlorine bubbled through solution.	
Amount determined by reaction with	No details given.
Potassium iodide and titration of	
iodine with sodium thiosulfate	t L
solution.	
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.2; \delta \alpha/\alpha = \pm 0.02$
	(compiler's estimate).
	REFERENCES:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Pydrochloric acid; HCl; [7647-01-0]

ORIGINAL MEASUREMENTS:

Sherrill, M. S.; Izard, E. F.

J. Am. Chem. Soc.

1928, 50, 1665-1675 and

J. Am. Chem. Soc. 1931, 53, 1667-1674.

VARIABLES:

Concentration of acid

PREPARED BY:

C. L. Young

EXPERIMENTAL VA	LUES:		
T/K	Concentration of acid /mol kg ⁻¹ (H ₂ O)	Concentration of chlorine /mol kg ⁻¹ (H ₂ O)	Mole fraction _§ of chlorine, ^x Cl ₂
298.15	0.000	0.0923	0.001660
	0.010	0.08264	0.001486
	0.100	0.06394	0.001146
	0.200	0.0619	0.00111
	0.496	0.0630	0.00112
	1.019	0.0665	0.00118
ł	1.991	0.0737	0.00128
	2.990	0.0824	0.00141
	3.989	0.0914	0.00153
	* 4.903	0.0978	0.00162
	5.180	0.1004	0.00165
	* 7.016	0.1150	0.00184
ĺ	* 8.163	0.1219	0.00191
ļ	* 8.854	0.1281	0.00199
	* 9.805	0.1326	0.00203
i			

 $^{^{\}S}$ at a partial pressure of chlorine of 101.3 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine bubbled through solution. Absorption train painted black to prevent decomposition of chlorine by light. Before the liquid sample was analysed the saturated solution was allowed to equilibrate for at least 3 hours without chlorine being bubbled through. Amount of chlorine determined by reaction with potassium iodide and titrating liberated iodine with sodium thiosulfate.

SOURCE AND PURITY OF MATERIALS:

 Chlorine prepared by action of hydrochloric acid on chromic acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$; $\delta x_{\text{Cl}_2} = \pm 2\%$ (estimated by compiler).

^{*} taken from earlier reference at a partial pressure of chlorine of 101.3 kPa.

*Water 347

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Hine, F.; Inuta, S.
2. Water; H ₂ O; [7732-18-5]	Bull. Chem. Soc. Japan
3. Hydrochloric acid; HCl; [7647-01-0]	1968, 41, 71-75.
VARIABLES:	PREPARED BY:
Temperature, pressure, concentration of component 3	C. L. Young

EXPERIMENTAL VALUES:

These workers presented data in graphical form for the solubility of chlorine at partial pressures up to 10^5 Pa in hydrochloric acid of concentrations in the range 2 to 10 moles per litre at temperatures between 30 to 90 °C. They proposed the following smoothing equation for the solubility of chlorine

$$S = (\alpha C + \beta) p \qquad \dots (1)$$

where p is the pressure in units of atmosphere. C is the concentration of hydrogen chloride in molality or g dm⁻³. α and β were functions of temperature and when C was expressed in g dm⁻³

$$\log \alpha = -1.21 \times 10^{-2} \text{ t} - 1.603$$
 and $\beta = 2.14 \times 10^{2} \text{ t}^{-1.21}$ where t = Temperature in °C.

The constants for equation (1) are given below.

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Flow system similar to that used by Whitney and Vivian (1). Chlorine and nitrogen mixture of known composition and pressure bubbled through acid of known composition. After one hour, samples of saturated liquid analysed by adding to excess potassium iodide and titrating the liberated iodine with sodium thiosulfate. Partial pressure of chlorine varied by adjusting proportion in nitrogen chlorine mixture.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

REFERENCES:

Whitney, R. P.; Vivian, J. E. Ind. Eng. Chem.
 1941, 33, 741.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Hydrochloric acid; HCl; [7647-01-0]

ORIGINAL MEASUREMENTS:

Hine, F.; Inuta, S.

Bull. Chem. Soc. Japan

1968, 41, 71-75.

EXPERIMENTAL VALUES:

t/°C	(K/T) × 10 ³	α α (†) \times 10 ³	α (*) \times 10 ²	β β(§) × 10 ²	β(#)
30	3.300	6.57	1.08	4.85	3.42
40	3.195	5.11	0.844	3.49	2.46
50	3.096	3.65	0.592	2.72	1.92
70	2.915	2.20	0.350	1.76	1.22
90	2.755	1.38	0.204	1.32	0.916

 $^{^{\}dagger}$ $\alpha/(\text{mole Cl}_2 \text{ per 1000 gm solvent})/(\text{mole HCl per 1000 gm solvent})$ (atm))

^{*} $\alpha/(g Cl_2 per dm^3 solvent)/(g HCl per dm^3 solvent)(atm))$

 $[\]beta$ β /(mole Cl₂ per 1000 gm solvent/atm)

 $^{^{\}sharp}$ $\beta/(g Cl_2 per dm^3 solvent/atm)$

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Electrolyte solutions

EVALUATOR:

Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia. June 1981.

CRITICAL EVALUATION:

Note on the data of Karapysh and coworkers

Karapysh and coworkers have made fairly extensive studies of the solubility of chlorine in aqueous solutions but the data are, in general, presented in a graphical form or the work was presented in journals which are not readily available. In many cases the information was presented in an ambiguous manner and the meaning of the tables and graphs was not clear.

The solubility of chlorine in perchloric acid has been investigated by Semchenko et al. (1), Loseva et al. (2), Levchenko and Karapysh (3) and Semchenko and Karapysh (4). In reference (1) a graph of solubility (g dm $^{-3}$) versus chlorine pressure was given.

In a later paper Smirnov et al. (5) presented the solubility of Chlorine in hydrochloric acid. The data were presented only in graphical form.

Smirnov and Aliev (6) presented results for the solubility of chlorine in aqueous solutions of lithium chloride, sodium chloride and of potassium chloride. The results were presented in graphical form. Atable was given in the paper but the values do not agree, even approximately, with the data presented in the graphs.

Aliev et al. (7) studied the solubility of chlorine in water and in aqueous sodium chloride solution. Blaznina et al. (8) studied the solubility of chlorine in aqueous barium chloride at concentrations in the range 0.1 to 3.0 mol dm $^{-3}$ and temperatures in the range 10 to 50 °C. Karapysh and Semchenko (9) studied the solubility of chlorine in aqueous solutions of lithium chloride, strontium chloride and barium chloride. Karapysh and Semchenko (10) also studied the solubility of chlorine in aqueous solutions of lithium and sodium perchlorates. The papers (7) to (10) could not be obtained by us despite considerable effort.

References

- Semchenko, D. P.; Smirnov, V. A.; Aliev, Z. M.; Karapysh, V. V. Zh. Fiz. Khim. 1974, 48, 1002; Russ. J. Phys. Chem. 1974, 48, 580-581.
- Loseva, G. K.; Semchenko, D. P.; Il'in, K. G. Tr. Novocherk. Politekh. Inst. <u>1969</u>, 197, 37.
- 3. Levchenko, V. M.; Karapysh, V. V. Gidrokhim. Mater. 1969, 51, 153.
- Semchenko, D. P.; Karapysh, V. V. Tr. Novocherk. Politekh. Inst. 1956, 48, 19.
- Smirnov, V. A.; Aliev, Z. M.; Karapysh, V. V.; Gurchin, I. I.
 Zh. Fiz. Khim. 1974, 48, 1241; Russ. J. Phys. Chem. 1974, 48, 720.
- 6. Smirnov, V. A.; Aliev, Z. M. Zh. Fiz. Khim. 1976, 50, 1132; Russ. J. Phys. Chem. 1976, 50, 684.
- Aliev, Z. M.; Karapysh, V. V.; Smirnov, V. A. Tr. Novocherk. Politekh. Inst. 1972, 266, 155.
- 8. Blaznina, V. A.; Fedorina, V. F.; Shul'gina, G. A.; Karapysh, V. V. Nauch. Raboty Stud. Khim.-Tekhnol.Fak., Novocherkasshii Politekh. Inst. im. S. Ordzhonikidze 1959, 7, 17.
- Karapysh, V. V.; Semchenko, D. P. Tr. Novocherk. Politekh. Inst. 1960, 98, 173.
- 10. Karapysh, V. V.; Semchenko, D. P. Tr. Novocherk. Politekh. Inst. 1959, 65, 111.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Sulfuric acid; H₂SO₄; [7664-93-9]

ORIGINAL MEASUREMENTS:

Sherrill, M. S.; Izard, E. F.

J. Am. Chem. Soc.

1931, 53, 1667-1674.

VARIABLES:

Concentration of acid

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol kg ⁻¹ (H ₂ O)	Conc. of chlorine /mol kg ⁻¹ (H ₂ O)	Mole fraction of chlorine $^x\mathrm{Cl}_2$
298.15	0.0000 0.4995 1.0240 1.9686 3.0090 3.9934 4.9901	0.0923 0.06272 0.05617 0.04973 0.04550 0.04278	0.001660 0.001119 0.000993 0.000865 0.000777 0.000718

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine bubbled through solution.

Absorption train painted black to prevent decomposition of chlorine by light. Before the liquid sample was analysed the saturated solution was allowed to equilibrate for at least 3 hours without chlorine being bubbled through. Amount of chlorine determined by reaction with potassium iodide and titrating liberated iodine with sodium thiosulfate.

SOURCE AND PURITY OF MATERIALS:

 Chlorine prepared by action of hydrochloric acid on chromic acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$; $\delta x_{Cl_2} = \pm 2\%$ (estimated by compiler).

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Sherrill, M. S.; Izard, E. F. 2. Water; H₂O; [7732-18-5] J. Am. Chem. Soc. 3. Barium chloride; BaCl₂; [10361-37-2] 1931, 53, 1667-1674. VARIABLES: PREPARED BY: Concentration of salt C. L. Young EXPERIMENTAL VALUES:

EXPERIMENTAL V	/ALUES:		
T/K	Conc. of salt /mol kg ⁻¹ (H ₂ O)	Conc. of chlorine /mol kg ⁻¹ (H ₂ O)	Mole fraction of chlorine ^x Cl ₂
298.15	0.000 0.330 0.667 1.000	0.0923 0.06216 0.05494 0.04924 0.04468	0.001660 0.001112 0.000977 0.000871 0.000785

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine bubbled through solution.
Absorption train painted black to
Prevent decomposition of chlorine
by light. Before the liquid sample
Was analysed the saturated solution
Was allowed to equilibrate for at
least 3 hours without chlorine being
bubbled through. Amount of
chlorine determined by reaction with
Potassium iodide and titrating
liberated iodine with sodium
thiosulfate.

SOURCE AND PURITY OF MATERIALS:

 Chlorine prepared by action of hydrochloric acid on chromic acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$; $\delta x_{Cl_2} = \pm 2\%$ (estimated by compiler).

ORIGINAL MEASUREMENTS: 1. Chlorine; Cl₂; [7782-50-5] Sherrill, M. S.; Izard, E. F. 2. Water; H₂O; [7732-18-5] J. Am. Chem. Soc. 3. Sodium chloride; NaCl; [7647-14-5] 1931, 53, 1667-1674. VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

т/к	Conc. of salt /mol kg ⁻¹ (H ₂ O)	Conc. of chlorine /mol kg ⁻¹ (H ₂ O)	Mole fraction of chlorine ^x Cl ₂
298.15	0.000	0.0923	0.001660
	0.501	0.06575	0.001183
	0.998	0.05795	0.001025
	2.991	0.04161	0.000711
	3.989	0.03601	0.000605
	4.989	0.03087	0.000510

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine bubbled through solution. Absorption train painted black to prevent decomposition of chlorine by light. Before the liquid sample was analysed the saturated solution was allowed to equilibrate for at least 3 hours without chlorine being bubbled through. Amount of chlorine determined by reaction with potassium iodide and titrating liberated iodine with sodium thiosulfate.

SOURCE AND PURITY OF MATERIALS:

 Chlorine prepared by action of hydrochloric acid on chromic acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01;$ $\delta x_{Cl_2} = \pm 2\%$ (estimated by compiler).

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Water; H₂O; [7732-18-5]
- 3. Potassium chloride; KCl; [7447-40-7]

ORIGINAL MEASUREMENTS:

Sherrill, M. S.; Izard, E. F.

J. Am. Chem. Soc.

1931, 53, 1667-1674.

VARIABLES:

Concentration of salt

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

т/к	Conc. of salt /mol kg ⁻¹ (H ₂ O)	Conc. of chlorine /mol kg ⁻¹ (H ₂ O)	Mole fraction of chlorine "Cl ₂
298.15	0.000	0.0923	0.001660
	0.500	0.06610	0.001179
	1.000	0.06109	0.001080
	2.013	0.05388	0.000936
	3.014	0.04865	0.000831
	3.913	0.04724	0.000794

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine bubbled through solution. Absorption train painted black to prevent decomposition of chlorine by light. Before the liquid sample was analysed the saturated solution was allowed to equilibrate for at least 3 hours without chlorine being bubbled through. Amount of chlorine determined by reaction with potassium iodide and titrating liberated iodine with sodium thiosulfate.

SOURCE AND PURITY OF MATERIALS:

 Chlorine prepared by action of hydrochloric acid on chromic acid.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$; $\delta x_{Cl_2} = \pm 2\%$ (estimated by compiler).

COMPONENTS:

1. Chlorine; Cl₂; [7782-50-5]

2. Organic liquids

EVALUATOR:

P. G. T. Fogg,
Department of Chemistry,
Polytechnic of North London,
Holloway,
London, U.K.
September 1980

CRITICAL EVALUATION:

It is not possible, in general, to judge between the merits of different apparatus from the information which has been given by authors. In the descriptions of technique it has not always been clearly stated or implied whether or not allowance has been made for the partial pressure of the solvent in the calculation of the partial pressure of chlorine. In the case of solvents which have low volatility at the temperature of measurement such correction is of little importance. However, at a temperature of about 50 K below the normal boiling point of a typical solvent the partial vapor pressure of the solvent is about 0.08 atm and appropriate correction becomes increasingly important for measurements at higher temperatures. Uncertainty as to whether appropriate correction has been made by authors leads to corresponding uncertainty in the significance of the results which have been reported.

Where solubilities have been reported for a range of temperatures and the partial pressure of chlorine equal to 1 atm or a sum of partial pressures of chlorine and solvent equal to 1 atm, the evaluator has carried out a least squares analysis to fit values of $\mathrm{RTln}x_{\mathrm{Cl}_2}$ to equations of the form:

$$-RTlnx_{Cl_2} = a + bT$$

where x_{Cl_2} is the mole fraction solubility of chlorine at a temperature T. In several cases solubilities were measured at an unstated barometric pressure. Any differences between a standard atmosphere and barometric pressure have been neglected for the purpose of general comparison of results.

If $\Delta \overline{G}^{\circ}$, $\Delta \overline{H}^{\circ}$ and $\Delta \overline{S}^{\circ}$ are defined as the change in Gibbs free energy, enthalpy and entropy for the hypothetical process:

$$Cl_2$$
 (1 atm) \rightarrow Cl_2 (solution, $x_{Cl_2} = 1$)

it follows that:

 $\Delta \overline{G}^{\circ}$ \simeq $-RTlnx_{Cl_2}$ $\Delta \overline{H}^{\circ}$ \simeq a $\Delta \overline{S}^{\circ}$ \simeq -b

provided that the solubility is measured at a partial pressure of chlorine equal to 1 atm (1). Values of α and b are given in table I.

In the cases where it appears to the evaluator that no allowance has been made by the authors for the vapor pressure of a volatile solvent, "corrected" solubility values have been determined. These "corrected" solubilities have been calculated using published vapor pressure data (2). It has been assumed that dissolution of chlorine lowers the partial vapor pressure of the solvent in accordance with the relationship:

$$p_{\text{solvent}} = p_{\text{solvent}}^{\circ} (1 - x_{\text{Cl}_2})$$

and that x_{Cl_2} (p_{Cl_2} = 1 atm) may be calculated from x_{Cl_2} (p_{Cl_2} + p_{Solvent} = 1 atm) by assuming that x_{Cl_2} is directly proportional to p_{Cl_2} over a small pressure range. This procedure, used by Hildebrand, is subject to limitations (3), (4). The "corrected" solubilities have been subjected to least squares analysis and fitted to equations of the form:

$$-RTlnx$$
Cl₂(corrected) = $a' + b'T$.

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COMPONENTS:	EVALUATOR:
 Chlorine; Cl₂; [7782-50-5] Organic liquids 	P. G. T. Fogg, Department of Chemistry, Polytechnic of North London, Holloway, London, U.K.
	September 1980

CRITICAL EVALUATION:

Values of a' and of b' are also given in table I. In view of the uncertainties involved they are not necessarily better constants than values of a and b.

Solubility measurements made at a single temperature have been collected together in table II and values of $x_{\rm Cl_2}$ (corrected) are given where appropriate.

The average value of α is -18935 J mol⁻¹. The average is -17284 J mol⁻¹ if the "corrected" values, α ', are taken into account. The enthalpy of vaporization of liquid chlorine, calculated from the variation of vapor pressure with temperature (2), is 19912 J mol⁻¹ at 298.16 K. The average value of b is 80.10 J K⁻¹ mol⁻¹ or 74.43 J K⁻¹ mol⁻¹ if "corrected" values of b' are taken into account. These values can be compared with the value of Δ S° for the process:

$$Cl_2$$
 (liquid) \rightarrow Cl_2 (vapor; 1 atm) at 298.16 K.

The value of this entropy change, calculated by the evaluator from the variation of vapor pressure of chlorine with temperature (2), is 83.68 $^{\circ}$ J K $^{-1}$ mol $^{-1}$. It follows that, on average, for the solvents under consideration there is no great difference between the values of $\Delta \overline{\rm G}^{\circ}$, $\Delta \overline{\rm H}^{\circ}$, and $\Delta \overline{\rm S}^{\circ}$ for the hypothetical process:

$$Cl_2(gas, l atm) \rightarrow Cl_2(solution, x_{Cl_2} = 1)$$

and the corresponding values for the process:

$$Cl_2(gas, 1 atm) \rightarrow Cl_2(liquid)$$
.

Experimental measurements of solubilities of chlorine which have led to values of a or a' and b or b' which differ appreciably from mean values are not necessarily unreliable but ought to be used with caution. Measurements which have given large standard deviations from the smoothing equations should also be treated with similar caution.

Experimental values of x_{Cl_2} (1 atm) as a function of T for various systems are shown in figs. 1 and 2. On these graphs are also plotted reference lines corresponding to the equation:

$$x_{\text{Cl}_2} = p_{\text{Cl}_2}/p^{\circ}_{\text{Cl}_2}$$

where $p^{\circ}_{\text{Cl}_2}$ is the vapor pressure of liquid chlorine at temperature T. As explained by Gerrard (4), comparison of experimental results with reference lines can give an estimation of the reliability of the measurements.

Experimental curves showing the variation of the mole fraction solubility of a gas as a function of temperature at constant pressure are often similar in shape to the corresponding reference lines. Solvents of similar structure usually show similar behavior relative to the reference line for a particular gas.

The general considerations outlined above lead to the following detailed observations on the results which have been reported:

Trichloromethanesulfenyl chloride

Values of α and b are large compared with average values. There is nothing unusual in the graph of x_{Cl_2} against T and the measurements (5) are classified as tentative.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Organic liquids

EVALUATOR:

P. G. T. Fogg, Department of Chemistry, Polytechnic of North London, Holloway, London, U.K. September 1980

CRITICAL EVALUATION: Carbon disulfide

Values of α and b are large compared with the average. "Corrected" values, a' and b' are a little closer in line with the average. "Uncorrected" values of x_{Cl_2} become increasingly lower than corresponding points on the reference line with increasing temperature. In contrast, "corrected" values become increasingly higher than the reference line with increasing temperature. The data of Raskina $et\ al$. (5) are classified as tentative.

Tetrachloromethane

The solubilities of chlorine in this liquid are evaluated on page 395.

Mixtures of tetrachloromethane, trichloromethanesulfenyl chloride and carbon disulfide

The solubilities of chlorine in six mixtures of the three solvents were measured by Raskina $et\ al.$ (5). In the case of two of the mixtures there is a discrepancy between solubilities given by the authors as mole fractions and those given as weight fractions. It is not clear which figures are erroneous.

Each mole fraction solubility, x_{Cl_2} , reported by the authors is close to the sum of the solubilities, x'_{Cl_2} , in the separate portions of the pure solvents which were used to make up the mixture. (Coef. corr. 0.8731; $x_{\text{Cl}_2}/x'_{\text{Cl}_2} = 1.01 \pm 0.03$.) The agreement between weight fraction solubilities, w_{Cl_2} , given by the authors and the sum weight fraction solubilities, w'_{Cl_2} , in separate portions of the pure liquid is not as good. (Coef. corr. 0.3772; $w_{\text{Cl}_2}/w'_{\text{Cl}_2} = 0.97 \pm 0.07$.)

Tetrachloroethene

The standard deviation of uncorrected values of $\mathrm{RTln}x_{\mathrm{Cl}_2}$ is about 8%. Corrected values have a standard deviation of about 3%. Uncorrected values of a and b are above average whereas corrected values are about average. A plot of uncorrected values of x_{Cl_2} crosses the reference line, i.e., exhibits both positive and negative deviations from Raoult's law. Corrected values of x_{Cl_2} fall on a curve which approaches but does not cross the reference line as the temperature is increased. The "corrected" values are to be preferred (6).

1,1,2,2-Tetrachloroethane

Standard deviations of both uncorrected and corrected values of $RT \ln x_{Cl_2}$ are about 6%. Corrected and uncorrected values of α and b are clearly considerably smaller than in any other similar system. The measurements (7) must therefore be considered doubtful.

Acetic acid

Values of α and b based on measurements by Kumar and Gehlawat (8) are appreciably greater than mean values. A plot of "uncorrected" values of x_{Cl_2} (1 atm) against T is close to a straight line which would indicate a very unusual temperature dependence of solubility. "Corrected" values of solubility do not show such an unusual temperature dependence and are deemed more reliable. Jones (9) measured solubilities at 289.2 K and low pressures of chlorine. Extrapolation of these results to 1 atm gives a value close to that obtained by extrapolating the results of Kumar and Gehlawat (8) to 289.2 K by use of the "corrected" smoothing equation.

Alkanes

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COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] 2. Organic liquids EVALUATOR: P. G. T. Fogg, Department of Chemistry, Polytechnic of North London, Holloway, London, U.K. September 1980

CRITICAL EVALUATION:

However, in view of uncertainty of the "correction" to Kumar and Gehlawat (8) values and the extrapolation from low pressure needed to compare Jones (9) values, both sets of data are classified as doubtful.

1,1,2,3,4,4-Hexachloro-1,3-butadiene

The measurements of Kogan et~al. (10) indicate that $x_{\rm Cl_2}$ is proportional to $p_{\rm Cl_2}$ in the range 408 mmHg to 974 mmHg at 303 K with $p_{\rm Cl_2}/x_{\rm Cl_2}$ equal to 4827 ± 17 mmHg. Values of $x_{\rm Cl_2}$ (1 atm) for temperatures in the range 253 K to 365 K are close to corresponding values for tetrachloromethane and are classified as tentative.

Chlorobenzene

Values of α and b based on the measurements by Cervinka (11) at three temperatures are well below average and differ appreciably from values based upon measurements by Krentsel et αl . (12) and by Zetkin et αl . (13). However, with the exception of a measurement at 298 K by Cervinka (11) which appears to be erroneous and which distorts the pattern of his results, solubilities reported by the different authors fall into a consistent pattern. "Corrected" smoothing equation constants, α' and b', from Zetkin's results agree more closely than "uncorrected" values with the corresponding constants based upon the work of Krentsel et αl . (12). However, because of the low volatility of the solvent at the temperature of measurement, such correction for the vapor pressure of the solvent is of little significance. The following equation, based upon "corrected" measurements by Zetkin et αl . (13) and measurements by Krentsel et al. (12), is recommended:

$$\Delta G^{\circ}/J \text{ mol}^{-1} = (-RTlnx_{Cl_2})/J \text{ mol}^{-1} = -19804 + 81.654T/K$$

Std. dev. $\Delta G^{\circ}/J \text{ mol}^{-1} = 154;$ Coef. corr. = 0.9951.

Benzene

There is appreciable disagreement between results over a range of temperatures which have been published by different authors. Corresponding values of a and b are inconsistent. However "corrected" solubilities based upon measurements by Zetkin $et\ al$. (13) are close to the values based upon the results of Cervinka (11). To estimate solubilities at 1 atm from the results given by Krivonos (14), it is assumed that Bunsen coefficients are independent of the pressure at which they are measured. This procedure may introduce considerable error and explain why these solubilities are appreciably greater than those based upon the work of Cervinka (11) and Zetkin $et\ al$. (13). Nevertheless, the measurement at 1 atm and 293 K by Pozin and Opykhtina (15) is close to the value based upon Krivonos' (14) work. The following equation is based upon a combination of "corrected" measurements by Zetkin $et\ al$. (13) and measurements by Cervinka (14):

$$\Delta G^{\circ}/J \text{ mol}^{-1} = (-RTlnx_{Cl_2})/J \text{ mol}^{-1} = -15043 + 66.633T/K$$

Std. dev. $\Delta G^{\circ}/J \text{ mol}^{-1} = 192$; Coef. corr. = 0.9872.

Values of $x_{\rm Cl_2}$ measured by Pozin and Opykhtina (15) at 293 K for the range 49 mmHg to 763 mmHg give a standard deviation of 9.6% when expressed as a linear function of $p_{\rm Cl_2}$.

COMPONENTS:	EVALUATOR:
 Chlorine; Cl₂; [7782-50-5] Organic liquids 	P. G. T. Fogg, Department of Chemistry, Polytechnic of North London, Holloway, London, U.K.
	September 1980

CRITICAL EVALUATION:

Mixtures of trifluoromethylbenzene and its ring substituted chlorinated derivatives

Solubilities of chlorine in pure trifluoromethylbenzene and in mixtures with chlorinated derivatives were measured by Ushakov et~al. (16). Solubilities increased with the proportion of chlorinated derivatives present. In each case plots of $x_{\rm Cl_2}$ against T fall on a smooth curve which tends to approach the reference line with increase in temperature. Data for the smoothing equation:

$$-RTln x_{Cl_2} = a + bT$$

are as follows:

	omposition before passage of chlorine (wt-%)				b	Coef.	(Std. dev.) /J mol ⁻¹
$C_7H_5F_3$	C7H4ClF3	C ₇ H ₃ Cl ₂ F ₃	/J mol ⁻¹	/JK ⁻¹ mol ⁻¹		of RTlnxCl2	
100	•••	_	-22918	94.563	0.9972	184	
84.84 58.29	15.16 39.47	- 2.24	-20233 -20851	84.933 86.514	0.9982 0.9994	105 65	
22.82	60.86	16.32	-16565	71.346	0.9989	70	

The proportions of the different isomers having the same empirical formulae were not determined.

Cyclohexane

Solubilities at three temperatures, 283 K, 293 K and 313 K, over a range of pressures were measured by Tsiklis and Svetlova (17). In each case a plot of $x_{\rm Cl_2}$ vs. $p_{\rm Cl_2}$ (T const.) is a curve which, when extrapolated, cuts the reference line for constant temperature at values of $x_{\rm Cl_2}$ ranging from about 0.1 to about 0.16. This behavior is unusual and the data ought to be used with caution. The data are classified as doubtful.

Methylbenzene

Values of a and b are high compared with the average. "Corrected" values, a' and b', while still above the average values appear to be reasonable. A plot of "uncorrected" values of $x_{\rm Cl_2}$ against T cuts the reference line. "Corrected" values fall on a curve which approaches but does not cut the reference line. These values seem to be more acceptable than the "uncorrected" values (18).

Heptane

Solubilities measured by Semb (19) are consistent with those measured by Zetkin et al. (20) over a shorter temperature range and with the measurement by Taylor and Hildebrand (3) at the single temperature of 273 K. Values above about 333 K should be used with caution because of uncertainties associated with the effect of the vapor pressure of the solvent and the difficulties of making satisfactory corrections as the

Alkanes

COMPONENTS:

- 1. Chlorine; Cl_2 ; [7782-50-5]
- 2. Organic liquids

EVALUATOR:

September 1980

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Department of Chemistry,
Polytechnic of North London,
Holloway,
London, U.K.

CRITICAL EVALUATION:

temperature approaches the b.p. of the solvent. The values of a and b based on Zetkin et al. results lie close to values for other hydrocarbons also based upon Zetkin et al. results. "Correction" of results leads to some inconsistencies between values of a' and b' for different hydrocarbons. It may therefore be preferable to use "uncorrected" values of solubilities of heptane and other hydrocarbons studied by Zetkin et al. (20).

Dichlorodioxochromium

A plot of $x_{\rm Cl_2}$ (1 atm) against T based upon measurements by Roozeboom (21) approaches the reference line with increase in temperature and values are acceptable. Values of $x_{\rm Cl_2}$ at 273.2 K for the pressure range 753 to 1302 mmHg differ from values given by the equation:

$$x_{\text{Cl}_2} = p_{\text{Cl}_2}/p^{\circ}_{\text{Cl}_2}$$

by about 4% and can be fitted to a curve which cuts the reference line for a constant temperature of 273.2 K at $x_{\rm Cl_2} = 0$ and $x_{\rm Cl_2} = 1$. This is a good indication that the measurements are acceptable (4) and add support to the validity of the way in which the original measurements were interpreted when the data were compiled.

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- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Organic liquids

EVALUATOR:

P. G. T. Fogg, Department of Chemistry, Polytechnic of North Soldon, Holloway, London, U.K. September 1980

CRITICAL EVALUATION:

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Table I. Quantitative evaluation of measurements of the solubility of chlorine in liquids at 1 atm.

					Sn	noothing	equati	on	Corre	cted smo	othing	equation
					Consta	ints			Const	ants		4
Solvent	b.p. /K	Authors	Temp. range /K	Allowance for v.p. of solvent	a /J mol ⁻¹	b /JT ⁻¹ mol ⁻¹	Coef.	(Std.dev.) /J mol ⁻¹ of RTlnxCl ₂	a	b /JT ⁻¹ mol ⁻¹	Coef.	(Std.dev.) /J mol ⁻¹ of RTlnxCl ₂
CHCl ₃ ; Trichloromethane	335	VK	257-298	Yes	-19788	84.219	0.9973	108			····	
CH ₂ Cl ₂ ; Dichloromethane	313.	VK	254-298	Yes	-17147	76.348	0.9996	42				
CCl ₄ ; Tetrachloromethane	349	†	253-353	Yes	-18728	78.052	0.9995	83				
CCl ₄ S; Trichloromethane- sulfinyl chloride	422	RZZKK	275-308	No	-23717	98.600	0.9906	159				
CS ₂ ; Carbon disulfide	319	RZZKK	275-298	No	-24996	102.504	0.9995	30	-14570	63.636	0.997	43
C ₂ Cl ₄ ; Tetrachloroethene	394	СН	273-363	No	-22825	92.530	0.9920	387	-18750	78.377	0.9983	3 151
C ₂ H ₂ Cl ₄ ; 1,1,2,2-Tetrachloro- ethane	419	KN	298-383	No	-12509	62.349	0.9721	502	-8674	50.056	0.9612	2 479
C ₂ H ₄ Br ₂ ; 1,2-Dibromoethane	405	TH	293;313	Yes	-18257	75.999	_	_				
C ₂ H ₄ O ₂ ; Acetic acid	391	KG	303-333	No	-26872	111.932	0.9926	176	-24136	102.76	0.9935	5 151
C4Cl6; 1,1,2,3,4,4-Hexa- chloro-1,3- butadiene	488	KKL	253-365	No	-17228	72.090	0.9997	66	-17082	71.570	0.9997	7 72
C ₆ H ₃ Cl ₃ ; 1,2,4-Trichloro- benzene	487	zksd	288-333	No	-22450	89.500	0.9995	48				
C ₆ H ₃ Cl ₂ NO ₂ ; l,2-Dichloro-4- nitrobenzene		ZKZD	333-433	No	-17771	78.307	0.9999	30				(cont.)

Table I (cont.)										·		
					Sı	moothing	equation	on	Correc	ted smo	othing	equation
					Const	ants			Consta	nts		
Solvent	b.p. /K	Authors	Temp. range /K	Allowance for v.p. of solvent	a /J mol ⁻¹	b /JT ⁻¹ mol ⁻¹		(Std.dev.) /J mol ⁻¹ of RTlnx _{Cl2}	a /J mol ⁻¹	b /JT ⁻¹ mol ⁻¹	Coef.	(Std.dev.) /J mol ¹ of RTlnx _{Cl2}
C6H3Cl2NO2; l,4-Dichloro-2- nitrobenzene	540	ZKZD	333-433	No	-18585	78.712	0.9999	9 31		30° 00° 00° 00° 00° 00° 00° 00° 00° 00°		
C ₆ H ₄ ClNO ₂ ; 1-Chloro-2- nitrobenzene	519	ZKZD	313-433	No	-17700	78.794	0.9999	9 41				
C ₆ H ₄ ClNO ₂ ; 1-Chloro-3- nitrobenzene	508	ZKZD	333-433	No	-19424	84.055	0.9999	e 36				
C ₆ H ₄ ClNO ₂ ; 1-Chloro-4- nitrobenzene	51.5	ZKZD	373-433	No	-22866	91.459	1.0000) 12				
C ₆ H ₄ Cl ₂ ; 1,2-Dichlorobenzene	454	ZKSD	288-333	No	-20174	81.553	0.9967	7 117	-19930	80.718	0.99	66 117
C ₆ H ₅ Cl; Chlorobenzene	405	С	298-338	Yes	-13327	62.404	0.9943	3 134				
C ₆ H ₅ Cl; Chlorobenzene	405	KLS	313-343	Yes	-17357	74.542	0.9999	9 10				
C ₆ H ₅ Cl; Chlorobenzene	405.	ZKSD	283-333	No	-20090	82.631	0.997	L 199	-18919	78.541	0.99	60 131
C ₆ H ₅ NO ₂ ; Nitrobenzene	484	ZKZD	313-433	No	-19405	82.342	0.9996	5 102	-16838	74.745	0.99	78 213
C ₆ H ₆ ; Benzene	353	С	298-341	Yes	-13448	62.072	0.9970	82				
C ₆ H ₆ ; Benzene	353	K	283-323	Yes	-11182	50.557	0.9963	3 69				
C ₆ H ₆ ; Benzene	353	ZKSD	283-333	No	-23857	97.081	0.9991	L 78	-14836	65.573	0.99	16 160
C ₇ H ₅ Cl ₃ ; Trichloromethyl benzene	494	EKRG	303-423	No	-19730	81.311	0.9955	5 287				
C ₇ H ₅ F ₃ ; Trifluoro- methyl benzene	375	UKSM	279-353	No	-22918	94.563	0.9972	2 184	-16158	71.402	0.99	66 155

(cont.)

					S	moothing	equation	ı	Corre	cted smoo	othing e	quation
					Const	ants			Const	ants		
Solvent	b.p. /K	Authors	Temp. range /K	Allowance for v.p. of solvent	a /J mol ⁻¹	b /JT ⁻¹ mol ⁻¹	Coer.	Std.dev.) /J mol ⁻¹ f RTlnxCl ₂	a /J mol ⁻¹	b /JT ⁻¹ mol ⁻¹	coer.	(Std.dev.) /J mol ⁻¹ of RTlnx _{Cl2}
C ₇ H ₆ Cl ₂ ; Dichloromethyl benzene	478	EKRG	303-403	No	-18877	78.531	0.9957	235				
C ₇ H ₇ Cl; Chloromethyl benzene	452	EKRG	303-383	No	-18003	75.960	0.9958	191				
C ₇ H ₈ ; Methyl benzene	384	EKRG	303-353	No	-26746	104.440	0.9967	158	-19709	81.343	0.9932	179
C7H16; Heptane	372	s	254-358	No	-18261	77.873	0.9947	278	-12108	55.750	0.9883	298
C ₇ H ₁₆ ; Heptane		ZKZMD	283-323	No	-15768	69.270	0.9998	19	-12660	58.281	0.9990	40
C ₇ F ₁₆ ; Hexadeca- fluoro heptane	356	GH	273-298	Yes	-13666	65.106	0.9964	24				
C ₈ H ₁₈ ; Octane	399	ZKZMD	283-323	No	-15972	69.416	0.9994	38	-14882	65.579	0.9988	51
C ₈ H ₁₈ ; 2,2,4-Trimethyl pentane	372	ZKZMD	283-323	, No	-15022	66.962	0.9996	28	-11914	55.928	0.9976	61
C ₁₀ H ₂₄ ; Decane	447	ZKZMD	283-323	No	-16770	71.116	0.9994	39	-16613	70.582	0.9993	43
C ₁₄ H ₃₀ ; Tetradecane	527	ZKZMD	283-323	No	-16899	69.183	0.9994	37	-16899	69.183	0.9994	37
Cl ₂ CrO ₂ ; Dichloro- dioxo chromium *	390	R	247-273	No	-19362	82.241	0.9954	65				
Cl ₄ Ti; Titanium chloride *	410	KM	293;303	No	-21816	89.226	_	-				

[†] See evaluation of CCl, by W. Gerrard. b.p. - boiling point at 1 atm pressure. v.p. - vapor pressure.

Solubilities at 1 atm estimated from values at other pressures.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Organic liquids

EVALUATOR:

P. G. T. Fogg, Department of Chemistry, Polytechnic of North London, Holloway, London, U.K. September 1980.

TABLE II

Quantitative evaluation of measurements of the solubility of chlorine in liquids.

Solvent	b.p. /K	Authors	Temp.	Allowance for v.p. of solvent	^x Cl ₂ (1 atm)	"Cl ₂ (corrected) (l atm)
C ₃ H ₇ NO; N,N-dimethyl- formamide	422	DuP	273	-	0.569	
C ₆ H ₆ ; Benzene	353	PO	293	No	0.2081*	0.2254
C ₇ H ₁₆ ; Heptane Cl ₂ O ₂ S;	372	тн	273	Yes		
Sulfuryl chloride	343	Sch	273	No	0.206	
Cl,Si; Tetrachloro- silane	331	TH	273	Yes	0.288	
l,2-Benzene- dicarboxylic acid esters:		PMBK	323	-		
C ₁₀ H ₁₀ O ₄ dimethyl ester	557				0.116*	
C ₁₂ H ₁₄ O ₄ diethyl ester	571				0.124*	
C ₁₆ H ₂₂ O ₄ dibutyl ester	613				0.144*	
C _{2 4} H _{3 8} O ₄ dioctyl ester					0.175*	
C ₂₆ H ₄₂ O ₄ dinonyl ester					0.180*	
C30H50O4 diundecyl ester					0.192*	

estimated from measurements made at other pressures.
b.p. boiling point at 1 atm pressure.

Alkanes

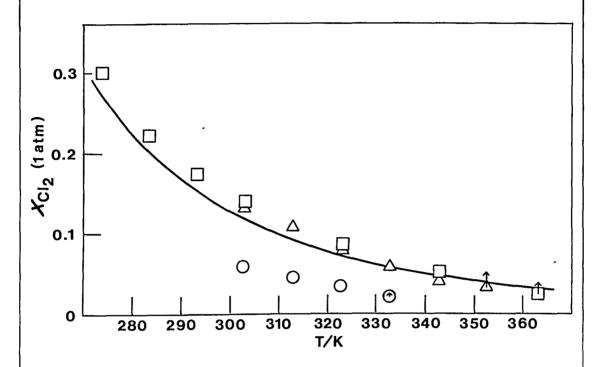
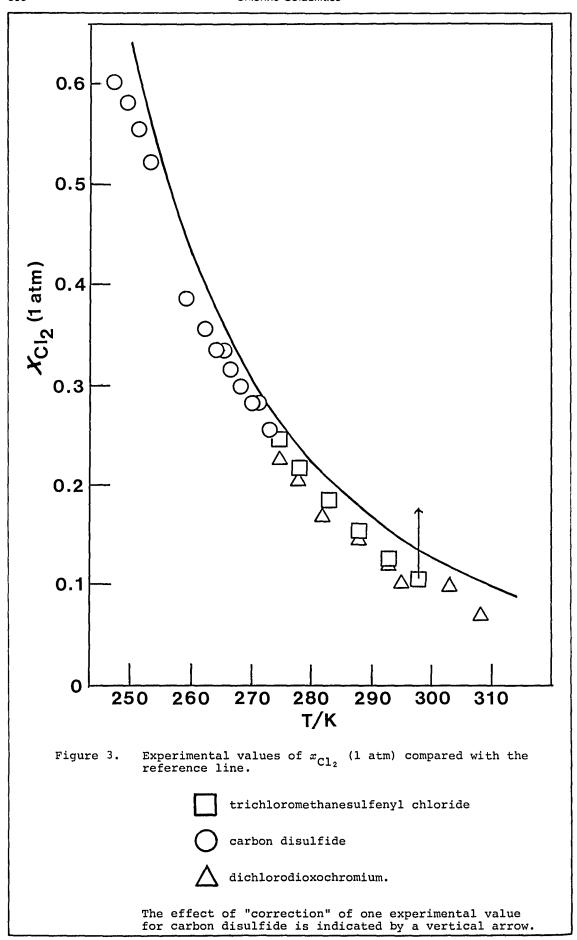


Figure 2. Experimental values of x_{Cl_2} (1 atm) compared with the reference line.

tetrachloroethene
acetic acid
methylbenzene.

The effects of "correction" of one experimental value for each compound are indicated by vertical arrows.



COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Taylor, N. W.; Hildebrand, J. H. J. Amer. Chem. Soc. 1923, 45,
2. Heptane; C ₇ H ₁₆ ; [142-82-5]	682-694.
VARIABLES:	PREPARED BY:
	P. G. T. Fogg
EXPERIMENTAL VALUES:	

T/K	g Cl_2/g of solution	$p_{{\tt Cl_2}}/{\tt mmHg}$	Mol ^x Cl ₂	e fractions x_{Cl_2} (1 atm)
273.16	0.2036	750	0.265	0.270

760 mmHg = 1 atm 1 atm = 1.013×10^5 Pascal

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturator tube (1). Chlorine was bubbled through liquid. Samples of saturated liquid were run into a weighed flask containing aqueous KI, and iodine was titrated with standard solution of thiosulfate. Temperature control was manual to 0.1 K. Saturation was at barometric pressure, $p_{\rm total}$. The value of $p_{\rm C_7H_{16}}$ was estimated by Raoult's law from vapor pressure data for $\rm C_7H_{16}$ in ref. (2). Hence:

 $p_{\text{Cl}_2} = p_{\text{total}} - p_{\text{C}_7\text{H}_{16}}$

SOURCE AND PURITY OF MATERIALS:

- 1. Cl_2 : from an electrolytic supply; contained less than 0.1% of free acid.
- 2. C7H16: not specified.

ESTIMATED ERROR:

- Bichowsky, F. R.; Storch, H. J. Amer. Chem. Soc. 1915, 37, 2695.
- 2. Landolt-Börnstein Tabellen.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl,; [7782-50-5]	Semb, J. J. Am. Pharm. Assoc. 1935, 24,
2. Heptane; C ₇ H ₁₆ ; [142-82-5]	547-553.
VARIABLES:	PREPARED BY:
VARIABLEO.	PREPARED BI:
Temperature	P. G. T. Fogg
EXPERIMENTAL VALUES:	
T/K g Cl ₂ /100 cm ³ s	solution Mole fraction, x_{Cl_2}
254.2 32.9	0.394
262.2 25.9	0.340
273.2 17.9 12.0	0.265 0.197
293.2	0.173
303.2 7.7	0.139
313.2 5.4	0.103
313.7 5.6	0.106
333.2 334.2 334.2	0.0646 0.0604
349.2 2.25	0.0478
350.2	0.0384
358.2	0.0359

The pressure of chlorine plus heptane was equal to barometric pressure (unspecified).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was passed into about 5 cm³ of heptane in a 25 cm³ graduated cylinder until the solution was saturated. The volume of solution was recorded and the dissolved chlorine determined iodometrically. Light was excluded as far as possible but the formation of HCl was detected in all cases.

SOURCE AND PURITY OF MATERIALS:

- Cl₂: from a cylinder purified and dried.
- 2. C₇H₁₆: isolated from a commercial oil and purified by chemical treatment and fractional distillation; b.p. 96.8-97.4 °C (743 mmHg).

ESTIMATED ERROR:

REFERENCES:

1. J. Timmermans, "Physico-Chemical Constants of Pure Organic Compounds", Vol. 2, Elsevier, London. 1965.

^{*} Calculated by compiler using published densities of heptane (1) and assuming that dissolution of chlorine causes no change of volume of the liquid phase.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Zetkin, V. I.; Kosorotov, V. I.; Zakharov, E. V.; Martynov, Yu. M.; Dzhagatspanyan, R. V.
2. Heptane; C ₇ H ₁₆ ; [142-82-5]	Zh. Fiz. Khim. 1970, 44, 830-831. (Complete article deposited at VINITI. No. 1480-70, dep. from 24 Feb. 1970.)
VARIABLES:	PREPARED BY:
Temperature, pressure	P. G. T. Fogg

T/K	Mole fraction, x_{Cl_2} (1 atm)	
283 293	0.195 0.157	760 mmHg = 1 atm
303 313 323	0.125 0.104 0.085	1 atm = 1.013×10^5 Pascal

The authors gave the following equation:

$$\log_{10}(x_{Cl_2}/p_{Cl_2}) = (930/(T/K)) - 3.97$$

where p_{Cl_2} is the pressure of Cl_2 in atm.

This equation cannot be tested because only measurements made at a pressure of chlorine equal to one atmosphere were reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is described in ref. (1). Chlorine at a pressure of 1 atm ± 10 mmHg was absorbed by heptane in a thermostatted vessel of capacity 100 cm³. Chlorination of the heptane was prevented by addition of phenol. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.

It was stated that the system obeys Henry's law as shown by the variation of the absorption when the partial pressure of chlorine was varied by dilution with air. However only measurements made at a partial pressure of one atmosphere were reported.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: to USSR standard GOST 6718-53. Dried by passing through H₂SO₄.
- 2. C₇H₁₆: "Chemically pure" grade dried with molecular sieve.

ESTIMATED ERROR:

REFERENCES:

 Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.; Dzhagatspanyan, R.V. Khim. Promst. (Moscow) 1966, 42 (8), 624.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Zetkin, V. I.; Kosorotov, V. I.; Zakharov, E. V.; Martynov, Yu. M.; Dzhagatspanyan, R. V.
2. Octane; C ₆ H ₁₆ ; [111-65-9]	Zh. Fiz. Khim. 1970, 44, 830-831. (Complete article deposted at VINITI. No. 1480-70, dep. from 24 Feb. 1970.)
VARIABLES:	PREPARED BY:
Temperature, pressure	P. G. T. Fogg

T/K	Mole fraction, x_{Cl_2} (1 atm)	
283 293 303 313	0.210 0.168 0.134 0.107	760 mmHg = 1 atm 1 atm = 1.013 × 10 ⁵ Pascal
323	0.092	

The authors gave the following equation:

$$\log_{10}(x_{\text{Cl}_2}/p_{\text{Cl}_2}) = (950/(\text{T/K})) - 4.02$$

where p_{Cl_2} is the pressure of Cl_2 in atm.

This equation cannot be tested because only measurements made at a pressure of chlorine equal to one atmosphere were reported.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus is described in ref. ('). Chlorine at a pressure of 1 atm ± 10 mmHg was absorbed by octane in a thermostatted vessel of capacity 100 cm³. Chlorination of the octane was prevented by addition of phenol. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.

It was stated that the system obeys Henry's law as shown by the variation of the absorption when the partial pressure of chlorine was varied by dilution with air. However only measurements made at a partial pressure of one atmosphere were reported.

It is not clear whether allowances were made for the contribution of the vapor pressure of octane to the total pressure.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: to USSR standard GOST 6718-53. Dried by passing through H₂SO₄.
- 2. C_8H_{18} : "Chemically pure" grade dried with molecular sieve.

ESTIMATED ERROR:

REFERENCES:

1. Zetkin, V. I.; Kolesnikov, I. M.;
 Zakharov, E. V.; Dzhagatspanyan,
 R.V.
 Khim. Promst. (Moscow) 1966, 42
 (8), 624.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Zetkin, V. I.; Kosorotov, V. I.; Zakharov, E. V.; Martynov, Yu. M.;
2. 2,2,4-Trimethylpentane;	Dzhagatspanyan, R. V. Zh. Fiz. Khim. 1970, 44, 830-831.
C ₈ H ₁₈ ; [540-84-1]	(Complete article deposited at VINITI No. 1480-70, dep. from 24 Feb. 1970.)
VARIABLES:	PREPARED BY:
Temperature, pressure	P. G. T. Fogg

T/K	Mole fraction, x_{Cl_2} (1 atm)	
283 293 303	0.187 0.154	760 mmHg = 1 atm
313 323	0.123 0.101 0.086	1 atm = 1.013×10^5 Pascal

The authors gave the following equation:

$$\log_{10}(x_{\text{Cl}_2}/p_{\text{Cl}_2}) = (870/(\text{T/K})) - 3.77$$

where p_{Cl_2} is the pressure of Cl_2 in atm.

This equation cannot be tested because only measurements made at a pressure of chlorine equal to one atmosphere were reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is described in ref. (1). Chlorine at a pressure of 1 atm ± 10 mmHg was absorbed by isoctane in a thermostatted vessel of capacity 100 cm³. Chlorination of the iso-octane was prevented by addition of 0.5 wt-% of phenol. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.

It was stated that the system obeys Henry's law as shown by the variation of the absorption when the partial pressure of chlorine was varied by dilution with air. However only measurements made at a partial pressure of 1 atm were reported.

It is not clear whether allowances were made for the contribution of the vapor pressure of iso-octane to the total pressure

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: to USSR standard GOST
 6718-53. Dried by
 passing through H₂SO₄.
- 2. C_8H_{18} : "Chemically pure" grade dried with molecular sieve.

ESTIMATED ERROR:

REFERENCES:

 Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.; Dzhagatspanyan, P. B. Khim. Promst. (Moscow) 1966, 42 (8), 624.

3/2 Chlorin	ne Solubilities
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Chlorine; Cl₂; [7782-50-5] Decane; C₁₀H₂₂; [124-18-5] 	Zetkin, V. I.; Kosorotov, V. I.; Zakharov, E. V.; Martynov, Yu. M.; Dzhagatspanyan, R. V. Zh. Fiz. Khim. 1970, 44, 830-831.
	(Complete article deposited at VINITI. No. 1480-70, dep. from 24 Feb. 1970.)
VARIABLES:	PREPARED BY:
Temperature, pressure	P. G. T. Fogg

T/K	p _{Cl₂} /mmHg	Mole fraction $^x\mathtt{Cl}_2$	T/K	$p_{\mathtt{Cl}_2}/\mathtt{mmHg}$	Mole fraction ^x Cl ₂
283	150 275	0.058 0.105	303	550 760	0.115 0.151
	400 550 760	0.150 0.190 0.237	313	150 275 400	0.031 0.053 0.067
293	150 275 400	0.050 0.083 0.101	323	550 760 150	0.092 0.119 0.021
	550 760	0.147 0.192	323	275 400	0.035 0.052
303	150 275 400	0.034 0.058 0.088		550 760	0.074 0.100

The authors have given the following equation:

 $\log_{10}(x_{\rm Cl_2}/p_{\rm Cl_2}) = (1010/(\rm T/K)) - 4.16$ where $p_{\rm Cl_2}$ is the pressure of Cl₂ in atm.

The compiler has calculated that experimental values of $x_{\rm Cl_2}$ for this equation with a standard deviation of 0.008.

760 mmHg = 1 atm

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is described in ref. (1). Chlorine was absorbed by decane in a thermostatted vessel of capacity 100 cm³. Chlorination of the decane was prevented by addition of 0.5 wt-% of phenol. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained. The partial pressure of chlorine was varied by dilution with air. Pressures were controlled to ± 10 mmHg.

It is not clear whether allowances were made for the contribution of the vapor pressure of decane to the total pressure.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: to USSR standard GOST 6718-53. Dried by passing through H₂SO₄.
- 2. $C_{10}H_{22}$: "Chemically pure" grade dried with molecular sieve.

ESTIMATED ERROR:

REFERENCES:

 Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.; Dzhagatspanyan, P. B. Khim. Promst. (Moscow) 1966, 42 (8), 624.

COMPONENTS: 1. Chlorine; Cl ₂ ; [7782-50-5] 2. Tetradecane; C ₁₄ H ₃₀ ; [629-59-4]	ORIGINAL MEASUREMENTS: Zetkin, V. I.; Kosorotov, V. I.; Zakharov, E. V.; Martynov, Yu. M.; Dzhagatspanyan, R. V. Zh. Fiz. Khim. 1970, 44, 830-831. (Complete article deposited at VINITI. No. 1480-70, dep. from 24 Feb. 1970.)
VARIABLES: Temperature, pressure	PREPARED BY: P. G. T. Fogg

T/K	Mole fraction, x_{Cl_2} (1 atm)	
283	0.316	760
293 303	0.254 0.202	760 mmHg = 1 atm
313 323	0.158 0.132	1 atm = 1.013 × 10 ⁵ Pascal

The authors gave the following equation:

$$\log_{10}(x_{\text{Cl}_2}/p_{\text{Cl}_2}) = (1090/(\text{T/K})) - 4.32$$

where p_{Cl_2} is the pressure of Cl_2 in atm.

This equation cannot be tested because only measurements made at a pressure of chlorine equal to one atmosphere were reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is described in ref. (1). Chlorine at a pressure of 1 atm ± 10 mmHg was absorbed by tetradecane in a thermostatted vessel of capacity 100 cm³. Chlorination of the tetradecane was prevented by addition of 0.5 wt-% of phenol. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.

It was stated that the system obeys Henry's law as shown by the variation of the absorption when the partial pressure of chlorine was varied by dilution with air. However only measurements made at a partial pressure of one atmosphere were reported.

It is not clear whether allowances were made for the contribution of the vapor pressure of tetradecane to the total pressure.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl_2 : to USSR standard GOST 6718-53.

ESTIMATED ERROR:

REFERENCES:

 Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.; Dzhagatspanyan, P. B. Khim. Promst. (Moscow) 1966, 42 (8), 624.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Cyclohexane; C_6H_{12} ; [110-82-7]

ORIGINAL MEASUREMENTS:

Tsiklis, D. S.; Svetlova, G. M.; Zh. Fiz. Khim. 1958, 32, 1476.

VARIABLES:

Temperature, pressure

PREPARED BY:

P. G. T. Fogg

EXPERIMENTAL VALUES: T/K pCl ₂ /mmHg	283.2 Mole fraction x Cl ₂	293.2 Mole fraction x Cl ₂	313.2 Mole fraction ^x Cl ₂
100 200 300 400 500 600 700 800 760	0.0129 0.0287 0.0465 0.0692 0.110 mmHg = 1 atm m = 1.013 × 10 ⁵ Pa	0.0092 0.0200 0.0321 0.0472 0.0699 0.111	0.0061 0.0134 0.0213 0.0300 0.0400 0.0515 0.0665 0.0867

The authors gave the following equation:

$$\log_{10} \left\{ \frac{p_{\text{Cl}_2}/\text{mmHg}}{x_{\text{Cl}_2}} \right\} = \log_{10} K - \beta (1 - x_{\text{C}_6 \text{H}_{12}}^2)$$

where K has the values 8240, 12180 and 17400 at 283.2 K, 293.2 K and 313.2 K, respectively and β has the values 1.250, 1.706 and 1.700 at 283.2 K, 293.2 K and 313.2 K, respectively. The compiler has calculated that values of $p_{\text{Cl}_2}/\text{mmHg}$ fit the equation with a standard deviation of 8. The authors have given the head of solution of chlorine calculated from the variation of solubility with temperature as -4500 cal mol $^{-1}$ (± 10-15%).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known weight of chlorine was dissolved in a known weight of cyclohexane and the resulting total pressure was measured by a manometer. The pressure of chlorine was equal to the total pressure minus the vapor pressure of the cyclohexane. Temperatures were controlled to ± 0.1 °C.

SOURCE AND PURITY OF MATERIALS:

Not stated.

ESTIMATED ERROR:

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Pozin, M. E.; Opykhtina, M. A. 2h. Prik. Khim. (Leningrad) 1947, 2. Benzene; C₆H₆; [71-43-2] 20, 523-531. VARIABLES: Pressure Pressure P. G. T. Fogg

EXPERIMENTAL VALUES:

$p_{\text{Cl}_2}/\text{mmHg}$	Mole fraction, x_{Cl_2}	
48.8	0.0152	
53.6 123.4	0.0115 0.0367	Temperature = 293.2 K
263.5 282.5	0.0687 0.0684	760 mmHg = 1 atm
311.5 416	0.0775 0.1091	$1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$
460 494	0.1287 0.1378	
663	0.1708	
693 730	0.1809 0.1978	
763	0.2089	•

The authors gave the Henry's law constant as:

$$H = 3.8 \times 10^3 \text{ mmHg/}x_{\text{Cl}_2}$$

The compiler has calculated that the mean value of $(p_{\rm Cl_2}/{\rm mmHg})/x_{\rm Cl_2}$ is 3788 with a standard deviation of 362.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The volume of chlorine absorbed by a measured quantity of benzene was determined by use of apparatus described in ref. (1). The absorbing liquid was stirred and maintained at a temperature constant to within 2 °C.

SOURCE AND PURITY OF MATERIALS:

2. C_6H_6 : b.p. 80.5 °C (barometric pressure unspecified); density (20 °C) 0.8796 g cm⁻³.

ESTIMATED ERROR:

REFERENCES:

Pozin, M. E.
 Zh. Prik. Khim. (Leningrad)
 1947, 20, 345.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Krivonos, F. F. J. Appl. Chem. USSR 1958, 31,
2. Benzene; C ₆ H ₆ ; [71-43-2]	487-491.
VARIABLES:	PREPARED BY:
Temperature	P. G. T. Fogg
EXPERIMENTAL VALUES:	

т/к	Bunsen coefficient	Mole fraction, $x_{\text{Cl}_2}^*$ (1 atm) (calculated by compiler)
283.2	95	0.274
293.2	69	0.217
303.2	57	0.189
313.2	49	0.168
323.2	42	0.149

Values of x_{Cl_2} (1 atm) have been calculated by the compiler on the assumption that the Bunsen coefficient is independent This is equivalent to assuming the validity of pressure. of Henry's law (mole ratio form).

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: A mixture of chlorine and air was admitted into a round bottomed flask of known volume. quantities of the two were calculated from the total weight, total volume and total pressure of the Not specified mixture (measured by a manometer). A measured volume of benzene was introduced and the total pressure measured after equilibrium had been reached. The partial pressure of chlorine, p_{Cl2}, was calcu-ESTIMATED ERROR: lated from: $p_{\text{total}} = p_{C_6H_6} + p_{\text{air}} + p_{Cl_2}$ It was assumed that $p_{\ensuremath{\mathrm{C_6H_6}}}$ was equal REFERENCES: to the vapor pressure of pure benzene. Temperatures were controlled by a thermostat bath and

light was excluded as far as possible. The authors claimed that reproducible results indicated that no irreversible reaction between benzene and chlorine took place

	0.110	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,
COMPONENTS:		ORIGINAL MEASUREMENTS:
 Chlorine; 	Cl ₂ ; [7782-50-5]	Cervinka, M.
2. Benzene,	C ₆ H ₆ ; [71-43-2]	Chem. Prum. <u>1960</u> , 10, 249-251.
VARIABLES:		PREPARED BY:
Pre	ssure, temperature	P. G. T. Fogg
EXPERIMENTAL VALU	JES:	
T/K	H/mmHg	Mole fraction, x_{Cl_2} (l atm) (calculated by compiler)
<u> </u>		
298.3	5.74×10^3 7.33×10^3	0.132 0.104
308.2 314.2	7.60×10^{3}	0.100
329.2 341.2	9.45×10^{3} 11.8×10^{3}	0.0804 0.0644

The Henry's law constant, H, was taken to be the slope of a plot of pressure of Cl_2 in the gas phase against mole fraction of Cl_2 in the liquid phase. The author has given the following equation:

$$log_{10}H = 6.1227 - 701.9/(T/K)$$

The compiler has calculated that the experimental values of H quoted above fit this equation with a standard deviation of 0.27 \times 10 3 .

The heat of solution of chlorine, calculated by the author from the variation of H with temperature, is -3.20 kcal mol⁻¹.

760 mmHg = 1 atm 1 atm = 1.013×10^5 Pascal

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption of chlorine at partial pressures up to 1 atm was determined by passing mixtures of chlorine and air into benzene in an absorption vessel. The apparatus is described in ref. (1).

Temperatures were controlled to ± 0.5 K. The chlorine content of the gas

phase and the liquid phase were determined by iodometry.

SOURCE AND PURITY OF MATERIALS:

- Cl₂ & air: dried with concentrated H₂SO₄.
- 2. C₆H₆: distilled before use.

ESTIMATED ERROR:

REFERENCES:

Balej, J.; Regner, A.
 Chem. Listy <u>1956</u>, 50, 1374.

ne; Cl ₂ ; [7782-50-5] le; C ₆ H ₆ ; [71-43-2] emperature VALUES:	ORIGINAL MEASUREMENTS: Zetkin, V.I.; Kosorotov, V.I.; Stul, B.Ya.; Dzhagatspanyan, R.V.; Khim. Prom. 1971, 47, 102-103. PREPARED BY: P.G.T. Fogg
mperature	Stul, B.Ya.; Dzhagatspanyan, R.V.; Khim. Prom. 1971, 47, 102-103. PREPARED BY:
mperature	Khim. Prom. <u>1971</u> , 47, 102-103. PREPARED BY:
-	PREPARED BY:
-	
-	
-	P.G.T. Fogg
VALUES:	
T/K	^x Cl ₂
283.2	0.209
	0.154 0.107
313.2	0.083
	0.063 0.045
The pressure of Cl ₂ prequal to barometric pre	ressure.
The following equation	n was given :
$\log_{10} x_{\text{Cl}_2} = 1250/$	(T/K) - 5.08.
The heat of solution of variation of solubiligiven as - 5700 cal m	of Cl_2 calculated from the ty with temperature was ol^{-1} .
	293.2 303.2 313.2 313.2 323.2 333.2 The pressure of Cl_2 p equal to barometric p The following equatio $log_{10} {}^{x}Cl_{2} = 1250/$ The heat of solution variation of solubili

METHOD/APPARATUS/PROCEDURE:

The method and apparatus were d scribed in ref. (1). Chlorine was bubbled through a measured quantity of benzene in a thermostatted vessel of capacity 100 cm³. Chlorination of the benzene was prevented by addition of 0.5 wt % of phenol. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.

SOURCE AND PURITY OF MATERIALS:

Cl₂: to USSR standard GOST 6718-53. Dried by passing through H₂SO₄.

C6H6: 99% pure. Dried with CaCl2.

ESTIMATED ERROR:

REFERENCES:

1. Zetkin, V.I. et al.

Zh. Fiz. Khim. 1970, 44, 830.

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Lohse, M.; Deckwer, W.-D. J. Chem. Eng. Data 2. Benzene; C₆H₆; [71-43-2] 1981, 26, 159-161. VARIABLES: PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
288.15	3.590
298.15	2.521
308.15	1.780
318.15	1.110
328.15	0.841
338.15	0.503

 $^{^\}S$ at a partial pressure of Cl2 of 101.3 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solvent saturated with chlorine in dark (~1% phenol added to prevent photochemical chlorination).

Samples withdrawn added to known amount of additional solvent and then 250 cm³ of potassium iodide solution. Released iodine titrated with thiosulfate.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta S = \pm 3\%$ (estimated by compiler).

ov, A. V.; Konobeev, B. I.; ov, E. A.; Gubanova, T. I. Prik. Khim. (Leningrad) 1973,
· · · · · · · · · · · · · · · · · · ·
.855-1856.
D BY:

EXPERIMENTAL VALUES:

T/K	Mole fraction, x _{Cl2}
303.2	0.132
313.2	0.106
323.2	0.080
333.2	0.054
343.2	0.039
353.2	0.032

The partial pressure of chlorine plus partial pressure of toluene was apparently equal to barometric pressure (unspecified).

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorine was bubbled through a weighed portion of the solvent (15-20 g) until a differential manometer registered no pressure drop when the chlorine supply was discontinued. The chlorine content of the solution was determined from the increase in weight and also argentometrically. Loss of solvent in the gas stream was shown to be negligible in comparison with other errors which the authors estimate to be ± 5%. Light was excluded and 1-2 wt-% of phenol was added to inhibit chlorination of toluene. The chlorination products which were formed were estimated by gas chromatography and appropriate corrections made during calculation of solubility.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl_2 : from a cylinder; dried over H_2SO_4 .
- 2. C7H8: "chemically pure" grade.

ESTIMATED ERROR:

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] 2. Methylbenzene (toluene); C₇H₈; [108-88-3] Cariables: Components: ORIGINAL MEASUREMENTS: Lohse, M.; Deckwer, W.-D. J. Chem. Eng. Data 1981, 26, 159-161. PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
288.15	2.570
298.15	1.905
308.15	1.479
318.15	1.122
328.15	0.771
338.15	0.611
348.15	0.464

 $[\]S$ at a partial pressure of Cl_2 of 101.3 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solvent saturated with chlorine in dark (~1% phenol added to prevent photochemical chlorination).

Samples withdrawn added to known amount of additional solvent and then 250 cm³ of potassium iodide solution. Released iodine titrated with thiosulfate.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta S = \pm 3\%$ (estimated by compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Lohse, M.; Deckwer, WD. J. Chem. Eng. Data
2. 1,2-Dimethylbenzene; C ₈ H ₁₀ ; [95-47-6]	<u>1981</u> , 26, 159-161.
VARIABLES:	PREPARED BY:
Temperature	C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
308.15	1.124
328.15	0.765

 $[\]S$ at a partial pressure of 101.3 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solvent saturated with chlorine in dark (01% phenol added to prevent	
photochemical chlorination).	No details given.
Samples withdrawn added to known	
amount of additional solvent and	
then 250 cm³ of potassium iodide solution. Released iodine	
titrated with thiosulfate.	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1; \delta S = \pm 3\%$
	(estimated by compiler).
	REFERENCES:

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Lohse, M.; Deckwer, W.-D. J. Chem. Eng. Data 2. 1,3-Dimethylbenzene; C₈H₁₀; [108-38-3] VARIABLES: Temperature PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
298.15	1.373
318.15	0.915
338.15	0.627

 $[\]S$ at a partial pressure of 101.3 kPa.

AUXILIARY INFORMATION

Solvent saturated with chlorine in
dark (∿1% phenol added to prevent
photochemical chlorination).
Samples withdrawn added to known
amount of additional solvent and
then 250 cm3 of potassium iodide
solution. Released iodine
titrated with thiosulfate.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S = \pm 3\%$ (estimated by compiler).

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
288.15	1.693
298.15	1.397
308.15	1.127
318.15	0.921
328.15	0.767
338.15	0.623
348.15	0.484

[§] at a partial pressure of Cl of 101.3 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solvent saturated with chlorine in dark (~1% phenol added to prevent photochemical chlorination).

Samples withdrawn added to known amount of additional solvent and then 250 cm³ of potassium iodide solution. Released iodine titrated with thiosulfate.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S = \pm 3\%$ (estimated by compiler).

ORIGINAL MEASUREMENTS:
Lohse, M.; Deckwer, WD. J. Chem. Eng. Data
<u>1981</u> , 26, 159-161.
PREPARED BY:
C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
288.15 298.15 308.15 318.15 328.15 338.15 348.15	2.193 1.657 1.228 0.980 0.779 0.660 0.528

 $^{^{\}S}$ at a partial pressure of Cl_2 of 101.3 kPa.

AUXILIARY INFORMATION

Solvent saturated with chlorine in
dark (~1% phenol added to prevent
photochemical chlorination).
Samples withdrawn added to known
amounts of additional solvent and
then 250 cm3 of potassium iodide
solution. Released iodine
titrated with thiosulfate.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta S = \pm 3\%$ (estimated by compiler).

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Chlorine; Cl₂; [7782-50-5] Jones, W. J. J. Chem. Soc. 1911, 99, 392-404. 2. Acetic acid; C₂H₄O₂; [64-19-7] VARIABLES: PREPARED BY: P. G. T. Fogg Concentration EXPERIMENTAL VALUES: p_{Cl₂}/Pa* Mole fraction, x_{Cl_2} S T/K 289.2 36.6 948 0.00086 0.00095 289.2 36.9 1038 289.2 36.9 1739 0.00160 289.2 36.4 2395 0.00218

 $S = \frac{\text{concentration of } Cl_2 \text{ in mol } dm^{-3} \text{ of the solution}}{\text{concentration of } Cl_2 \text{ in mol } dm^{-3} \text{ of the gas phase}}$

Extrapolation to $p_{Cl_2} = 1$ atm is not valid.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The apparatus consisted of a bubbler and wash bottles. The concentration of the original solution was determined by iodometry. Chlorine, carried away from the solution in a stream of air, was also determined by iodometry. The results were given as a partition coefficient, S. S was deemed to be constant and independent of pressure p_{Cl_2} .

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: not specified.
- 2. C₂H₄O₂: some prepared in the laboratory; some obtained from Kahlbaum. Both samples said to be "specially purified".

ESTIMATED ERROR:

Calculated by the compiler from the volumes of titrant given in the original paper. It has been assumed that the volume of the solution is equal to the volume of the original liquid at these low concentrations.

Organic compounds containing oxygen/nitrogen 387 COMPONENTS: ORIGINAL MEASUREMENTS: Kumar, S.; Gehlawat, J.K.; 1. Chlorine; Cl₂; [7782-50-5] J. Chem. Technol. Biotechnol. 1979 2. Acetic acid; C₂H₄O₂; [64-19-7] 29, 353-360. VARIABLES: PREPARED BY: P.G.T. Fogg. Temperature EXPERIMENTAL VALUES: $^{\text{mol}}_{\text{Cl}_2}$ dm $^{-3}$ * Mole fraction** x_{Cl_2} 0.058 1.06 303 0.81 0.045 313

0.59

0.38

Total pressure = 101 kPa.

323

333

It is not clear whether values refer to ${\rm mol}_{{\rm Cl}_2}{\rm dm}^{-3}$ (solution) or to ${\rm mol}_{{\rm Cl}_2}{\rm dm}^{-3}$ (solvent).

0.034

0.022

Calculated by the compiler using published values of densities of acetic acid (ref. 1) and assuming that dissolution of chlorine causes no change in the volume of the liquid phase.

The authors stated that the solubility data were unlikely to be in error by more than 15%. No basis for this statement was given.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: The authors stated that the : analytical grade. solutions were saturated with chlorine at a specified temperature C2H4O2 : analytical grade. and the dissolved chlorine was determined by standard iodometric titration. No further details were given. ESTIMATED ERROR: REFERENCES: J. Timmermans, "Physico-Chemical Constants of Pure Organic Compounds", Vol. 2, Elsevier, London. 1965.

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5]

Acetic acid, anhydride; C₄H₆O₃;

ORIGINAL MEASUREMENTS:

Jones, W. J.

J. Chem. Soc. 1911, 99, 392-404.

[108-24-7]

PREPARED BY:

P. G. T. Fogg

Concentration

EXPERIMENTAL VALUES:

VARIABLES:

т/к	conc. Cl ₂ in soln. /mol dm ⁻³	s	p _{Cl2} /Pa*	Mole fraction, *
288.2	0.01574	39.6	953	0.00148
288.2	0.01015	40.1	606	0.00095
288.2	0.00403	38.8	249	· 0.00038

 $S = \frac{\text{concn. Cl}_2 \text{ in mol dm}^{-3} \text{ solution}}{}$ concn. Cl₂ in mol dm⁻³ gas phase

Extrapolation to p_{Cl} , = 1 atm is not valid.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus consisted of a bubbler and wash bottles. The concentration of the original solution was determined by iodometry. Chlorine, carried away from the solution in a stream of air, was also determined by iodometry. The results were given as a partition coefficient, S. S was deemed to be constant and independent of pressure p_{Cl_2} .

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: not specified.
- 2. $C_4H_6O_3$: supplied by Kahlbaum.

ESTIMATED ERROR:

Calculated by the compiler on the assumption that the volume of the solution is equal to that of the original liquid at these $\frac{1}{2}$ low concentrations.

0.124

0.144

0.175

0.180

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Chlorine; Cl₂; [7782-50-5] 1,2-Benzenedicarboxylic acid esters. 	Prokop'eva, M. F.; Mar'yanovskaya, K. Sh.; Bukina, V. K.; Korol', A. N. Zh. Fiz. Khim. 1971, 45, 722. (Complete article deposited at VINITI. No.2400-70, dep. from 17 Dec. 1970).
VARIABLES:	PREPARED BY:
None	P. G. T. Fogg
EXPERIMENTAL VALUES:	
Temperatu	re = 323.2 K
Stationary phase	Specific retention Mole fraction, volume x_{Cl_2} (1 atm)
Dimethyl ester, C ₁₀ H ₁₀ O ₄ [131-11-3]	14.92 0.116

14.10

13.34

12.00

11.59

11.01

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:

AUXILIARY INFORMATION

Retention volumes for chlorine were determined for the various stationary phases using conventional gas chromatographic techniques.

Diethyl ester, $C_{12}H_{14}O_{4}$ [84-66-2]

Dibutyl ester, $C_{16}H_{22}O_{4}$ [84-74-2]

Dinonyl ester, $C_{26}H_{42}O_{4}$ [84-76-4]

Dioctyl ester, C24H38O4 [117-84-0]

Diundecyl ester, C₃₀H₅₀O₄ [3648-20-2]

No information.

ESTIMATED ERROR:

REFERENCES:

Ambrose, D.; Keulemans, A. I. M.;
 Purnell, J. H.
 Anal. Chem. <u>1958</u>, 30, 1582.

^{*} Values of $x_{\rm Cl_2}$ (1 atm) have been calculated by the compiler on the assumption that specific retention volumes given above are in units of cm³ g⁻¹ and that these values can be equated with the volume of gas, corrected to 273.2 K, absorbed by 1 g of solvent (see ref. 1). It has also been assumed that this volume is independent of pressure. This last assumption may have introduced appreciable error and the values of $x_{\rm Cl_2}$ (1 atm) given above can only be thought of as approximate values.

COMPONENTS:		ORIGINAL MEASURE	MENTS:		
1. Chlorine	e; Cl ₂ ; [7782-5	50-5] DuPont de No	emours and Co. (Inc.);		
2			Chem. Eng. News 1955, 33, 2366.		
2. <i>N</i> , <i>N</i> -Dime	thyl formamide;				
C ₃ H ₇ NO;	[68-12-2]				
VARIABLES:		PREPARED BY:			
			D C III II		
			P. G. T. Fogg		
EXPERIMENTAL V	ALUES:				
T/K	$p_{\mathtt{Cl}_2}$	Vol of Cl ₂ absorbed	Mole fraction*,		
	CI2	per vol. of DMF	x _{Cl₂} (1 atm)		
273.2	1 atm	385	0.569		
	l atr	$m = 1.013 \times 10^5 \text{ Pascal}$			
		•			
* Calc	rulated by compi	ler on the assumption tha	at the volume of		
gas	absorbed is inde	ependent of pressure and	that the density		
of I publ	DMF at 273.2 K is Lished values at	s given by a linear extra 293.2 K (1) and 298.2 K	apolation of (2).		
£					
		AUXILIARY INFORMATION			
METHOD/APPARAT	US/PROCEDURE:	SOURCE AND PURIT	Y OF MATERIALS:		
l					
No	ot stated.	No	ot stated.		
		ESTIMATED ERROR			
		REFERENCES:			
		1. "Handbook	k of Chemistry & Physics"		
			tion), C.R.C. Press, 1, Ohio. <u>1976</u> .		
		2. "Lange's	Handbook of Chemistry"		
		(12th edi New York	tion), McGraw-Hill,		

Organic compounds containing oxygen/nitrogen 391 COMPONENTS: ORIGINAL MEASUREMENTS: Zetkin, V.I.; Kolesnikov, I.M.; Chlorine; Cl₂; [7782-50-5] Zakharov, E.V.; Dzhagatspanyan, Nitrobenzene; C6H5NO2; [98-95-3] Khim. Prom. 1966, 42, 624-626 VARIABLES: PREPARED BY: Temperature P.G.T. Fogg EXPERIMENTAL VALUES: Mole fraction a g_{C1},/100g_{C6H5NO2} T/K mol_{Cl},/mol_{C6H5NO} xCl2 5.138 0.0818 0.0891 313 0.0575 0.0610 3.518 333 2.353 0.0392 0.0408 353 0.0257 0.0264 1.522 373

The total pressure was apparently equal to barometric pressure (unspecified).

1.096

0.825

0.646

0.0187

0.0141

0.0110

The heat of solution of Cl_2 calculated from the variation of solubility with temperature was given by the authors as - 4680 cal mol^{-1} .

Calculated by compiler.

0.0190

0.0143

0.0111

393

413

433

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: : to USSR standards GOST Chlorine was bubbled through Cl₂ 6718-53. Dried with nitrobenzene in a thermostatted H2SO and with CaCl2. vessel of capacity 100 cm3. Samples were withdrawn periodically for iodometric analysis until consistent : Dried with CaCl2. $C_6H_5NO_2$ Distilled through a 20results were obtained. plate column before use. ESTIMATED ERROR: REFERENCES:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Carbon disulfide; CS₂; [75-15-0]

ORIGINAL MEASUREMENTS:

Raskina, A.D.; Zetkin, V.I.; Zakharov, E.V.; Kolesnikov, I.M. Kosorotov, V.I.;

Zh. Prik. Khim. (Leningrad), 1972, 45, 1333-1334.

VARIABLES:

Temperature

PREPARED BY:

P.G.T. Fogg

EXPERIMENTAL VALUES:

т/к	g _{Cl2} /100 g of solution	Mole fraction $^x\mathrm{Cl}_2$
275	23.0	0.246
278	20.4	0.218
283	17.2	0.184
288	14.4	0.154
293	11.7	0.125
298	9.9	0.106

The total pressure was apparently equal to barometric pressure (unspecified).

The authors have given the following equation:

$$\log_{10} (100x_{\text{Cl}_2}) = (1250/(\text{T/K})) - 3.18$$

The compiler has calculated that values of $x_{\rm Cl_2}$ quoted above fit this equation with a standard deviation of 0.011. The compiler has also calculated that the equation:

 \log_{10} (100 $x_{\rm Cl_2}$) = (1304/(T/K)) - 3.55 fits the data better (standard deviation 0.002).

The authors have given the heat of solution of chlorine, calculated from the variation of solubility with temperature, as -5.7 kcal mol⁻¹.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorine or chlorine/nitrogen mixtures were bubbled through carbon disulfide until the concentration of chlorine in the liquid phase, as determined by iodometry, was constant. The apparatus was protected from light. The total pressure of gas was apparently equal to barometric pressure although this is not explicitly stated. Variations of solubility when chlorine was diluted with nitrogen is said to indicate that Henry's law is obeyed although these experimental measurements are not reported. No allowances seem to have been made for the partial pressure of the carbon disulfide.

SOURCE AND PURITY OF MATERIALS:

- Cl₂: to USSR standard GOST 6718-53; additionally dried over H₂SO₄.
- N₂: to GOST 9293-59; dried over H₂SO₄.
- CS₂: to GOST 1541-42; distilled and dried over ignited CaCl₂.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Chlorine; Cl₂; [7782-50-5] Vdovichenko, V. T.; Kondratenko, v. I. 2. Dichloromethane; CH₂Cl₂; [75-09-2] Khim. Promst. 1967, 43, 290-291. VARIABLES: PREPARED BY: Temperature P. G. T. Fogg

EXPERIMENTAL VALUES:

T/K	Mole fraction, x_{Cl_2} (1 atm)
254.2	0.338
273.2	0.198
283.2	0.152
298.2	0.102

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method described by Taylor and Hildebrand was used (1).	1. Cl ₂ : to USSR standard GOST 6718-53. 2. CH ₂ Cl ₂ : b.p. 40.0-40.3 °C (barometric pressure unspecified); density (20 °C) 1.3260 g cm ⁻³ ; n _D (20 °C) 1.4245.
	ESTIMATED ERROR: REFERENCES:
	1. Taylor, N. W.; Hildebrand, J. H. J. Amer. Chem. Soc. 1923, 45, 682.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Vdovichenko, V. T.; Kondratenko, V. I.
2. Trichloromethane; CHCl ₃ ; [67-66-3]	Khim. Promst. <u>1967</u> , 43, 290-291.
VARIABLES:	PREPARED BY:
Temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

T/K	Mole fraction, x_{Cl_2} (1 atm)
257.2	0.399
273.2	0.259
283.2	0.178
298.2	0.114

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY	INFORMATION
METHOD APPARATUS PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method described by Taylor and Hildebrand was used (1).	1. Cl ₂ : to USSR standard GOST 6718-53. 2. CHCl ₃ : b.p. 61.1-61.2 °C; density (293.2 K) 1.4892 g cm ⁻³ ; n _D (293.2 K) 1.4464.
	REFERENCES: 1. Taylor, N. W.; Hildebrand, J. H.
	J. Amer. Chem. Soc. 1923, 45,

682.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl4;
 [56-23-5]

EVALUATOR:

W. Gerrard, Department of Chemistry, The Polytechnic of North London, Holloway, London, N7 8DB UNITED KINGDOM

CRITICAL EVALUATION:

Only five sets of values need be considered in arriving at an average plot of x_{Cl_2} vs. T/K from which the recommended values are taken. The original data are given as referring to a partial pressure of 1 atm. i.e. $p_{\text{Cl}_2} = 1$ atm. The uncertainty in these values for $p_{\text{Cl}_2} = 1$ atm, lies in two assumptions. Firstly, the total pressure $p_{\text{T}} = p_{\text{Cl}_2} + p_{\text{CCl}_4}$ was measured, and p_{CCl_4} was estimated by assuming Raoult's law, although this is not explicitly stated in every paper. Secondly, the derived p_{Cl_2} value is taken to adjust the corresponding p_{Cl_2} value to that at 1 atm, on the assumption that Henry's law, mole fraction form, holds; but this assumption is frequently not valid, although it may be used with caution.

Data used in the construction of the average curve are shown in Fig. 1, and are taken from the following contributors: Taylor and Hildebrand (1) (T-H), Smith (2) (S), Kogan, Kol'tsov, and Litvinov (3) (K-K-L), Vdovichenko and Kondratenko (4) (V-K), Raskina, Zetkin, Zakharov, Kolesnikov, and Kosorotov (5) (not shown on diagram because the numbers are identical with the K-K-L values, although three T/K values are slightly different). The derived plot is shown in Fig. 2.

Data by Curda and Holas (6) are for a total pressure, $p_{\rm T}$, about 1 atm, see line C-H in Fig. 1. and are excluded from the mean line. Data by Blair and Yost (7) should not be used for extrapolation beyond the highest $p_{\rm Cl_2}$ = 73.4 mm Hg. Data by Jones (8) should not be used for extrapolation beyond $p_{\rm Cl_2}$ = 13 mm Hg. Jakowkin's isolated value (9) is for similar low $p_{\rm Cl_2}$. Perkin's (10) and Egunov et al. (11) data are for total pressure about 1 atm. and serve to support the average line. Value by Schwab and Hantke (12) is out-of-line.

- 1. Taylor, N.W.; Hildebrand, J.H. J. Amer. Chem. Soc. 1923, 45, 682.
- 2. Smith, T.L. J: Phys. Chem. 1955, 59, 188.
- 3. Kogan, L.M.; Kol'tsov, N.S.; Litvinov, N.D. Zh. Fiz. Khim. 1963, 37, 1914.
- 4. Vdovichenko, V.T.; Kondratenko, V.I. Khim. Prom. 1967, 43, 290.
- Raskina, A.D.; Zetkin, V.I.; Zakharov, E.V.; Kolesnikov, I.M.; Kosorotov, V.I. Zh. Prikl. Khim. 1972, 45, 1333.
- 6. Curda, M; Holas, J. Chem. Prumysl. 1964, 14, 547.
- 7. Blair, M.C. Jr.; Yost, D.M. J. Amer. Chem. Soc. 1933,55,4489.
- 8. Jones, W.J. J. Chem. Soc. 1911,99,392.
- 9. Jakowkin, A.A. Z. Phys. Chem. 1899, 29,613.
- 10. Perkin, W.H. J. Chem. Soc. 1894,65,20.
- Egunov, A.V.; Konobeev, B.I.; Ryabov, E.A.; Gubanova, T.I. Zh. Prikl. Khim. <u>1973</u>, 46, 1855.
- 12. Schwab, G.M.; Hantke, G. Z. Phys. Chem. 1924, 114, 251.

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl₄;
 [56-23-5]

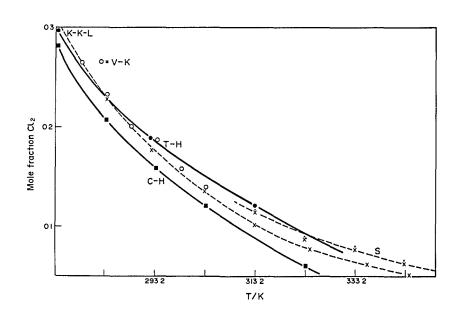
EVALUATOR:

W. Gerrard, Department of Chemistry, The Polytechnic of North London, Holloway, London, N7 8DB. UNITED KINGDOM:

CRITICAL EVALUATION:

RECOMMENDED NUMERICAL VALUES

T/K	x _{Cl₂} (1 atm)	
253.16 263.16 273.16 283.16 293.16 303.16 313.16 323.16 333.16 343.16 343.16	0.600 0.434 0.305 0.262 0.181 0.142 0.112 0.088 0.072 0.058	

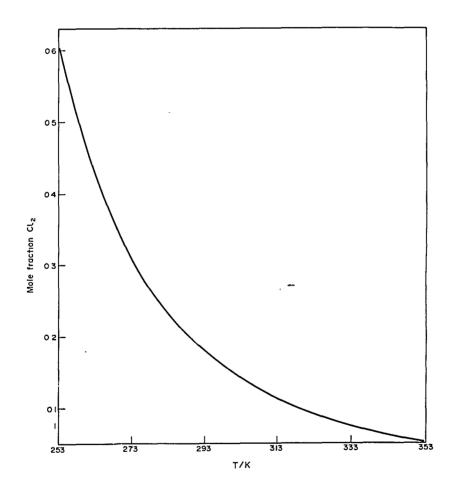


- Chlorine; Cl₂; [7782-50-5] Tetrachloromethane; CCl₄; 2. [56-23-5]

EVALUATOR:

W. Gerrard, Department of Chemisty, The Polytechnic of North London, Holloway, London, N7 8DB UNITED KINGDOM

CRITICAL EVALUATION:



	ORIGINAL MEASURE	MENTS:	
1. Chlorine; Cl ₂ ; [7782-50-5]		Perkin, W. H.	
2. Tetrachloromethane; CCl4; [56-23-5]		J. Chem. Soc.	
	1034, 00, 20		
	PREPARED BY:		
		W. Gerrard	
.ues:			
wt~%	в*	x Cl $_2$	
10.29 9.88	4.02 4.204	0.199 0.192	
	TUES: wt-%	Cl ₂ ; [7782-50-5] Perkin, W. Foromethane; CCl ₄ ; J. Chem. Society 1894, 65, 20 PREPARED BY: Wt-% B* 10.29 4.02	

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: No details except as below. The amount of chlorine taken up by the solvent was determined by introducing a weighed quantity of the solution into a bottle containing Not specified. potassium iodide, and titrating with sodium thiosulfate. pressure was not mentioned; it was presumably barometric. ESTIMATED ERROR: NOTE: The pressure was presumably total (approximately 1 atm). The solu-REFERENCES: bility was expressed as a mole ratio: 1-Cl₂ + B-CCl₄, B being the number of moles of CCl4 for each mole of Cl2. The wt-% was also given.

see note below.

COMPONENTS: ORIGINAL MEASUREMENTS: Chlorine; Cl₂; [7782-50-5] Jakowkin, A.A. 2. Tetrachloromethane; CCli; Z. Phys. Chem. 1899, 29,613. [56-23-5] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: x_{Cl_2} (approximate, assuming p_{Cl_2} is about T/K Absorption coefficient, 1 atm and the coefficient is independent of pressure). 273.16 83.3 (83.3 = 1/0.012)0.267 $760 \text{ mmHg} = 1 \text{ atm} = 1.013 \times 10^5 \text{ Pa}$ Solubility expressed as absorption coefficient: $\frac{\text{concn. in gas}}{\text{concn. in liquid}} = 0.012 \text{ (average)}$ AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Two bulbs, one connected to an Cl₂ : Self-prepared. Purity not ordinary pipette carrying a tap. specified. Absorption was at a pressure of about 15 mm Hg. Amount absorbed was determined by a titration (potassium CCl4: Not specified. iodide-thiosulfate). ESTIMATED ERROR: REFERENCES:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Jones, W. J.

J. Chem. Soc.

1911, 99, 392-404.

VARIABLES:

Pressure

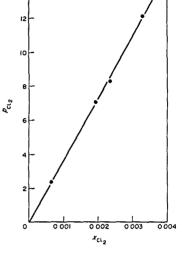
PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	S	$p_{\mathrm{Cl}_2}/\mathrm{mmHg}$	x _{Cl₂}
288.16	50.7	2.34	0.000634
	51.4	7.03	0.00193
	53.7	8.29	0.00237
	51.0	12.14	0.00331

(Extrapolation to p_{Cl_2} = 1 atm is not valid.) 760 mmHg = 1 atm = 1.013 × 10 5 Pascal



AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Bubbler and wash bottles. Concentration of the original solution determined iodometrically. Chlorine, carried away from the solution in a stream of air, was determined by iodometric titration. The results were given as a partition coefficient,

- $S = \frac{\text{concn. Cl}_2 \text{ in moles/dm}^3 \text{ solution}}{\text{concn. Cl}_2 \text{ in moles/dm}^3 \text{ gas phase}}.$
- s was deemed to be constant and independent of pressure, $p_{{\rm Cl}_2}$. NOTES: Compiler has given the approximate $p_{{\rm Cl}_2}$ and $x_{{\rm Cl}_2}$ values on the assumption that the volume of solution is equal to that of the original liquid for these low concentrations.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: not specified.
- 2. CCl4: redistilled.

ESTIMATED ERROR:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Taylor, N. W.; Hildebrand, J. H. J. Amer. Chem. Soc. 1923, 45, 682-694.

VARIABLES:

Temperature

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	g Cl ₂ /g of solution	p _{gas} /mmHg	^x gas	^x gas (1 atm)
273.16	0.156	729	0.286	0.298
292.16	0.0848	680	0.163	0.187
313.16	0.0433	557	0.0892	0.1215

760 mmHg = 1 atm = 1.013×10^5 Pascal

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturator tube (1). Chlorine was bubbled through liquid. Samples of saturated liquid were run into a weighed flask containing aqueous KI, and iodine was titrated with standard solution of thiosulfate. Temperature control was manual to 0.1 K. Saturation at barometric pressure, ptotal, partial pressure, pgas, estimated by Raoult's law to give p_{CC1} . Hence $p_{qas} = p_{total}$ x_{gas} (1 atm) estimated by $_{b}$ CCl". Henry's law, mole fraction form.

SOURCE AND PURITY OF MATERIALS:

- 1. Chlorine was from an electrolytic supply; it contained less than 0.1% of free acid.
- Purity of CCl, not specified.
 Vapor pressure data from ref. 2.

ESTIMATED ERROR:

- Bichowsky, F. R.; Storch, H. J. Amer. Chem. Soc. 1915, 37, 2695.
- 2. Young, S. J. Chem. Soc. 1891, 59, 911.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Chlorine; Cl₂; [7782-50-5] Schwab, G.M.; Hantke, G. Z. Phys. Chem. 1924, 114,251. Tetrachloromethane; CCl4; [56-23-5] VARIABLES: PREPARED BY: W. Gerrard EXPERIMENTAL VALUES: 1/s T/K Approx.x_{Cl}, (1 atm) 0.031 292.16 32.26 0.116 $760 \text{ mmHg} = 1 \text{ atm} = 1.013 \times 10^5 \text{ Pa}$ Solubility was expressed as an absorption coefficient $s = \frac{\text{concn. of Cl}_2 \text{ in gas}}{\text{concn. of Cl}_2 \text{ in liquid}}$ Actual pressure was about 700 mm Hg. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Liquid held in small bulb of 1 cm3 Cl2 : Gas from liquid passed through calcium chloride. capacity connected to manometer assembly. Diagram given in original CCl4: Not specified. paper. Absorption coefficient determined by measurement of the decrease of pressure with time in an apparatus of known volume connected with a small bulb containing a small amount of CClu. ESTIMATED ERROR: ±10% (Compiler) REFERENCES:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Blair, M.C. Jr.; Yost, D.M.

J. Amer. Chem. Soc. 1933, 55, 4489-96.

VARIABLES:

Pressure

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

p _{Cl2} /mmHg	x _{Cl₂} at p _{Cl₂}	Henry's Constant* HCl ₂
18.6	0.00394	4730
22.8	0.00448	5080
28.0 (a)	0.00609	4600
30.4	0.00615	4940
32.2	0.00690	4670
39.8	0.00781	5100
64.6	0.01245	5180
69.0	0.01363	5070
73.4	0.01391	5280

- (a) Given as 2.80 in the original. The lowest value of ${}^{\rm H}{\rm Cl}_2$ gives ${}^{\rm x}{\rm Cl}_2$
- = 0.165; the highest value gives x_{Cl_2} = 0.144, for p_{Cl_2} = 1 atm.

760 mmHg = 1 atm. 1 atm = 1.013×10^5 Pascal.

* H_{Cl_2} defined as $H_{\text{Cl}_2} = p_{\text{Cl}_2}/x_{\text{Cl}_2}$

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

The vapor pressures, p_{Cl_2} , were determined by the iodometric determination of chlorine carried away in a stream of nitrogen (see ref. 1), at 298.16 K. The pressures were not greater than 74 mmHg.

SOURCE AND PURITY OF MATERIALS:

All reagents were stated to be of the highest purity obtainable.

ESTIMATED ERROR:

- 1. Bichowsky, F.R.; Storch, H.
 - J. Amer. Chem. Soc. 1915,37, 2696.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Chlorine; Cl₂; [7782-50-5] Tetrachloromethane; CCl₄; [56-23-5] 	Smith, T. L. J. Phys. Chem. 1955, 59, 188-189.
VARIABLES:	PREPARED BY:
Temperature	W. Gerrard

EXPERIMENTAL V	ALUES:		
T/K	Total pressure $p_{\mathrm{T}}^{\prime}/\mathrm{atm}$	Moles ${\rm Cl}_2/$ (kg solution)/atm ${\rm Cl}_2$	a $x_{\mathrm{Cl}_2}/\mathrm{atm}~\mathrm{Cl}_2$
313.16	2.02 2.36	0.797 0.789	0.115
323.16	2.02 2.36	0.590 0.602	0.0875
333.16	2.02 2.36	0.522 0.522	0.0771
343.16	2.36 2.36	0.417 0.433	0.0632
353.16	2.36 2.70	0.340 0.329	0.0502
363.16	2.70	0.269	0.0444

 $^{\rm a}$ at 1 atm partial pressure of chlorine

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Two bulbs separated by stopcock. Bulbs are detachable for weighing. Bourdon gauge. Chlorine passed into liquid in upper bulb until constant gauge reading attained. Sample then run into lower bulb for	 Cl₂: from cylinder (The Matheson Co.). CCl₄: distilled.
weighing and iodometric titration. Saturation at a total pressure $p_{\rm T}$ of about 2 atm. Partial pressure $p_{\rm Cl_2}$ derived from $p_{\rm Cl_2} = p_{\rm T} - p_{\rm CCl_4}$, assuming Raoult's law. Basis of	ESTIMATED ERROR:
adjustment to $p_{Cl_2} = 1$ atm probably Henry's law, mole fraction form.	REFERENCES:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl4;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Kogan, L.M.; Kol'tsov, N.S.; Litvinov, N.D.

Zh. Fiz. Khim. 1963, 37,1914-7.

VARIABLES:

Temperature

PREPARED BY:

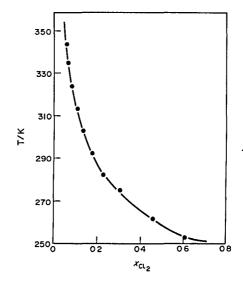
W. Gerrard

EXPERIMENTAL VALUES:

	Mole fraction	of
T/K	chlorine, x_{Cl}	2

253.16 262.16 273.16 283.46 292.36 303.16 313.16 324.16 335.66	0.603 0.456 0.309 0.228 0.177 0.136 0.102 0.0755 0.0625	
344.16	0.0518	

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$



AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Thermostatted double gas buret, null manometer, magnet-striker and stirrer. Diagram of elaborate assembly is given in the original paper.

A weighed amount of liquid in a sealed tube was placed in the absorption vessel. The system was evacuated, filled with gas, and the sealed tube was broken. The volume of gas absorbed was measured at a fixed pressure (total). Light was excluded.

Volume of chlorine measured at constant pressure, which was not stated. Henry's law was used to calculate the mole fraction values for $p_{\rm Cl_2}=1$ atm; but details were not disclosed. Allowance for $p_{\rm CCl_4}$ was not mentioned.

SOURCE AND PURITY OF MATERIALS:

 Cl_2 conformed with USSR standard GOST 6718-53; purity stated to be 99.97.

CCl4 was dried, distilled and checked by physical data.

ESTIMATED ERROR:

Temperature control was ± 0.02 to ± 0.05 °C. Volume could be read to 0.05 cm³. The reproducibility of the volume measurements was stated to be within ± 0.25 %.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
1. Chlorine; Cl ₂ ; [7782-50-5]	Curda, M., Holas, J.	
2. Tetrachloromethane; CCl ₄ ;	Curda, M., Holas, J. Chem. Prumys1. 1964, 14, 547-8.	
[56-23-5]	5.15.1. 11 angov. 1504, 14, 547-0.	
VARIABLES: Temperature	PREPARED BY: W. Gerrard	
16.11.50.11.01	5522512	
EXPERIMENTAL VALUES:		
T/K $ ext{Cl}_2$ wt % $ ext{(p_{ extbf{T}}$ about 1}$	atm) x_{Cl_2} (Calc. by compiler)	
	0.000	
273.16 15.4 283.16 10.8	0.283 0.208	
293.16 8.0 303.16 6.0	0.159 0.122	
323.16 2.9	0.0609 0.0129	
$1 \text{ atm} = 1.013 \times 10^5 \text{ Pa}$	ascal.	
AUXILIARY	INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Jacketted bubbler tube. Diagram in original paper.	Cl ₂ , of technical grade, of 99.2% purity.	
Sample removed by a tap at the bottom	CCl4, distilled, b.p. 77°C.	
of the tube. Chlorine determined iodometrically. Temperature measured within 0.5°C.		
Saturation at barometric pressure,		
total.		
	ESTIMATED ERROR:	
	REFERENCES:	
1		

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Tetrachloromethane; CCl4;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Vdovichenko, V. T.; Kondratenko,

v. I.

Khim. Prom.

1967, 43, 290-291.

VARIABLES:

PREPARED BY:

W. Gerrard

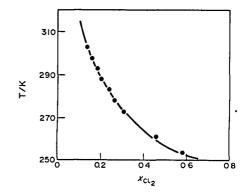
EXPERIMENTAL VALUES:

T/K	x _{Cl₂}
253.16 261.16 273.16 278.16 283.16 288.16 293.16 298.16 303.16	0.592 0.464 0.303 0.264 0.232 0.201 0.186 0.158

Temperature

Note: Mole fraction values, $x_{\rm Cl_2}$ are for $p_{\rm Cl_2}$ = 1 atm.

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$



AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method described by Taylor and Hildebrand was used (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: GOST 6718-53 (All Union Standard).
- 2. CCl4: b.p., d_4 , and n_D^{20} given as 76.7-76.8 °C, 1.5970 and 1.4602, respectively.

ESTIMATED ERROR:

REFERENCES:

Taylor, N. W.; Hildebrand, J. H. J. Amer. Chem. Soc.
 1923, 45, 682.

- Chlorine; Cl₂; [7782-50-5]
- Tetrachloromethane; CCl4; [56-23-5]

ORIGINAL MEASUREMENTS:

Raskina, A.D; Zetkin, V.I.; Zakharov, E.V.; Kolesnikov, I.M.; Kosorotov, V.I.

Zh. Prikl. Khim. 1972, 45,1333-4.

VARIABLES:

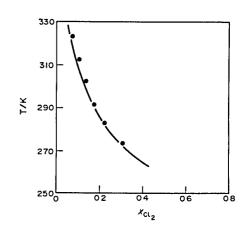
Temperature

PREPARED BY:

W. Gerrard.

EXPERIMENTAL VALUES:

T/K		xCl ₂	
273.16 283.16 292.16 303.16 313.16 324.16	(283.46) (292.36) (303.06)	0.309 0.228 0.177 0.136 0.102	_
1 atm =	= 1.013 x	10 ⁵ Pasca	1



AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Chlorine bubbled through liquid until saturated at total pressure, p_m , apparently atmospheric.

Thermostatted cylinder, 100 cm³ capacity protected from light. Reflux condenser, bubbler fitted Schott porous plate. Cl_2 or $(Cl_2 + N_2)$ passed through liquid (70 cm³). Samples withdrawn periodically for iodometric analysis, until constant result obtained. Three successive analyses stated to show satisfactory reproducibility.

From the variation of the partial pressure, p_{Cl_2} , by dilution with nitrogen it was concluded that Henry's law was obeyed. Allowance for the partial pressure of CCl4 was not mentioned. Results were given as mole %, presumably for $p_{Cl_2} = 1$ atm, but this was not explicitly stated. The numbers are identical with those of ref. 1, cited by authors, but three T/K () are slightly different.

SOURCE AND PURITY OF MATERIALS:

- : GOST 6318-55 standard. Dried by sulfuric acid.
- CCl: technical grade, GOST 4-65, dried and distilled.

ESTIMATED ERROR:

REFERENCES:

1. Kogan, L.M.; Kol'tsov, N.S.; Litvinov, N.D.;

Zh. Fiz. Khim. 1963, 37,1914.

COMPONENTS: 1. Chlorine; Cl ₂ ; [7782-50-5] 2. Tetrachloromethane; CCl ₄ ; [56-23-5]	ORIGINAL MEASUREMENTS: Egunov, A. V.; Konobeev, B. I.; Ryabov, E. A.; Gubanova, T. I. Zh. Prikl. Khim. 1973, 46, 1855-6.
VARIABLES: Temperature	PREPARED BY: W. Gerrard
EXPERIMENTAL VALUES:	
T/K w	t-%
313,10	.27 0.108
323.16	.9 0.081

^{*} $p_{\text{total}} \approx 1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal (calculated by compiler)}$

3.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

unspecified).

333.16

Bubbler tube, differential manometer, and rheometer. Diagram given in paper. Chlorine from cylinder was passed through concentrated sulfuric acid and a rheometer into a known weight of liquid (15-20 g) until equilibrium was reached as indicated by a differential manometer.

Amount absorbed was determined by increase in weight. Light was excluded.

Chlorine bubbled through liquid until equilibrium attained at a total pressure (barometric,

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: Unspecified.
- 2. CCl4: Chemically pure grade.

0.073

ESTIMATED ERROR:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Trichloromethanesulfenyl
 chloride; CCl₄S; [594-42-3]

ORIGINAL MEASUREMENTS:

Raskina, A.D.; Zetkin, V.I.; Zakharov, E.V.; Kolesnikov, I.M.; Kosorotov, V.I.;

Zh. Prik. Khim. (Leningrad), 1972, 42, 1333-1334.

VARIABLES:

Temperature

PREPARED BY:

P.G.T. Fogg

EXPERIMENTAL VALUES:

T/K	$g_{{ m Cl}_2}/{ m 100g}$ of solution	Mole fraction $^x\mathtt{Cl}_2$	
275	16.0 *	0.225	
278	8.9	0.204	
283	7.4	0.168	
288	6.0	0.145	
293	5.0	0.121	
295	4.1	0.102	
303	3.4 *	0.098	
308	2.8	0.070	

The total pressure was apparently equal to barometric pressure (unspecified).

* these values are not consistent with the corresponding values of the mole fraction given by the authors.

The authors have given the following equation:

$$\log_{10} (100x_{\text{Cl}_2}) = (1250/(\text{T/K})) - 3.20$$

The compiler has calculated that values of $x_{\rm Cl_2}$ quoted above fit this equation with a standard deviation of 0.007.

The authors have given the heat of solution of chlorine, calculated from the variation of solubility with temperature, as - $5.7~\rm kcal~mol^{-1}$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorine or chlorine/nitrogen mixtures were bubbled through CCl₄S until the concentration of chlorine in the liquid phase, as determined by iodometry, was constant. The apparatus was protected from light. The total pressure of gas was apparently equal to barometric pressure although this is not explicitly stated. Variations of solubility when chlorine was diluted with nitrogen is said to indicate that Henry's law is obeyed although these experimental measurements are not reported. No allowances seem to have been made for the partial pressure of the CC1₄S.

SOURCE AND PURITY OF MATERIALS:

C1₂: to USSR standard GOST 6718-53 dried over H₂SO₄.

 N_2 : to GOST 9293-59; dried over H_2SO_4 .

CCl.S: made by chlorination of CS₂; purified by distill-ation to 99.5%

ESTIMATED ERROR:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. Carbon disulfide; CS₂; [75-15-0]
- 3. Trichloromethanesulfenyl chloride; CCl₄S; [594-42-3]
- 4. Tetrachloromethane; CCl₄; [56-23-5]

ORIGINAL MEASUREMENTS:

Raskina, A.D.; Zetkin, V.I.

Zakharov, E.V.; Kolesnikov, I.M.; Kosorotov, V.I.

Zh. Prik. Khim. (Leningrad), 1972, 45, 1333-1334.

VARIABLES:

Composition

PREPARED BY:

P.G.T. Fogg

EXPERIMENTAL VALUES:

Composition before passage of chlorine (mole %)		g Cl ₂ /100g solution	Mole fraction x Cl $_2$	
CS ₂	CC14S	CCl ₄		
15.6	18.4	66.0	14.3	0.263
15.6	66.0	18.4	12.2	0.240
62.5	7.5	30.0	21.8	0.263(0.297)
62.5	18.7	18.8	20.1	0.250(0.283)
88.0	5.4	6.6	21.4	0.248
42.7	23.0	34.3	16.4	0.263

Temperature: 275 K

The total pressure was apparently equal to barometric pressure (unspecified).

* values recalculated by the compiler from wt % of Cl_2 given by the authors.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was bubbled through the liquid until the concentration of chlorine in the liquid phase, as determined by iodometry, was constant. The apparatus was protected from light.

The total pressure of gas was apparently equal to barometric pressure although this is not explicitly stated.

SOURCE AND PURITY OF MATERIALS:

- Cl₂ : to USSR standard GOST 6718-53; additionally dried over H₂SO₄.
- CS₂ : to GOST 1541-42; distilled and dried over ignited CaCl₂.
- CC14S: made by chlorination of CS2; purified by distillation to 99.5%
- CCl₄ : technical grade (GOST 4-65);
 dried over ignited CaCl₂.

ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
l. Chlorine; Cl ₂ ; [7782-50-5]	Taylor, N. W.; Hildebrand, J. H. J. Amer. Chem. Soc. <u>1923</u> , 45,	
2. 1,2-Dibromoethane; C ₂ H ₄ Br ₂ ; [106-93-4]	682-694.	
VARIABLES:	PREPARED BY:	
Temperature	P. G. T. Fogg	

CVDC	RIMEN	TAT	17 A T	HEC.

T/K	g Cl ₂ /g of solution	p _{Cl₂} /mmHg	Mole fr	factions $x_{\operatorname{Cl}_2}(1 \text{ atm})$
293.16	0.0813	752	0.190	0.192
313.16	0.0469	736	0.1151	0.119

760 mmHg = 1 atm

 $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturator tube (1). Chlorine was bubbled through liquid. Samples of saturated liquid were run into a weighed flask containing aqueous KI, and iodine was titrated with standard solution of thiosulfate. Temperature control was manual to 0.1 K.

Saturation was at barometric pressure, $p_{\rm total}$. The value of

 $p_{C_2H_4Br_2}$ was estimated by Raoult's law from vapor pressure data given in ref. (2). Hence:

 $p_{\text{Cl}_2} = p_{\text{total}} - p_{\text{C}_2\text{H}_4\text{Br}_2}$

The authors then used Henry's law (mole fraction form) to calculate x_{Cl_2} (1 atm) from x_{Cl_2} .

SOURCE AND PURITY OF MATERIALS:

- 2. C₂H₄Br₂: not specified.

ESTIMATED ERROR:

- Bichowsky, F. R.; Storch, H. J. Amer. Chem. Soc. <u>1915</u>, 37, 2695.
- 2. Landolt-Börnstein Tabellen.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Curda, M.; Holas, J. Chem. Prum. 1964, 14, 547-548.
2. Tetrachloroethene; C ₂ Cl ₄ ; [127-18-4]	
VARIABLES: Temperature	PREPARED BY: P. G. T. Fogg
EXPERIMENTAL VALUES:	n. Mole fraction. $*x$

T/K	$g_{Cl_2}/100 \text{ g solm.}$	Mole fraction, * x_{Cl_2}	
273.2	15.4	0.299	
283.2	10.8	0.221	
293.2	8.1	0.171	
303.2	6.4	0.138	
323.2	3.8	0.085	
343.2	2.2	0.050	
363.2	1.0	0.023	

The pressure of Cl_2 plus C_2Cl_4 was equal to barometric pressure.

AUXILIARY INFORMATION

Chlorine was passed into the C2Cl4 in | 1. Cl2: technical grade, 99.2% a jacketted bubbler tube (diagram in original paper). Samples were withdrawn through a tap at the bottom of the tube. Temperature was controlled to ± 0.5 °C. The total pressure was equal to barometric pressure (unspecified).

METHOD /APPARATUS / PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

- pure.
- 2. C₂Cl₄: technical grade; distilled; b.p. 120 °C.

ESTIMATED ERROR:

^{*} Calculated by compiler.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Kalz, G.; Naumann, A. Plaste Kautsch. 1971, 18, 500-501.
2. 1,1,2,2-Tetrachloroethane; C ₂ H ₂ Cl ₄ ; [79-34-5]	
VARIABLES:	PREPARED BY:
Temperature	P. G. T. Fogg

EXPERIMENTAL VALUES:

T/K	g Cl ₂ dm ⁻³	Mole fraction*, x_{Cl_2}
298.2	51.77	· 0.072
323.2	50.25	0.071
348.2	33.05	0.049
363.2	18.72	0.029
383.2	17.87	0.028

The pressure of Cl_2 plus $\text{C}_2\text{H}_2\text{Cl}_4$ was apparently equal to barometric pressure (unspecified).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine from a cylinder was passed into 400 cm3 of the solvent in a flask fitted with stirrer and reflux condenser. Temperatures were controlled by a thermostat. The chlorine which dissolved was determined by iodometry. The extent of irreversible reaction between chlorine and tetrachloroethane was measured by estimation of chloride ions produced. At 90 °C about 3% of the tetrachloroethane reacted but at other temperatures there was less than 0.2% reaction.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: from a cylinder.
- 2. $C_2H_2Cl_4$: b.p. 146.2 °C (barometric pressure unspecified); density (20 °C) 1.5950 g cm⁻³; n_D (20 °C) 1.4938.

ESTIMATED ERROR:

REFERENCES:

1. J. Timmermans, "Physico-Chemical Constants of Pure Organic Compounds", Vol. 2, Elsevier, London. 1965.

Approximate values calculated by compiler on the assumption that dissolution of Cl_2 causes no change in volume of the liquid phase. Densities of $\text{C}_2\text{H}_2\text{Cl}_4$ at 293.2 K and 298.2 K are given in ref. (1). Densities at other temperatures were obtained by extrapolation.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
1. Chlorine; Cl ₂ ; [7782-50-5]	Kogan, L. M.; Kol'tsov, N. S.; Litvinov, N. D. Zh.	
<pre>2. 1,1,2,3,4,4-Hexachloro-1,3- butadiene; C₄Cl₆; [87-68-3]</pre>	Fiz. Khim. <u>1963</u> , 37, 1014-1016.	
VARIABLES:	PREPARED BY:	
Temperature, pressure	P. G. T. Fogg	

EXPERIMENTAL VALUES:

T = 303.2 K		$p_{Cl_2} = 7$	60 mmHg
p _{Cl₂} /mmHg	Mole fraction ^x Cl ₂	T/K	Mole fraction $^{x}\text{Cl}_{2}$
408.4 600.8 745.7 773.7 926.2 974.2	0.0844 0.125 0.155 0.160 0.191 0.202	253.5 261.7 266.0 271.8 272.8 283.0 293.4 303.2 334.4 352.9 365.3	0.607 0.467 0.421 0.358 0.353 0.250 0.199 0.158 0.083 0.059 0.052

760 mmHg = 1 atm \cdot 1 atm = 1.013 × 10⁵ Pascal

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The volumes of gas absorbed by weighed quantities of hexachlorobutadiene were determined by a static method using a thermostatted gas burette connected to absorption vessels and a vacuum line as described in ref. (1). Pressures were measured by a mercury manometer. Chlorine did not come into contact Temperawith any metal surfaces. tures were controlled to ± 0.02 K in the range 283 K - 353 K and to [±] 0.05 outside this range. apparatus was shielded from light.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: to USSR standard GOST 6718-53.
- 2. C₄Cl₆: m.p. 18.7 °C; density (20 °C) 1.6793 g cm⁻³; n_D (20 °C) 1.5558.

ESTIMATED ERROR:

REFERENCES:

Kogan, L. M.; Kol'tsov, N. S.;
 Litvinov, N. D.
 Zh. Fiz. Khim. 1963, 37, 1040.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Gjaldbaek, J. C.; Hildebrand, J. H.
2. Hexadecafluoroheptane; (Perfluoroheptane); C ₇ F ₁₆ ; [335-57-9]	J. Amer. Chem. Soc. <u>1950</u> , 72, 609-611.
VARIABLES:	PREPARED BY:
Temperature	P. G. T. Fogg

T/K	Bunsen coefficient	Mole fraction, x_{Cl_2} (1 atm)
273.16	20.1	0.164 ^a
288.76		0.1165
288.96		0.1174
292.96		0.1101,
293.16	12.3	0.110 ^D
295.16		0.1051
298.16	10.7	0.0977
298.46		0.0975
l .		

- a Extrapolated
- b Interpolated
- $1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorine was bubbled through solvent for about 1 hour and the chlorine in a weighed sample of the solution estimated by iodometry. Temperature control was manual to

0.1 K. Saturation was at barometric pressure, p_{total} . The value of $p_{\text{C}_7\text{F}_{16}}$ was estimated by Raoult's law from vapor pressure data for C_7F_{16} in ref. (1). Hence:

 $p_{\text{Cl}_2} = p_{\text{total}} - p_{\text{C}_7\text{F}_{16}}$

The authors then used Henry's law (mole fraction form) to calculate x_{Cl_2} (1 atm).

SOURCE AND PURITY OF MATERIALS:

- 2. C_7F_{16} : distilled, b.p. 355.49 355.58 K (753.8 mmHg).

ESTIMATED ERROR:

REFERENCES:

1. Fowler, R. D.; Hamilton, J. M.; Kasper, J. S.; Weber, C. E.; Burford, W. B.; Anderson, H. C. Ind. Eng. Chem. 1947, 39, 375.

COMPONENTS: 1. Chlorine; Cl ₂ ; [7782-50-5] 2. 1,2-Dichlorobenzene; C ₆ H ₄ Cl ₂ ; [95-50-1]	ORIGINAL MEASUREMENTS: Zetkin, V.I.; Kosorotov, V.I.; Stul, B.Ya.; Dzhagatspanyan, R.V.; Khim. Prom. 1971, 47, 102-103.
VARIABLES: Temperature	PREPARED BY: P.G.T. Fogg.
EVENEZA WAY WES	
EXPERIMENTAL VALUES: T/K	[∞] Cl₂
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	
AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method and apparatus were described in ref. (1). Chlorine was bubbled through a measured quantity of dichlorobenzene in a thermostatted vessel of capacity 100 cm³. Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.	Cl ₂ : to USSR standard GOST 6718-53. C ₆ H ₄ Cl ₂ : 99% pure. Dried with CaCl ₂
	ESTIMATED ERROR: REFERENCES:
	1. Zetkin, V.I. et. al.

Zetkin, V.I. et. al.
 Zh. Fiz. Khim. 1970, 44, 830.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Zetkin, V.I. Kosorotov, V.I.; Stul, B.Ya.; Dzhagatspanyan, R.V.;
 1,2,4-Trichlorobenzene; C₆H₃Cl₃; [120-82-1] 	Khim. Prom. 1971, 47, 102-103.
0,1,01,, [110 01 1]	<u> </u>
VARIABLES:	PREPARED BY:
Temperature	P.G.T. Fogg.
EXPERIMENTAL VALUES:	
T/K	^x Cl ₂
288.2	0.254 0.210
293.2 303.2	0.151
313.2 323.2	0.117
323.2 333.2	0.091 0.070
The pressure of Cl	
apparently equal to	o barometric pressure.
The following equa-	tion was given :
$\log_{10} x_{\text{Cl}_2} = (105)$	0/(T/K)) - 4.29
10 °C1 ₂ (233	
	on of Cl ₂ calculated from
was given as - 480	olubility with temperature 0 cal mol-1.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method and apparatus were	Cl ₂ : to USSR standard GOST
described in ref. (1). Chlorine was	6718-53.
bubbled through a measured quantity of trichlorobenzene in a thermostatt-	C ₆ H ₃ Cl ₃ : 99% pure. Dried with CaCl
ed vessel of capacity 100 cm3.	Consciss. 338 pare. Brica with cac.
Samples were withdrawn periodically for iodometric analysis until	
consistent results were obtained.	
	ESTIMATED ERROR:
	January British
	REFERENCES:
	l. Zetkin, V.I. et. al.;
	Zh. Fiz. Khim. <u>1970</u> , 44, 830.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Chlorine; Cl₂; [7782-50-5] Chlorobenzene; C₆H₅Cl; [108-90-7] 	Silberstein, B.; Date, R. V.; Butt, J. B. J. Chem. Engng. Data 1969, 14, 253-4.
VARIABLES:	PREPARED BY: C. L. Young

T/K	Solubility [†] , S/mol dm ⁻³	Mole fraction of chlorine in liquid, $^{x}_{\text{Cl}_{2}}$
303.15	1.56	0.138
318.15	1.10	0.103
333.15	0.78	0.076

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorobenzene saturated with gas by bubbling chlorine through at 283 K. Temperature then raised to experimental temperature and chlorine allowed to equilibriate. Then stannic chloride in chlorobenzene solution added to cause chlorine to react with chlorobenzene to give dichlorobenzene.

SOURCE AND PURITY OF MATERIALS:

- Matheson high purity grade; purity better than 99.5 mole per cent.
- Fisher Scientific certified reagent, dried over CaCl₂, distilled middle fraction stored over calcium hydride in dark.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05; \quad \delta x_{Cl_2} = \pm 3\%.$

 $^{^{\}dagger}$ at a partial pressure of 101.3 kPa.

 $^{^{\}star}$ calculated by compiler assuming solubility is given as mol dm $^{-3}$ (solvent).

COMPONENTS:		ORIGINAL MEASUREMENTS:
1. Chlorine;	Cl ₂ ; [7782-50-5]	Cervinka, M. Chem. Prum. 1960, 10, 249-251.
2. Chloroben [108-90-7	zene; C ₆ H ₅ Cl;	
VARIABLES:		PREPARED BY:
Pressure, temperature		P. G. T. Fogg
EXPERIMENTAL VAL	UES:	
T/K	H/mm H g	Mole fraction, x_{Cl_2} (1 atm) (calculated by compiler)
298.2	6.61 × 10 ³	0.115
317.2	8.32×10^{3}	0.0913
338.2	12.4×10^3	0.0613

The Henry's law constant, H, was taken to be the slope of a plot of pressure of Cl_2 in the gas phase against mole fraction of Cl_2 in the liquid phase. The author has given the following equation:

$$log_{10}H = 6.0234 - 659.8/(T/K)$$

The compiler has calculated that the experimental values of H quoted above fit this equation with a standard deviation of 0.54 \times 10 3 .

The heat of solution of chlorine, calculated by the author from the variation of H with temperature, is -3.01 kcal mol⁻¹.

760 mmHg = 1 atm 1 atm = 1.013×10^5 Pascal

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The absorption of chlorine at partial pressures up to 1 atm was determined by passing mixtures of chlorine and air into chlorobenzene in an absorption vessel. The apparatus is described in ref. (1). Temperatures were controlled to ± 0.5 K. The chlorine content of the gas phase and the liquid phase were determined by iodometry.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl_2 & air: dried with concentrated H_2SO_4 .
- 2. C6H5Cl: distilled before use.

ESTIMATED ERROR:

REFERENCES:

Balej, J.; Regner, A.
 Chem. Listy <u>1956</u>, 50, 1374.

Organic compounds	s containing naiogen 42
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Chlorine; Cl₂; [7782-50-5] Chlorobenzene; C₆H₅Cl; 	Zetkin, V.I.; Kosorotov, V.I.; Stul, B.Ya.; Dzhagatspanyan, R.V.;
[108-90-7]	Khim. Prom. <u>1971</u> , 47, 102-103.
VARIABLES:	PREPARED BY:
Temperature	P.G.T. Fogg.
EXPERIMENTAL VALUES:	<u> </u>
`т/к	x _{Cl₂}
283.2 293.2 303.2	0.250 0.178 0.141
313.2 323.2 333.2	0.112 0.079 0.071
The pressure of Cl apparently equal t	₂ plus C ₆ H ₅ Cl was o barometric pressure.
The following equa	tion was given :
$\log_{10} x_{\text{Cl}_2} = 980$	/(T/K) - 4.08
The heat of solution of Cl_2 calculated from the variation of solubility with temperature was given as - 4500 cal mol^{-1} .	
	·
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method and apparatus were described in ref. (1). Chlorine was bubbled through a measured quantity of chlorobenzene in a thermostatted vessel of capacity 100 cm ³ . Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.	Cl ₂ ; to USSR standard GOST 6718-5 Dried by passing through H ₂ SO ₄ . C ₆ H ₅ Cl:99% pure. Dried with CaCl ₂ .
-courts were obtained.	
	ESTIMATED ERROR:
	REFERENCES: 1. Zetkin, V.I.; et al.; 2h. Fiz. Khim. 1970, 44, 830

ORIGINAL MEASUREMENTS:
Krentsel, L. B.; Litmanovich, A. D.; Shtern, V. Ya.
Zh. Prik. Khim. (Leningrad) <u>1972</u> , 45, 1875-1876.
PREPARED BY:
P. G. T. Fogg

T/K	H/mmHg ·	Mole fraction, x_{Cl_2} (1 a	tm) (calculated by compiler)
313.2 323.2 333.2 343.2	7.6×10 ³ 9.3×10 ³ 11.4×10 ³ 13.5×10 ³	0.100 0.082 0.067 0.056	760 mmHg = 1 atm 1 atm = 1.013 × 10 ⁵ Pascal

The Henry's law constant, H, was taken to be the slope of a plot of pressure of Cl_2 in the gas phase against mole fraction of Cl_2 in the liquid phase. The authors stated that values fit the equation:

$$log_{10}H = 6.83 - 925/(T/K)$$
).

The compiler has calculated that the values of ${\it H}$ which have been given fit this equation with a standard deviation of 0.09 \times 10 3 .

The heat of solution of chlorine in chlorobenzene, calculated by the authors from the variation of ${\it H}$ with T, was given as -4.3 kcal mol⁻¹.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

A high vacuum assembly was used. The amount of chlorine dissolved by a measured volume of chlorobenzene was calculated from the decrease in pressure of a known volume of chlorine. Pressures were measured by a mercury manometer but direct contact between mercury and chlorine was prevented by the use of a glass Bourdon type gauge as a null instru-Benzoquinone (0.1 wt-%) was ment. added to the chlorobenzene and experiments were conducted in a darkened room.

The authors stated that reproducible results were obtained and that this was evidence that there was no irreversible reaction between chlorine and chlorobenzene under the conditions of the experiment.

SOURCE AND PURITY OF MATERIALS:

- Cl₂: condensed and degassed under vacuum.
- C₆H₅Cl: degassed under vacuum; vapor pressure agreed with literature values in ref. (1).

ESTIMATED ERROR:

REFERENCES:

Stull, D. R.
 Vapor Pressures of Pure
 Substances (Russian translation),
 Izd. Inostr. Lit. 1949.

COMPONENTS: ORIGINAL MEASUREMENTS: Ushakov, A.A.; Kosorotov, V.I.; Chlorine; Cl₂; [7782-50-5] Stul, B. Ya.; Motsarev, G.V.; (Trifluoromethyl)benzene; 2. Dzhagatspanyan, R.V. (Benzotrifluoride); C7H5F3; [98-08-8] Zhur. Prikl. Khim. 1977, 50, 425-7. VARIABLES: PREPARED BY: C.L. Young Temperature EXPERIMENTAL VALUES: Mole fraction of + T/K Mole ratio Wt. solubility chlorine in liquid, solubility $g Cl_2/g C_7H_5F_3$ x_{Cl_2} 0.2550 12.40 0.2035 6.84 298 0.1406 0.1235 4.36 0.0824 313 0.0896 0.0608 323 0.0646 3.14 0.0468 333 0.0489 2.38 0.0261 0.0276 1.30 353 + calculated by compiler AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Dried with sulfuric acid and Solvent saturated with gas by bubbling chlorine through at a rate of 0.3 mol h⁻¹. Samples calcium chloride. withdrawn and concentration of 2. Distilled, purity not less than 99.5 mole per cent. chlorine determined by iodometric titration. ESTIMATED ERROR: $\delta T/K = \pm 0.3; \ \delta x_{Cl_2} = \pm 2\%.$ (estimated by compiler). REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Egunov, A. V.; Konobeev, B. I.; Ryabov, E. A.; Gubanova, T. I.
2. (Trichloromethyl)benzene; C ₇ H ₅ Cl ₃ ; [98-07-7]	Zh. Prik. Khim. (Leningrad) <u>1973</u> , 46, 1855-1856.
VARIABLES:	PREPARED BY:
Temperature	P. G. T. Fogg

т/к	Mole fraction, x _{Cl2}
303.2 313.2 323.2 333.2 343.2 353.2 363.2 373.2 393.2 423.2	0.124 0.105 0.084 0.071 0.060 0.050 0.047 0.035 0.022
-	

The partial pressure of chlorine plus the partial pressure of benzotrichloride was apparently equal to barometric pressure (unspecified).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was bubbled through a weighed portion of the solvent (15-20 g) until a differential manometer registered no pressure drop when the chlorine supply was discontinued. The chlorine absorbed was found from the increase in weight of the solution. Loss of solvent in the gas stream was shown to be negligible in comparison with other experimental errors which the authors estimate to be ± 5%. Light was excluded. Products of further chlorination were estimated by gas chromatography and appropriate corrections made.

SOURCE AND PURITY OF MATERIALS:

- 2. C7H5Cl3: "pure" grade.

ESTIMATED ERROR:

T/K	Mole fraction, x _{Cl2}
303.2 313.2 323.2 333.2 343.2 353.2 363.2 373.2 383.2	0.124 0.107 0.089 0.072 0.067 0.053 0.045 0.034
403.2	0.020

The partial pressure of chlorine plus partial pressure of benzal chloride was apparently equal to barometric pressure (unspecified).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was bubbled through a weighed portion of the solvent $(15-20\ g)$ until a differential manometer registered no pressure drop when the chlorine supply was The chlorine discontinued. absorbed was found from the increase in weight of the solution. of solvent in the gas stream was shown to be negligible in comparison with other experimental errors which the authors estimate to be ± 5%. Products of Light was excluded. further chlorination were estimated by gas chromatography and appropriate corrections made.

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: from a cylinder; dried over H₂SO₄.
- 2. C₇H₆Cl₂: by fractionation of
 products of chlorina tion of toluene;
 contained 1.2 wt-% of
 benzotrichloride.

ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Chlorine; Cl ₂ ; [7782-50-5]	Egunov, A. V.; Konobeev, B. I.; Ryabov, E. A.; Gubanova, T. I.
2. (Chloromethyl)benzene; C ₇ H ₇ Cl ; [100-44-7]	Zh. Prik. Khim. (Leningrad) <u>1973</u> , 46, 1855-1856.
VARIABLES:	PREPARED BY:
Temperature	P. G. T. Fogg

T/K	Mole fraction, x _{Cl2}
303.2	0.125
313.2	0.108
323.2	0.087
333.2	0.074
343.2	0.062
353.2	0.052
363.2	0.044
373.2	0.037
383.2	0.027

The partial pressure of chlorine plus the partial pressure of benzyl chloride was apparently equal to barometric pressure (unspecified).

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorine was bubbled through a weighed portion of the solvent (15-20 g) until a differential manometer registered no pressure drop when the chlorine supply was The chlorine discontinued. absorbed was found from the increase in weight of the solution. Loss of solvent in the gas stream was shown to be negligible in comparison with other experimental errors which the authors estimate to be ± 5%. Light was excluded. Products of further chlorination were estimated by gas chromatography and appropriate corrections made during calculation of solubility.

SOURCE AND PURITY OF MATERIALS:

- Cl₂: from a cylinder; dried over H₂SO₄.
- 2. C7H7Cl: "pure" grade.

ESTIMATED ERROR:

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Lohse, M.; Deckwer, W.-D. J. Chem. Eng. Data 2. 1-Chloro-2-methylbenzene (2-Chlorotoluene); C₇H₇Cl; [95-49-8] VARIABLES: PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³	(soln.)
288.15	2.306	
298.15	1.745	
308.15	1.311	
318.15	1.036	
328.15	0.842	
338.15	0.674	
348.15	0.547	

 $[\]S$ at a partial pressure of 101.3 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solvent saturated with chlorine in dark (~1% phenol added to prevent photochemical chlorination).

Samples withdrawn added to known amount of additional solvent and then 250 cm³ of potassium iodide solution. Released iodine titrated with thiosulfate.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta S = \pm 3\%$ (estimated by compiler).

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Lohse, M.; Deckwer, W.-D. 2. 1-Chloro-3-methylbenzene J. Chem. Eng. Data (3-Chlorotoluene); C₇H₇Cl; 1981, 26, 159-161. [108-41-8] VARIABLES: PREPARED BY: Temperature C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³ (soln.)
298.15 308.15 318.15 338.15 348.15	1.398 1.180 0.940 0.624 0.499

 $^{^{\}S}$ at a partial pressure of 101.3 kPa.

AUXILIARY INFORMATION

Solvent saturated with chlorine in
dark (~1% phenol added to prevent
photochemical chlorination).
Samples withdrawn added to known
amount of additional solvent and
then 250 cm ³ of potassium iodide
solution. Released indine

titrated with thiosulfate.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta S = \pm 3\%$ (estimated by compiler).

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Lohse, M.; Deckwer, W.-D. 2. 1-Chloro-4-methylbenzene J. Chem. Eng. Data (4-Chlorotoluene); C₇H₇Cl; [106-43-4] VARIABLES: Temperature PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Solubility, S/mol dm ⁻³	(soln.)
298.15 318.15 328.15 338.15 348.15	1.386 0.884 0.741 0.552 0.479	

 $[\]S$ at a partial pressure of 101.3 KPa.

AUXILIARY INFORMATION

Solvent saturated with chlorine in
dark (~1% phenol added to prevent
photochemical chlorination).
Samples withdrawn added to known
amount of additional solvent and
then 250 cm³ of potassium iodide
solution. Released iodine
titrated with thiogulfate

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta S = \pm 3\%$ (estimated by compiler).

430		•	Chlorine	Solubiliti	es				
1.	 (Trifluoromethyl) benzene, (Benzotrifluoride); C₇H₅F₃; [98-08-8] Chloro(trifluoromethyl)benzene; C₇H₄Cl₃F; [52181-51-8] Dichloro(trifluoromethyl)benzene; C₇H₃Cl₂F₃; 			Ushako Stul, Dzhag Zhur.	ov, A. B. Ya atspar	UREMENTS: A.; Koson A., Motsan nyan, R.V. L. Khim.	cev, G	.V.;	25-7
VARIA	ABLES: Temperature, co	omposition		PREPARE	D BY:	C.L. Y	oung/		
EXPER	•	ole ratio olubility	solu	% bility 00g(2+3	c	Mole fract of chloring liquid, x_0	ne in		
Mix C ₇ H	ture containing 3Cl ₂ F ₃ .	58.29 Wt	% C ₇ H ₅ F ₃ ,	39.47	Wt %	C7H4ClF3	and 2	.24 W	t %
	298 313 323 333 353	0.1543 0.1040 0.0799 0.0604 0.0381	4. 3. 2.	80 58 52 66 68		0.1325 0.0933 0.0733 0.0563 0.0363			
	ture containing 3Cl ₂ F ₃ .	22.82 Wt	% C ₇ H ₅ F ₃ ,	60.86	Wt %	C ₇ H ₄ ClF ₃ ,	and	16.32	Wt
	298 313 323 333 353	0.1727 0.1255 0.1024 0.0833 0.0587	5. 4.	32		0.1457 0.1102 0.0918 0.0760 0.0517			
	+ cai	lculated b	y compile	r.					

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solvent saturated with gas by bubbling chlorine through at a rate of 0.3 mol h⁻¹. Samples withdrawn and concentration of chlorine determined by iodometric titration.

SOURCE AND PURITY OF MATERIALS:

- 1. Dried with sulfuric acid and calcium chloride.
- 2. Distilled, purity not less than 99.5 mole per cent.
- 3. and 4. Prepared by chlorination of benzotrifluoride in presence of ferric chloride at 60°C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.3; \ \delta x_{Cl_2} = \pm 2\%.$

(estimated by compiler).

COMPONENTS:

- 1. Chlorine; Cl₂; [7782-50-5]
- 2. (Trifluoromethyl)benzene;
 (Benzotrifluoride); C₇H₅F₃;
 [98-08-8]
- Chloro(trifluoromethyl)benzene; C7H4ClF2

ORIGINAL MEASUREMENTS:

Ushakov, A.A.; Kosorotov, V.I.; Stul, B.Ya.; Motsarev, G.V. Dzhagatspanyan, R.V.

Zhur. Prikl. Khim. 1977, 50, 425-7.

VARIABLES:

Temperature

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

Mixture containing 84.84 weight percent of benzotrifluoride before passage of chlorine

Mole ratio solubility	Wt. % solubility g Cl ₂ /g (2+3)	Mole fraction of $^+$ chlorine in liquid, x Cl $_2$	
		•	
0.1340	6.60	0.1229	
0.0870	4.58	0.0886	
0.0660	3.62	0.0713	
0.0510	2.80	0.0561	
0.0324	1.70	0.0348	
	0.1340 0.0870 0.0660 0.0510	solubility solubility g Cl ₂ /g (2+3) 0.1340 6.60 0.0870 4.58 0.0660 3.62 0.0510 2.80	solubility solubility chlorine in liquid, g Cl ₂ /g (2+3) x _{Cl₂} 0.1340 6.60 0.1229 0.0870 4.58 0.0886 0.0660 3.62 0.0713 0.0510 2.80 0.0561

+ calculated by compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solvent saturated with gas by bubbling chlorine through at a rate of 0.3 mol h⁻¹. Samples withdrawn and concentration of chlorine determined by iodometric titration.

SOURCE AND PURITY OF MATERIALS:

- Dried with sulfuric acid and calcium chloride.
- Distilled, purity not less than 99.5 mole per cent.
- Prepared by chlorination of benzotrifluoride in presence of ferric chloride at 60°C.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.3; \ \delta x_{Cl_2} = \pm 2\%.$

(estimated by compiler)

COMPONENTS:	ORIGINAL MEASUREMENTS:		
 Chlorine; Cl₂; [7782-50-5] 3,4,5-Trichloro-2-(trichloro-methyl)-pyridine; C₆HCl₆N; [1201-30-5] 	Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V. Zh. Prikl. Khim. 1978, 51, 887-889 (J. Appl. Chem. USSR 1978, 51, 858-860).		
VARIABLES:	PREPARED BY:		
Temperature	C. L. Young		

Pressure, p = 101.3 kPa

T/K	Solubility, S/mol dm ⁻³	
 378.2	0.21	
393.2	0.17	
408.2	0.13	
423.2	0.11	
473.2	0.056	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was bubbled through the liquid until equilibrium was attained at a total pressure equal to the barometric pressure. The results were corrected to 101.3 kPa pressure. The chlorine in solution was determined by iodometry. Reaction of chlorine and solvent was minimised by 0.2 mole per cent phenol.

SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Purity 95-99 mole per cent as determined by chromatography.
 0.2 mole per cent phenol added as a chlorination inhibitor.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S/S = \pm 0.07.$

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Kosorotov, V. I.; Stul, B. Ya.; 2. 3,4,5-Trichloro-2-(dichloromethyl)pyridine; C₆H₂Cl₅N; Zh. Prikl. Khim. 1978, 51, 887-889 [7041-22-7] (J. Appl. Chem. USSR 1978, 51, 858860). VARIABLES: PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

Pressure, p = 101.3 kPa

T/K	Solubility, S/mol dm ⁻³	
333.2	0.51	
363.2	0.26	
378.2	0.19	
408.2	0.12	•

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was bubbled through the liquid until equilibrium was attained at a total pressure equal to the barometric pressure. The results were corrected to 101.3 kPa pressure. The chlorine in solution was determined by iodometry. Reaction of chlorine and solvent was minimised by 0.2 mole per cent phenol.

SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Purity 95-99 mole per cent as determined by chromatography.
 0.2 mole per cent phenol added as a chlorination inhibitor.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S/S = \pm 0.05.$

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] Kosorotov, V. I.; Stul, B. Ya.; 2. 3,5-Dichloro-2-(trichloromethyl)pyridine; C₆H₂Cl₅N; Zh. Prikl. Khim. 1978, 51, 887-889 [1128-16-1] (J. Appl. Chem. USSR 1978, 51, 858-860). VARIABLES: PREPARED BY: Temperature C. L. Young

EXPERIMENTAL VALUES:

Pressure, p = 101.3 kPa

T/K	Solubility, S/mol dm ⁻³	
333.2	0.50	
363.2	0.26	
393.2	0.15	
423.2	0.10	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Chlorine was bubbled through the liquid until equilibrium was attained at a total pressure equal to the barometric pressure. The results were corrected to 101.3 kPa pressure. The chlorine in solution was determined by iodometry. Reaction of chlorine and solvent was minimised by 0.2 mole per cent phenol.

SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Purity 95-99 mole per cent as determined by chromatography.
 0.2 mole per cent phenol added as a chlorination inhibitor.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S/S = \pm 0.05.$

COMPONENTS: 1. Chlorine; Cl₂; [7782-50-5] 2. 1,2-Dichloro-4-nitrobenzene; C₆H₃Cl₂NO₂; [99-54-7] VARIABLES: Temperature ORIGINAL MEASUREMENTS: Zetkin, V.I.; Kolesnikov, I.M. Zakharov, E.V.; Dzhagatspanyan, R.V. Khim. Prom. 1966, 42, 624-626. PREPARED BY: P.G.T. Fogg

EXPERIMENTAL VALUES:

T/K	mol _{Cl2} /mol _{C6H3Cl2NO2}	g _{Cl2} /100g _{C6H3} Cl2NO2	Mole fraction* **Cl2
333	0.0517	1.911	0.0492
353	0.0363	1.342	0.0351
373	0.0258	0.954	0.0252
393	0.0188	0.695	0.0185
413	0.0146	0.540	0.0144
433	0.0114	0.421	0.0113

The total pressure was apparently equal to barometric pressure (unspecified).

The heat of solution of Cl_2 , calculated from the variation of solubility with temperature, was given by the authors as - 4340 cal mol^{-1} .

Calculated by compiler.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Chlorine was bubbled through the solvent in a thermostatted vessel of capacity 100 cm ³ . Samples were withdrawn periodically for iodometric analysis until consistent results were obtained.	Cl ₂ : to USSR standard GOST 6718-53 C ₆ H ₃ Cl ₂ NO ₂ : prepared by chlorination of 1-chloro-4-nitro-benzene; recrystallised before use.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: Chlorine; Cl₂; [7782-50-5] Zetkin, V.I.; Kolesnikov, I.M.; 1. Zakharov, E.V.; Dzhagatspanyan, R.V. 2. 1,4-Dichloro-2-nitrobenzene; Khim. Prom. 1966, 42, 624-626. $C_6H_3Cl_2NO_2$; [89-61-2] VARIABLES: PREPARED BY: Temperature P.G.T. Fogg EXPERIMENTAL VALUES: Mole fraction T/K mol_{C12}/mol_{C6H3C12NO2} g_{C12}/100g_{C6H3C12NO2} x Cl₂ 0.0675 2.495 0.0632 333 353 0.0463 1.712 0.0443 373 1.168 0.0306 0.0316 393 0.0233 0.861 0.0228 0.0177 0.654 0.0174 413 433 0.0137 0.506 0.0135 The total pressure was apparently equal to barometric pressure (unspecified). The heat of solution of Cl_2 , calculated from the variation of solubility with temperature, was given by the authors as - 4580 cal mol^{-1} . * Calculated by compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: : to USSR standard GOST Chlorine was bubbled through the Cl_2 solvent in a thermostatted vessel 6718-53. Dried with of capacity 100 cm3. Samples were H2SO4 and with CaCl2. withdrawn periodically for iodometric analysis until consistent results $\text{C}_6\text{H}_3\text{Cl}_2\text{NO}_2$: to standard TU GAP-U were obtained. 539-54. Recrystallised before use. ESTIMATED ERROR: REFERENCES:

ORIGINAL MEASUREMENTS:
Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V. Zh. Prikl. Khim. 1978, 51, 887-889 (J. Appl. Chem. USSR 1978, 51, 858-860).
PREPARED BY:
C. L. Young

Pressure, p = 101.3 kPa

т/к	Solubility, S/mol dm ⁻³
363.2	0.13
393.2	0.10
423.2	0.08
443.2	0.066
473.2	0.05

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Chlorine was bubbled through the liquid until equilibrium was attained at a total pressure equal to the barometric pressure. The results were corrected to 101.3 kPa pressure. The chlorine in solution was determined by iodometry. Reaction of chlorine and solvent was minimised by 0.2 mole per cent phenol.

SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Purity 95-99 mole per cent as determined by chromatography.
 0.2 mole per cent phenol added as a chlorination inhibitor.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S/S = \pm 0.07.$

438 Chlorine Solubilities COMPONENTS: ORIGINAL MEASUREMENTS: Chlorine; Cl₂; [7782-50-5] Kosorotov, V. I.; Stul, B. Ya.; 2. 5-Chloro-2-(trichloromethyl)-Dzhagatspanyan, R. V. pyridine; C₆H₃Cl₄N; [1197-03-1] Zh. Prikl. Khim. 1978, 51, 887-889 3. 3,5-Dichloro-2-(dichloromethy1)-(J. Appl. Chem. USSR 1978, 51, 858pyridine; C₆H₃Cl₄N; [7041-25-0] 860). VARIABLES: PREPARED BY: C. L. Young Temperature EXPERIMENTAL VALUES: Pressure, p = 101.3 kPaSolubility, S/mol dm⁻³ T/K 0.57 333.2 0.36 363.2 0.26 393.2 0.17 423.2 0.12 443.2 AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS:

Chlorine was bubbled through the liquid until equilibrium was attained at a total pressure equal to the barometric pressure. results were corrected to 101.3 kPa pressure. The chlorine in solution was determined by iodometry. Reaction of chlorine and solvent was minimised by 0.2 mole per cent phenol.

- 1. No details given.
- 2. Purity 95-99 mole per cent as determined by chromatography. 0.2 mole per cent phenol added as a chlorination inhibitor.
- 3. As in 2 above.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S/S = \pm 0.05.$

Organic compounds containing halogen 439 COMPONENTS: ORIGINAL MEASUREMENTS: Chlorine; Cl₂; [7782-50-5] Zetkin, V.I.; Kolesnikov, I.M.; 1. Zakharov, E.V.; Dzhagatspanyan, R.V. 1-Chloro-2-nitrobenzene; Khim. Prom. 1966, 42, 624-626. C₆H₄ClNO₂; [88-73-3] VARIABLES: PREPARED BY: Temperature P.G.T. Fogg EXPERIMENTAL VALUES: gCl2/100gC6H4ClNO2 mol_{C1},/mol_{C6H4}ClNO₂ Mole fraction T/K x_{Cl_2} 0.0682 0.0732 3.298 313 333 0.0482 2.172 0.0460 0.0326 353 0.0337 1.518

The total pressure was apparently equal to barometric pressure (unspecified).

1.041

0.793

0.604

0.478

0.0226

0.0173

0.0132

0.0105

The heat of solution of Cl_2 calculated from the variation of solubility with temperature was given by the authors as - 4340 cal mol^{-1} .

Calculated by compiler.

0.0231

0.0176

0.0134

0.0106

373

393 413

433

AUXILIARY INFORMATION

110712 441111	2.11 Old MITON
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Chlorine was bubbled through the solvent in a thermostatted vessel of capacity 100 cm ³ . Samples were withdrawn periodically for iodometric analysis until consistent results	C ₆ H ₄ ClNO ₂ : to standard TU GAP-U
were obtained.	451-53. Recrystallised before use.
	ESTIMATED ERROR:
	REFERENCES:

440 Chlorine Solubilities ORIGINAL MEASUREMENTS: COMPONENTS: Chlorine; Cl₂; [7782-50-5] Zetkin, V.I.; Kolesnikov, I.M.; Zakharov, E.V.; Dzhagatspanyan, R.V. 1-Chloro-3-nitrobenzene; Khim. Prom. 1966, 42, 624-626. $C_6H_4C1NO_2$; [121-73-3] VARIABLES: PREPARED BY: Temperature P.G.T. Fogg EXPERIMENTAL VALUES: mol_{Cl2}/mol_{C6H4}ClNO₂ g_{Cl2}/100g_{C6H4}ClNO₂ Mole_fraction* T/K x_{Cl_2} 0.0447 333 0.0468 2.109 0.0321 1.446 0.0311 353 373 0.0219 0.987 0.0214 0.707 0.0154 393 0.0157 413 0.0117 0.527 0.0116 0.0090 0.0091 0.410 433 The total pressure was apparently equal to barometric pressure (unspecified). The heat of solution of Cl₂ calculated from the variation of solubility with temperature was given by the authors as - 4700 cal mol⁻¹. * Calculated by compiler. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: : to USSR standard GOST Cl₂ 6718-53. Chlorine was bubbled through the Dried with H₂SO₄ and solvent in a thermostatted vessel with CaCl2. of capacity 100 cm3. Samples were withdrawn periodically for iodometric C₆H₄ClNO₂: prepared by chlorination analysis until consistent results of nitrobenzene. were obtained. Purified by crystallis-

ation.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Chlorine; Cl₂; [7782-50-5] Zetkin, V.I. Kolesnikov, I.M.; Zakharov, E.V.; Dzhagatspanyan, R.V.; 2. 1-Chloro-4-nitrobenzene; C₆H₄ClNO₂; [100-00-5] Khim. Prom. 1966, 42, 624-626. VARIABLES: PREPARED BY: P.G.T. Fogg Temperature EXPERIMENTAL VALUES: Mole fraction* T/K x_{Cl_2} 0.0274 1.235 0.0267 373 393 0.0185 0.834 0.0182 0.0132 0.595 0.0130 413 433 0.0097 0.437 0.0096 The total pressure was apparently equal to barometric pressure (unspecified). The heat of solution of Cl2 calculated from the variation of solubility with temperature was given by the authors as -5560 cal mol⁻¹. * Calculated by compiler. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Cl_2 : to USSR standard GOST 6718-53. Dried with H_2SO_4 and with $CaCl_2$. Chlorine was bubbled through the solvent in a thermostatted vessel of capacity 100 cm3. Samples were C6H4ClNO2: to standard TU 9728-61. withdrawn periodically for iodometric Recrystallised before analysis until consistent results use. were obtained. ESTIMATED ERROR: REFERENCES:

Chloring Chloring	Chlorine Solubilities		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
 Chlorine; Cl₂; [7782-50-5] 2-(Trichloromethyl)-pyridine; C₆H₄Cl₃N; [4377-37-1] 	Kosorotov, V.I.; Stul, B. Ya.; Dzhagatspanyan, R. V. Zh. Prikl. Khim. 1978, 51, 887-889 (J. Appl. Chem. USSR 1978, 51, 858-860).		
VARIABLES:	PREPARED BY:		
Temperature	C. L. Young		
EXPERIMENTAL VALUES: Pressure	p = 101.3 kPa		
т/к	Solubility, S/mol dm ⁻³		
333.2	0.63		
363.2	0.38		
393.2	0.26		
423.2 443.2	0.19 0.15		
AUXILIA	RY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;		
Chlorine was bubbled through the liquid until equilibrium was	1. No details given.		

Chlorine was bubbled through the liquid until equilibrium was attained at a total pressure equal to the barometric pressure. The results were corrected to 101.3 kPa pressure. The chlorine in solution was determined by iodometry. Reaction of chlorine and solvent was minimised by 0.2 mole per cent phenol.

2. Purity 95-99 mole per cent as determined by chromatography.0.2 mole per cent phenol added as a chlorination inhibitor.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S/S = \pm 0.05.$

COMPONENTS:

- Chlorine; Cl₂; [7782-50-5] l.
- Dichlorodioxochromium; Cl₂CrO₂; [14977-61-8]

ORIGINAL MEASUREMENTS:

Roozeboom, H.W.B.;

Rec. Trav. Chim. 1885, 4, 379-381.

VARIABLES:

Temperature, concentration

PREPARED BY:

P.G.T. Fogg.

EXPERIMENTAL	VALUES:
_ ,	_

T/K	Quantity of chlorine en atomes.	$p_{\mathtt{Cl}_2}/\mathtt{mmHg}$	Mole fraction* Cl ₂
273.2	1.70	1302	0.459
273.2	1.43	1208	0.417
273.2	1.40	1198	0.412
273.2	1.35	1189	0.403
273.2	1.30	1150	0.394
273.2	1.25	1125	0.385
273.2	1.20	1101	0.375
273.2	1.16	1069	0.367
273.2	1.12	1051	0.359
273.2	1.04	1016	0.342
273.2	1.00	984	0.333
273.2	0.91	923	0.313
273.2	0.78	824	0.281
273.2	0.68	753	0.254
247.2	3.08	765	0.606
249.2	3.08	791	0.606
251.2	3.08	844	0.606
251.2	2.77	820	0.581
251.2	2.31	734	0.536
253.2	3.08	896	0.606
253.2	2.77	862	0.581
253.2	2.31	780	0.536
255.2	2.77	905	0.581
255.2	2.31	831	0.536
257.2	2.00	851	0.500
258.2	2.77	1002	0.581

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The pressure over a known weight of Cl₂ dissolved in a known weight of Cl₂CrO₂ in a small bulb at 247.2K to 273.2K was measured by a mercury manometer in which the mercury was protected by sulphuric acid. The concentration of Cl2 was changed by removing gas through a side tap and collecting it over brine saturated with chlorine. The weight of Cl2 removed, and the weight remaining in the flask, were calculated from the volume of gas collected. No allow-ance was made for the vapor pressure of Cl₂CrO₂.

SOURCE AND PURITY OF MATERIALS:

: not specified.

Cl₂CrCO₂: fractionally distilled under dry CO₂; b.p.117°C (barometric pressure

unspecified.)

ESTIMATED ERROR:

COMPONENTS:

ORIGINAL MEASUREMENTS:

1. Chlorine; Cl₂; [7782-50-5]

Roozeboom, H.W.B.;

2. Dichlorodioxochromium;

Rec. Trav. Chim. 1885, 4, 379-381.

Cl₂CrO₂; [14977-61-8]

EXPERIMENTAL VALUES:

T/K	Quantity of chlorine en atomes	$p_{\mathrm{Cl}_2}/\mathrm{mmHg}$	Mole fraction* **Cl2
259.2	2.00	902	0.500
259.2	1.24	754	0.383
261.2	2.77	1105	0.581
262.2	1.70	952	0.459
262.2	1.24	818	0.383
263.2	2.00	1015	0.500
264.2	1.70	995	0.459
264.2	1.24	870	0.383
265.2	1.39	930	0.410
266.2	1.39	948	0.410
266.2	1.24	921	0.383
268.2	1.24	975	0.383
270.2	1.24	1034	0.383
271.2	1.70	1232	0.459
273.2	1.70	1295	0.459
273.2	1.39	1185	0.410
273.2	1.24	1118	0.383
273.2	1.07	1031	0.349
273.2	0.76	825	0.275
!			

760 mmHg = 1 atm; 1 atm = 1.013×10^5 Pascal.

^{*} calculated by the compiler on the assumption that concentration *en atomes* is the ratio of atoms of dissolved chlorine to molecules of Cl₂CrO₂.

Miscellatieo	us compounds 440
COMPONENTS:	ORIGINAL MEASUREMENTS:
 Chlorine; Cl₂; [7782-50-5] Sulfuryl chloride; Cl₂O₂S; [7791-25-5] 	Schulze, H. J. Prakt. Chem. <u>1881</u> , 24, 168.
VARIABLES:	PREPARED BY: P. G. T. Fogg
EXPERIMENTAL VALUES:	
T/K Wt. of Cl ₂ absorbed per unit wt. of Cl ₂ O ₂ S	Vol. of Cl ₂ absorbed Mole fraction, per vol. of Cl ₂ O ₂ S x Cl ₂
273.2 0.136	71 0.206
AUXILIARY	INFORMATION
METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Chlorine was bubbled through a weighed quantity of sulfuryl chloride in a stoppered cylinder fitted with inlet and outlet tube. Passage of gas was continued until bubbles of gas no longer appeared to be absorbed. The amount of	No details given.
chlorine absorbed was found by weighing.	ESTIMATED ERROR:
•	REFERENCES:

446	Chlori	ne Solubilities	
COMPONENTS:		ORIGINAL MEASUREMENTS:	
1. Chlorine	e; Cl ₂ ; [7782-50-5]	Taylor, N. W.; Hildebrand, J. H. J. Amer. Chem. Soc. <u>1923</u> , 45,	
	lorosilane, (Silicon loride); SiCl ₄ ; 04-7]	682-694.	
VARIABLES:		PREPARED BY:	
		P. G. T. Fogg	
EXPERIMENTAL V	VALUES:		
T/K	g Cl_2/g of solution	$p_{\rm Cl_2}/\rm mmHg \qquad \qquad mole fractions \\ m_{\rm Cl_2} \sim m_{\rm Cl_2} (1)$	atm)

681

760 mmHg = 1 atm

0.131

$1 \text{ atm} = 1.013 \times 10^5 \text{ Pascal}$

AUXILIARY INFORMATION

METHOD 'APPARATUS / PROCEDURE:

273.16

Saturator tube (1). Chlorine was bubbled through liquid. Samples of saturated liquid were run into a weighed flask containing aqueous KI, and iodine was titrated with standard solution of thiosulfate. Temperature control was manual to 0.1 K. Saturation was at barometric pressure, The value of p_{SiCl_4} was $p_{\sf total}$. estimated by Raoult's law from vapor pressure data for SiCl, given in ref. (2). Hence:

p_{Cl2} = p_{total} - p_{SiCl4}

The authors also estimated x_{Cl_2} (1 atm) from x_{Cl_2} by Henry's law (mole fraction form).

SOURCE AND PURITY OF MATERIALS:

1. Cl₂: from an electrolytic supply; contained less than 0.1% of free acid.

0.266

0.288

2. SiCl4: not specified.

ESTIMATED ERROR:

- Bichowsky, F. R.; Storch, H. J. Amer. Chem. Soc. 1915, 37, 2695.
- 2. Landolt Börnstein Tabellen.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Chlorine; Cl₂; [7782-50-5] Krieve, W. F.; Mason, D. M. Titanium chloride; Cl₄Ti; J. Phys. Chem. 1956, 60, 374. [7550-45-0] VARIABLES: PREPARED BY: Temperature, pressure P. G. T. Fogg

EXPERIMENTAL	STATISTS.

т/к	$p_{\mathrm{Cl}_2}/\mathrm{atm}$	Mole fraction ^x Cl ₂	T/K	$p_{\mathrm{Cl}_2}/\mathrm{atm}$	Mole fraction x Cl ₂
293.2	1.50 2.20 2.71 3.13 3.67 4.24 4.76	0.2513 0.3585 0.4358 0.4964 0.5674 0.6499 0.7229	303.2	3.39 3.93 4.63 5.41 6.14	0.4227 0.4844 0.5571 0.6412 0.7107

The recovery of Cl_2 by dissolution in Cl_4Ti on an industrial scale has been reported (1).

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

A known weight of chlorine, determined by the change in pressure in the bomb containing the gas, was added to a known weight of titanium tetrachloride in a second bomb. When equilibrium had been attained the pressure in the second bomb was recorded. All pressures were measured by calibrated stainless steel Bourdon gauge to ± 0.5%. Temperatures were controlled to Solubilities were calculated from the pressure data using published gas density data (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Cl₂: A commercial sample was purified by fractional distillation to remove air and CO2.
- 2. TiCl4: from National Bureau of Standards; 99.999% pure.

ESTIMATED ERROR:

- 1. Anon.
 - Res. Discl. 1977, 157, 15.
- 2. Hulme, R.E.; Tillman, A.B. Chem. Eng. 1949,56,99.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Fluorine; F ₂ ; [7782-41-4]	Rewick, R. T.; Tolberg, W. E.;
2. Hydrogen fluoride; HF;	Hill, M. E.
[7664-39-3]	J. Chem. Engng. Data <u>1970</u> , 15,
	527-530.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young

EXPERIMENTAL	VALUES:			
T/K	Total pressure <i>P/</i> kPa	Partial pressure <i>P/</i> kPa	Conc. of fluorine /mol kg ⁻¹	Mole fraction * of fluorine, $^x{ m F}_2$
•	- /			- 2
292.95	280.0	177.3	0.0356	0.000713
	538.6	434.6	0.0925	0.00185
	799.9	695.9	0.150	0.00300
272.94	1064	959.9	0.204	0.00410
	1088	983.9	0.206	0.00414
	364.0	316.0	0.0690	0.00138
2/2,54	370.6	322.6	0.0697	0.00139
	729.3	681.3	0.148	0.00296
	950.6	903.0	0.196	0.00393
249.95 207.95 195.95	1192 815.9 637.3 204.0	1144 798.6 634.6 202.6	0.247 0.194 0.187 0.0675	0.00496 0.00389 0.00375 0.00135
	209.3	208.0	0.0678	0.00136
	440.0	438.6	0.144	0.00288
	735.9	734.6	0.243	0.00486

^{*} calculated by compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell made of Monel metal. Known amounts of fluorine added to known amount of hydrogen fluoride in cell. Quantity of gas absorbed calculated from equilibrium pressure and cell volume.

SOURCE AND PURITY OF MATERIALS:

- 1. Purity 98 mole per cent obtained from Allied Chemical Corp. Fractionally distilled final purity better than 99 mole per cent. Major impurities nitrogen and oxygen.
- 2. Anhydrous sample obtained from Olin Corp. Conductivity $3 \times 10^5 \text{ ohm}^{-1} \text{ cm}^{-1}$.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.02; \quad \delta x_{F_2} = \pm 3 \%$ (estimated by compiler).

COMPONENTS:			ORIGINAL MEASUREMENT	S:		
	ne monoxide; Cl ₂	0;	Ourisson, M.M.J	.; Kastne	r, M.	
[7791- 2. Water;	H ₂ O; [7732-18-5]	Bull. Soc. Chim. 1307-11.	. France.	1939,	6,
VARIABLES:			PREPARED BY:			
	Temperature		R. Ba	ttino.		
EXPERIMENTAL V						
т/к а	mb HOC1/mol 1000g H ₂ O ⁻¹	FCl ₂ /mm ^C	F _{Cl₂O^{/mm}d}	т/к	К 1	K 2
283,15	0.26 0.57 0.70 0.90 1.05 1.23 1.55 1.65 1.92 2.00 2.03	0.097 0.29 0.36 0.56 0.67 1.05 1.59 1.65 2.08 2.16	0.014 0.068 0.103 0.170 0.232 0.318 0.505 0.572 0.774 0.840 0.865	283.15 293.15		0.24 0.70
293.15	0.148 0.149 0.178 0.175 0.189 0.222 0.287 0.287 0.327 0.545 0.553 0.641 0.651	0.16 0.15 0.18 0.13 0.15 0.23 0.21 0.19 0.36 0.68 0.74 1.11	0.014 0.014 0.021 0.020 0.023 0.032 0.054 0.023 0.070 0.19 0.20 0.27			•
		AUXILIARY	INFORMATION			
METHOD APPARAT	US/PROCEDURE:		SOURCE AND PURITY OF	MATERIALS	:	
The amount is determi	of HOCl in soluned by chemical	tion titration.	No detail:	s given.		
			ESTIMATED ERROR:		-	
			δm _{HOC1} /m _{HOC}	c1 = 0.03		
			compiler's			
			REFERENCES:		<u></u>	
			,			

COMPONENTS:

- 1. Chlorine monoxide; Cl₂O;
- 2. Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS

Ourisson, M.M.J.; Kastner, M.

Bull. Soc. Chim. France. 1939, 6, 1307-11.

EXPERIMENTAL VALUES

T/K a	$_{\rm HOC1}/_{\rm mol\ 1000g\ H_20^{-1}}$	$P_{\text{Cl}_2}/\text{mm}$	PCl ₂ O/mm
293.15	0.672 0.747 0.771 0.812 0.842 0.943 0.941 1.22 1.52 2.55	1.2 1.0 1.1 1.2 1.4 1.5 2.7 4.1 10.3	0.29 0.36 0.39 0.43 0.46 0.58 0.58 0.97 1.50 4.23 4.67
283.15	60.16 ^e		760. e
293.15	34.19 e		760. e

- a. Temperature reported as 10 and 20° C.
- b. Molality (moles HOC1/1000g H2O) in solution.
- c. P_{Cl_2} is defined as $2P_{\text{Cl}_2\text{O}} + P_{\text{HOCl}}$. P_{Cl_2} is also defined as $P_{\text{Cl}_2} = 2K_1 [\text{HOCl}]^2 + K_2 [\text{HOCl}]$.

$$K_1 = P_{Cl_2O} / [HOC1]^2$$
. $K_2 = P_{HOC1} / [HOC1]$.

- d. P_{Cl_2O} calculated from $P_{\text{Cl}_2O} = \text{K [HOCl]}^2$
- e. Extrapolated values to $P_{\text{Cl}_2\text{O}} = 1$ atm. Since [Cl₂O] in solution were not given it was not possible to calculate a mole fraction solubility for Cl₂O.

COMPONENTS: (1) Chlorine monoxide; Cl₂O; Secoy, C.H.; Cady, G.H. [7791-21-1] J. Amer. Chem. Soc. 1941, 63, 2504-8. (2) Water; H₂O; [7732-18-5] VARIABLES: PREPARED BY: T/K: 276-293 p/mm Hg: 1-75

EXPERIMENTAL VALUES:

Solubility of Chlorine Monoxide as g Cl₂O/100 g H₂O

$p_{\mathrm{Cl}_2\mathrm{O/mm}}$	o ^o c ^b	10°C	20°C
1	7.6	5.2	3.5
5	16.7	12.3	8.0
10	23.7	17.4	11.1
20	33.6	24.2	15.4
30	40.7	29.2	18.7
40	46.9	33.0	21.3
50	52.4	36.2	23.7
60	56.7	39.0	25.8
70	60.2	41.4	27.7
75	61.6	42.5	28.6

- a. Actual measurements were made at 3.46°C (1.27 to 247.6 mm), 6.00°C (15.17 to 15.70 mm), 9.92°C (0.918 to 75.62 mm), 16.00°C (32.38 to 33.66 mm), and 19.98°C (1.11 to 87.49 mm). The numbers in parentheses give the range of partial pressure of Cl₂O at each temperature. The authors condensed these values to the above solubility table.
- b. Temperatures reported to 0.01°C.

contd.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two bulbs are connected by stop-cocks. A solution of hypochlorous acid is introduced in one and the apparatus rotated so the solution moves through both bulbs. After equilibration samples of the gas and liquid phases are chemically analysed. The analysis of the gas samples used the method of Spinks (1). The pressure was altered during the run.

SOURCE AND PURITY OF MATERIALS:

- (1) Cl₂O no comment by authors.
- (2) H_2O no comment by authors.

ESTIMATED ERROR:

 $\delta S/S = 0.02$ to 0.05 (estimated by compiler).

REFERENCES:

(1) Spinks J. Amer. Chem. Soc. <u>1931</u>, 53, 3015.

COMPONENTS:

- Chlorine monoxide; Cl₂O; [7791-21-1]
- Water; H₂O; [7732-18-5] (2)

ORIGINAL MEASUREMENTS:

Secoy, C.H.; Cady, G.H. J. Amer. Chem. Soc. 1941, 63, 2504-8.

Solubility^a of Chlorine Monoxide

T/K	<u>x</u> 1	r _c	s ^d
273.15	0.5259	1375	533.3
283.15	0.4273	962	359.9
293.15	0.3353	672	243.4

a. All values calculated by compiler.b. Mole fraction solubility (extrapolated) at 1 atm partial pressure of gas.

c.

Ostwald coefficient (extrapolated).
Solubility as g Cl₂O/100 g H₂O at 1 atm partial pressure of gas (extrapolated).

Equilibrium Constant Ka

t/°C		K	
3.46	0.41	±	0.01
6.00	0.48	±	0.01
9.92	0.62	±	0.01
16.00	1.01	<u>+</u>	0.01
19.98	1.47	+	0.01

a. $K = P_{Cl_2O} \times a_{H_2O}/(a_{HOCl})^2$ for 2 HOCl(aq) = $Cl_2O(g) + H_2O(l)$.

Assume $a_{H_2O} = 1$ and $K^1 = P_{Cl_2O}/m^2$ where m is the molal concentration of HOCl. The ${\rm K}^1$ values are plotted against m and extrapolated to infinite dilution to give the values of K in this table.

EXPERIMENTAL VALUES:

Solubility data at 3.46°C

_m a	mHOC1	mcl ₂ o	pCl ₂ O/mmHg	K(Henry) ^b
1.76 2.49 2.84 3.60 3.89 4.48 4.57 4.88 5.07	1.754 2.478 2.824 3.575 3.861 4.441 4.530 4.834 5.0205	0.012 0.024 0.031 0.050 0.058 0.078 0.080 0.092 0.099	1.27 2.54 3.40 5.31 6.31 8.27 8.46 10.10 10.62	0.00945 0.00945 0.0094 0.0092 0.0094 0.00945 0.0091 0.00935

- a. $m = m_{HOC1} + 0.5 m_{Cl_2O}$
- b. Henry's Law constant (= m_{Cl_2} 0/ p_{Cl_2} 0) refers to undissociated Cl₂0 only.
- c. The extrapolated solubility at $p_{\text{Cl}_2\text{O}} = 1$ atm is 7.12 moles $\text{Cl}_2\text{O}/\text{litre H}_2\text{O}$ or a mole fraction of 0.1137 for 1 atm partial pressure of gas. This is a mole fraction of 0.454 for total amount of Cl_2O dissolved at $p_{\text{Cl}_2\text{O}} = 1$ atm

 $p_{\text{Cl}_2\text{O}} = 1 \text{ atm}$ $K = m_{\text{HOCl}} \frac{2}{m_{\text{Cl}_2\text{O}}} = 255$

At 1 atm $m_{\text{Cl}_2\text{O}} = 7.21$ and $m_{\text{HOCl}} = 42.61$, therefore total Cl₂O = 28.42 moles/litre $^{\text{H}_2\text{O}}$, therefore x = 0.454.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Henry's Law constants determined from measuring hydrolysis constant of hydrolysis constant of hydrolysis constant of hypochlorous acid solutions at different molalities. Author points out systematic errors in work of Secoy and Cady (1).

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta K/K = 0.005$, estimate by author.

REFERENCES:

(1) Secoy, C.H.; Cady, G.H. J. Amer. Chem. Soc. 1941, 63, 2504-8.

COMPONENTS:	EVALUATOR:	
1. Chlorine dioxide; ClO ₂ ;	Rubin Battino,	
	Department of Chemistry,	
2. Water; H ₂ O; [7732-18-5]	Wright State University,	
	Dayton, Ohio, 45431,	
	U.S.A.	

CRITICAL EVALUATION:

Both the data of Kepinski and Trzeszcynski (1) and that of Haller and Northgraves (2) were used for the smoothing equation. This comprised six data points from the former and three from the latter. The standard deviation of the fit was 4.6% indicating rather poor data (but the only data available for this system). The fitting equation is:

ln x_1 = 7.91625 + 0.479133/(T/100K) - 11.0593 ln (T/100K) ...(1) where x_1 is the mole fraction solubility at 101.325 kPa (1 atm) partial pressure of gas. Table 1 gives smoothed values of the mole fraction (at 101.325 kPa) and the Ostwald coefficient at 5K intervals. Table 1 also gives the values of the thermodynamic functions $\Delta \overline{G}_1^{\circ}$, $\Delta \overline{H}_1^{\circ}$, $\Delta \overline{S}_1^{\circ}$ and $\Delta \overline{C}_{p_1}^{\circ}$ for the transfer of gas from the vapor phase at 101.325 kPa partial gas pressure to the (hypothetical) solution phase of unit mole fraction.

References

- 1. Kepinski, J.; Trzeszcynski, J. Rocz. Chem. 1964, 38, 201.10.
- 2. Haller, J. F.; Northgraves, W. W. Tappi 1955, 38, 199-202.

Table 1. Smoothed values of the solubility of chlorine dioxide in water and thermodynamic functions ^a at 101.325 kPa (1 atm) partial pressure of gas.

T/K	$x_1 \times 10^2$ b	r c	$\Delta \overline{G}_1^{\circ}/J \text{ mol}^{-1}$	$\Delta \overline{\text{H}}_1^{\circ}/\text{J mol}^{-1}$	$\Delta \overline{S}_{1}^{\circ}/J \text{ mol}^{-1} K^{-1}$
283.15	3.255	43.37	8.06	-26.43	-118.5
288.15	2.674	36.03	8.68	-26.89	-120.2
293.15	2.204	30.04	9.30	-27.35	-121.8
298.15	1.823	25.15	10.56	-27.81	-123.4
303.15	1.513	21.12	11.21	-28.27	-125.0
308.15	1.259	17.79	11.86	-28.73	-126.6
313.15	1.051	15.04	12.52	-29.19	-128.1
318.15	0.880	12.74	13.19	-29.65	-129.6
323.15	0.739	10.83	13.86	-30.11	-131.1
328.15	0.525	9.23	14.54	-30.57	-132.6
333.15	0.445	7.88	15.23	-31.03	-134.0

^a $\Delta \overline{C}_{p}$, was independent of temperature and had the value -92 J K⁻¹ mol⁻¹.

b Mole fraction solubility at 101.325 kPa partial pressure of gas.

C Ostwald coefficient.

Chlor	ine Dioxide Solubilities	450
COMPONENTS:	ORIGINAL MEASUREMENTS:	***************************************
 Chlorine dioxide; ClO₂; [10049-04-4] Water; H₂O; [7732-18-5] 	Haller, J.F.; Northgraves, Tappi. 1955, 38,199-202.	W.W.
VARIABLES: Temperature	PREPARED BY: R. Battino,	
experimental values:	PC10 $_2$ /mmHg Solubili / g l $^-$	ty 1

t/°C		PC10 ₂ /mmHg	Solubility / g l ⁻¹
25 25		34.5 22.1	3.01 1.82
25		13.4	1.13
25		8.4	0.69
40		56.2	2.63
40		34.3	1.60
40		18.9	0.83
40	9.9		0.47
60		105.9	2.65
60		53.7	1.18
60		21.3	0.58
60		12.0	0.26
T/K ^a	$X, \times 10^2$ b	<u>L</u> c	Solubility d
298.15	1.771	24.41	67.30
313.15	0.956	13.66	35.86
333.15	0.515	7.72	19.06

- a. Temperature reported as 24,40,60°C.
- b. Mole fraction solubility at 101.325kPa (1 atm) partial pressure of gas. Calculated by compiler. Extrapolated.
- c. Ostwald coefficient. Calculated by compiler. Extrapolated.
- d. Solubility in $g l^{-1}$. Extrapolated to 1 atm.

AUXILIARY INFORMATION

AUXILIARY	INFORMATION
METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The data are taken from reference (1). No other details supplied.	
	ESTIMATED ERROR:
	REFERENCES:
	l. Kirk, R.E.; Othmer, D.F. "Encyclopedia of Chemical Technology", Vol. 3., p.702. Interscience Publishers, (1952)

COMPONENTS: Chlorine dioxide; ClO₂; [10049-04-4] 2. Water; H₂O; [7732-18-5] VARIABLES:

ORIGINAL MEASUREMENTS:

Kepinski, J.; Trzeszcynski, J.

Rocz. Chem. 1964, 38, 201-10.

PREPARED BY:

Temperature

R. Battino.

EXPERIMENTAL VALUES:

T/K = 283-318

T/K a	$x_1 \times 10^2$ b	L C	_H d	Pressure ^e range /mm
283.15	3.271	43.60	0.1666	42-156
288.15	2.664	35.89	0.1347	14-163
293.15	2.208	30.09	0.1111	18-151
298.15	1.827	25.20	0.0914	21-154
308.15	1.296	18.32	0.0634	31-155
318.15	0.962	13.94	0.0474	38-154

- Temperature reported as 10, 15,...,45°C. a.
- b. Mole fraction solubility at 101.325 kPa (1 atm) partial pressure of gas. Calculated by compiler. Extrapolated.
- Ostwald coefficient. Calculated by compiler. Extrapolated. c.
- Henry's law constant. Units of (g $C10_4/$ liter) /mmHg $C10_4$. d.
- Pressure range of actual measurements. e.

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Used a dynamic saturation method along with a chemical method of analysis. A drawing and details given in the paper.

SOURCE AND PURITY OF MATERIALS:

- 1. Chlorine dioxide prepared according to reference (1).
- 2. Water no comment by authors.

ESTIMATED ERROR:

 $\delta H/H = 0.02$, compiler's estimate.

REFERENCES:

1. Kepinski, J. Przemysł. Chem. <u>1955</u>, 34,124.

SYSTEM INDEX

Underlined page numbers refer to evaluation text and those not underlined to compiled tables. All compounds are listed as in Chemical Abstracts. For example, toluene is listed as benzene, methyl- and dimethylsulfoxide is listed as methane, sulfinylbis-.

```
+ sulfur dioxide
  Acetamide, N,N-dimethyl-
                                                                                                 276, 297
                                                         + chlorine
  Acetic acid
                                                                                                 354 - 366,
                                                                                         386, 387
198, 200, 201
                                                        + sulfur dioxide
+ sulfur dioxide
  Acetic acid
 Acetic acid
Acetic acid (aqueous)
Acetic acid, anhydride
Acetic acid, anhydride
                                                                                                        199
                                                        + chlorine
                                                                                                        388
                                                        + sulfur dioxide
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Acetic acid, ethyl ester
Acetic acid, methyl ester
                                                     + sulfur dioxide
                                                                                                        218
                                                         + sulfur dioxide
                                                                                                218, 230
                                                         + sulfur dioxide
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Acetic acid, phenylmethyl ester + sulfur dioxide
                                                                                                179, 216
                                                                                                        253
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                                           see acetic acid, anhydride
 Acetone
                                            see 2-propanone
 Acetonitrile
                                                         + sulfur dioxide
                                                                                               267, 268
 Acetonitrile (aqueous)
                                                         + sulfur dioxide
                                                                                                        110
                                         see ethanone, 1-phenyl-
see ethane, 1,1,2,2-tetrachloro-
see under individual acids
 Acetophenone
 Acetylene tetrachloride
 Acids
                                          see under individual alcohols
 Alcohols
 Aluminium sulfate
                                         see sulfuric acid, aluminium salt
 2-Aminoethanol see ethanol, 2-amino-
Ammonium bisulfite see sulfurous acid, monoammonium salt
Ammonium bromide (aqueous) + sulfur dioxide 37 - 39,
Ammonium chloride (aqueous) + sulfur dioxide 37 - 39,
                                                                                                         55
Ammonium bromide (aqueous)
Ammonium chloride (aqueous)
Ammonium nitrate
Ammonium sulfate
Ammonium thiocyanate
iso-Amyl acetate
iso-Amyl alcohol
Aniline

+ sulfur dioxide
37 - 39,
37 - 39,

+ sulfur dioxide
37 - 39,

- see nitric acid, ammonium salt
- see sulfuric acid, ammonium salt
- see thiocyanic acid, ammonium salt
- see l-butanol, 3-methyl- acetate
- see benzenamine
Aniline
                                          see benzenamine
Anisole
                                          see benzene, methoxy-
                                                                                          Barium chloride (aqueous)
                                                        + chlorine
                                                        + sulfur dioxide
Benzenamine, N,N-diethyl-
Benzenamine, Ar,Ar-dimethyl-
Benzenamine, Ar
Benzenamine
                                                        + sulfur dioxide
                                                       + sulfur dioxide
                                                                                               287, 297
Benzenamine, Ar, Ar-dimethyl- (ternary)
                                                        + sulfur dioxide
                                                                                                       297
                                                                                        291 - \frac{261}{293}, \frac{262}{297},
                                                        + sulfur dioxide
Benzenamine, N, N-dimethyl-
Benzenamine, N,N-dimethyl- (ternary) + sulfur dioxide
Benzenamine, N-ethyl- + sulfur dioxide
Benzenamine, Ar-methyl- + sulfur dioxide
                                                                                                       297
                                                                                                       294
                                                                                                       287
Benzenamine, N-methyl-
                                                       + sulfur dioxide
                                                                                                      290
Benzene
                                                        + chlorine
                                                                                               \frac{354 - 366}{375 - 379}
Benzene
                                                       + sulfur dioxide
                                                                                               145 - 147
                                                                                               148 - 153
                                                   + sulfur dioxide
+ sulfur dioxide
Benzene, bis(l-methylethyl)-
                                                                                                      164
Benzene, bromo-
                                                                                                      311
Benzene, chloro-
                                                      + chlorine
                                                                                              \frac{354 - 366}{419 - 422}
Benzene, chloro-
Benzene, l-chloro-2-methyl-
                                                       + sulfur dioxide 298, 308 - 310
                                                      + chlorine
                                                                                                      427
                                                                                               (cont.)
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Benzene, 1-chloro-3-methyl-
Benzene, 1-chloro-4-methyl-
Benzene, 1-chloro-2-mitro-
                                                                                       + chlorine
                                                                                                                                                                   428
Benzene, 1,2-dichloro-
Benzene (dichloromethyl)-
Benzene, 1,2-dichloro-
Benzene (dichloromethyl)-
Benzene (dichloromethyl)
                                                                                     + chlorine
+ chlorine
+ chlorine
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Benzene, 1,4-dichloro-2-nitro- + chlorine
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Benzene, 1,3-dimethyl-
Benzene, 1,4-dimethyl-
Benzene, dimethyl-
Benzene, 1,3-dimethyl-
                                                                                        + chlorine
                                                                                                                                                                   382
Benzene, 1,2-dimethy1-
                                                                                                                                                                   383
                                                                                        + chlorine
                                                                                                                                                                   384
                                                                                        + chlorine
                                                                                       + sulfur dioxide
                                                                                                                                                                   151
                                                                                                                                                       146 - 147
                                                                                       + sulfur dioxide
                                                                                                                                                       158 - 160
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Benzene, 1,4-dimethoxy-
Benzene ethoxy-
                                                                                       + sulfur dioxide
+ sulfur dioxide
                                                                                                                                                                   252
                                                                                                                                                                   252
Benzene, ethoxy-
                                                                                       + sulfur dioxide
                                                                                                                                                                   249
                                                                                                                                                                   385
Benzene, ethyl-
                                                                                        + chlorine
                                                                                        + sulfur dioxide
+ sulfur dioxide
                                                                                                                                                                   312
Benzene, iodo-
Benzene, methoxy- + sulfur dioxide
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                                                                                        + chlorine
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                                                                                         + sulfur dioxide
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                                                                                        + sulfur dioxide
Benzene, nitro-
                                                                                       + chlorine
+ chlorine
+ chlorine
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Benzene, (trichloromethyl) -
Benzene, (trifluoromethyl) -
Renzene (trifluoromethyl)
Benzene, (trifluoromethyl) -, (ternary + quaternary)
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                                                                                         + sulfur dioxide
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1,2-Benzenedicarboxylic acid, dimethyl ester
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                                                                                         + chlorine
                                                                                        + chlorine
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                                                 + sulfur dioxide
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 Benzyl benzoate
 Benzyl cyanide
Benzyl ether
                                  see benzeneacetonitrile
                                  see benzene, 1,1-(methoxymethylene)bis-
 Bicyclo(2,2,1)heptan-2-one, 1,7,7-trimethyl-
                                                                                  \frac{190}{254}, \frac{191}{257},
                                                 + sulfur dioxide
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                                                                                         277
                                                 + sulfur dioxide
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                                                + sulfur dioxide
                                                                                         277
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Butane, 2-chloro-
Butane, 1,4-dichloro-
                                                + sulfur dioxide
+ sulfur dioxide
                                                                                           2/2/2
                                                + sulfur dioxide
 Butane, 1,1'-oxybis-
                                                + sulfur dioxide
                                                                                         25\overline{1}
 tert-Butanol
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1-Butanol, 3-methyl-, acetate
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                                                                                        193
                                                + sulfur dioxide
                                                                                        218
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                                                + sulfur dioxide
                                                                                        210
 (Z)-2-Butenedioic acid, dimethyl ester
                                                + sulfur dioxide
                                                                                        237
                                                + sulfur dioxide
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                                                                                         79
                                                                             \frac{37}{37} - 39
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                                                                                         78
                                                                               - 39,
                                                + sulfur dioxide
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                                                                           354 - 366, 392
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1-Chlorobutane
2-Chlorobutane
Chloroethane
Chloroform
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3-Chlorotoluene
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3-Chlorotoluene see benzene, l-chloro-3-methyl-
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2-Chloro-2-methylpropane see propane, 2-chloro-2-methyl-
1-Chloro-3-methylbenzene see benzene, 1-chloro-3-methyl-
                             see benzene, 1-chloro-2-nitro-
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1,2-Dichloroethane
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                             see ethene, 1,2-dichloro-, cis-
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trans-1,2-Dichloroethene see ethene, 1,2-dichloro-, trans-
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                              see benzene, 1,4-dichloro-2-nitro-
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                              see pyridine, 3,5-dichloro-2-
                                   (dichloromethyl) -
3,5-Dichloro-2-(trichloromethyl)pyridine
                              see pyridine, 3,5-dichloro-2-
                                   (trichloromethyl) -
1,2-Dichloro-4-nitrobenzene
                              see benzene, 1,2-dichloro-4-nitro-
Dichloro(trifluoromethyl)benzene
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Diethyl ether
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Dimethylamine
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                                                                         (cont.)
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Dimethylbenzene
Dimethyl aniline
Dimethyl formamide
Dimethyl ketone
Dimethyl maleate
Dimethyl phenylamine
Dimethyl phthalate
Dimethyl phthalate
See benzene, dimethyl-
see benzenamine, N,N-dimethyl-
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l,2-benzenecarboxylic acid,
dimethyl ester
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224, 225
                                                                                                                                                     + sulfur dioxide
   1,3-Dioxolan-2-one, 4-methyl-
                                                                                                                                                                                                                                                                \frac{116}{131}, \frac{117}{132}
                                                                                                                                                      + sulfur dioxide
   Dodecane
                                                                                                                                                    + sulfur dioxide
   Dodecanoic acid, ethyl ester
                                                                                                                                                      + sulfur dioxide
                                                                                                                                                                                                                                            \frac{1}{354 - 366}, \frac{2}{412}
   Ethane, chloro-
  Ethane, 1,2-dibromo-
Ethane, 1,1-dichloro-
Ethane, 1,2-dichloro-
                                                                                                                                                      + chlorine
                                                                                                                                                                                                                                                                       Ť,
Ī,
                                                                                                                                                     + sulfur dioxide
                                                                                                                                                    + sulfur dioxide
                                                                                                                                                                                                                                                                 306, 307
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                                                                                                                                                                                                                                                                           234
                                                                                                                                                     + sulfur dioxide
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                                                                                                                                                      + sulfur dioxide
                                                                                                                                                                                                                                            231, \overline{232}, \overline{234}
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Ethane, 1,1,2,2-tetrachloro-

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Ethane, 1,1,2-trichloro-

Eth
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   1,2-ethanediamine, N,N'-bis(2-aminoethyl)-
                                                                                                                                                                                                                                                                                 297
                                                                                                                                                       + sulfur dioxide
                                                                                                                                                                                                                                                                \frac{189}{203}, \frac{191}{206},
                                                                                                                                                       + sulfur dioxide
   1,2-Ethanediol
                                                                                                                                                                                                                                                                                    241
                                                                                                                                                     + sulfur dioxide
   1,2-Ethanediol, diacetate
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                                                                                                                                                      + sulfur dioxide
   Ethanol
                                                                                                                                                      + sulfur dioxide
                                                                                                                                                                                                                                                                111, 112
                                                                                                                                                      + sulfur dioxide
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   Ethanol, 2-amino-
Ethanol, 2-butoxy-
                                                                                                                                                     + sulfur dioxide
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Ethanol, ethoxy-, acetate
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Ethanol, 2,2-oxybis-
Ethanol, 2-phenoxy-
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Ethanone, 1-phenyl-
alloxide
sulfur dioxide
                                                                                                                                       + sulfur dioxide
+ sulfur dioxide
+ sulfur dioxide
                                                                                                                                                                                                                                                                                    241
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                                                                                                                                                                                                                                                                                    204
                                                                                                                                                                                                                                                                                    217
                                                                                                                                                                                                                                                                                    305
                                                                                                                                                                                                                                                                                    239
                                                                                                                                                                                                                                            354 - 36\overline{6}, 41\overline{3}
                                                                                                                                                    + sulfur dioxide
+ sulfur dioxide
                                                                                                                                                                                                                                                                       \frac{1}{2}, \frac{2}{306}
  Ethene, 1,1,2,2-tetrachier + sulfur dioxide = ...

Ethene, 1,1,2-trichloro- + sulfur dioxide = ...

Ethyl acetoacetate see 3-oxobutanoic acid, ethyl ester see benzenamine, N-ethyl-
   Ethylene glycol dimethyl ether
                                                                                                          see ethane, dimethoxy-
                                                                                                          see 1,2-ethanediol
   Ethylene glycol
   Ethylene glycol monoethyl monoacetate
  Ethyl benzene see ethanol, 2-ethoxy-, acetate
Ethyl benzene see benzene, ethyl
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Ethyl laurate see dodecanoic acid, ethyl ester
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Formamide, N,N-dimethyl-
                                        + chlorine
+ sulfur dioxide
                                                                    354 - 366, 390
                                                                    + sulfur dioxide
+ sulfur dioxide
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                                           + sulfur dioxide
                                                                                202
                                           + sulfur dioxide
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+ sulfur dioxide
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Glycol
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Heptane
                                           + chlorine
                                                                          367 - 369
                                           + sulfur dioxide
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Heptane
                                           + sulfur dioxide
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Heptane, hexadecafluoro-
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                                           + chlorine
                                                                                41\overline{6}
                                           + sulfur dioxide
                                                                                194
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Hexadecane + sulfur dioxide
                                                                          \frac{116}{136}, \frac{117}{138},
                                                                          \frac{116}{119}, \frac{117}{121},
Hexane
                                           + sulfur dioxide
                                                                                  2
                                           + sulfur dioxide
Hexane, 1-chloro-
                                           + sulfur dioxide
+ sulfur dioxide
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                                                                    344, 345 - 348,
                                           + chlorine
                                                                               349
                                           + sulfur dioxide
+ sulfur dioxide
                                                                           40, \overline{41}
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Hydrogen chloride (multicomponent)
                                                                                107
                                                                                448
Hydrogen fluoride
                                           + chlorine
Hydrogen fluoride
                                           + sulfur dioxide
                                                                                <u>2</u>
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Hydroterpin
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                                           + sulfur dioxide
                                                                                171
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Kerosene
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                                                                                172
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Methane, chloro-
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                                              + chlorine
                                              + sulfur dioxide
+ sulfur dioxide
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+ sulfur dioxide
+ sulfur dioxide
                                              + sulfur dioxide
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                                                                                      411
                                              + chlorine
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                                                                         \frac{1}{300}, \frac{2}{303}, \frac{298}{304}
                                               + sulfur dioxide
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Methane, trichloro-
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                                                                         106, 107
354 - 366, 410
                                               + sulfur dioxide
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Methanesulfenyl chloride, trichloro- (quaternary)
                                               + chlorine
                                                                                      411
                                                                         <u>174</u>, 175 - 177,
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Methanol (ternary)
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                                                                               178, 179
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Methylal
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Methylaniline
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Methyl benzoate
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                                                                               129, 140,
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                                                                         143, 144, \frac{147}{129}, 140, \frac{147}{62}
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Naphthalene, 1,2,3,4-tetrahydro- + sulfur dioxide
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Nitric acid, potassium salt (aqueous)
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2-Nitrotoluene
                                               + sulfur dioxide
                                                                         <u>116</u>, <u>117</u>, 127
Nonane
                                                                                (cont.)
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0
                                                      + chlorine
                                                                                     354 - 366, 370
Octane
                                                                                            \frac{116}{123}, \frac{117}{124}
                                                      + sulfur dioxide
Octane
Octane, 1-bromo-
Octane, 1-chloro-
                                                                                                   315
                                                      + sulfur dioxide
                                                      + sulfur dioxide
                                                                                                   314
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                                                                                            189, 191,
193, 195
                                                      + sulfur dioxide
1-Octanol
                                                                                                   250
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