#### INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

# ANALYTICAL CHEMISTRY DIVISION COMMISSION ON SOLUBILITY DATA

# **SOLUBILITY DATA SERIES**

Volume 50

# CARBON DIOXIDE IN NON-AQUEOUS SOLVENTS AT PRESSURES LESS THAN 200 KPA

# **SOLUBILITY DATA SERIES**

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A complete list of volumes published in the Solubility Data Series will be found on p. 484.

# **SOLUBILITY DATA SERIES**

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Volume 50

# CARBON DIOXIDE IN NON-AQUEOUS SOLVENTS AT PRESSURES LESS THAN 200 KPA

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# **FOREWORD**

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

The Solubility Data Series is a project of Commission V.8 (Solubility Data) of the International Union of Pure and Applied Chemistry (IUPAC). The project had its origins in 1973, when the Analytical Chemistry Division of IUPAC set up a Subcommission on Solubility Data under the chairmanship of the late Prof. A. S. Kertes. When publication of the *Solubility Data Series* began in 1979, the Committee became a full commission of IUPAC, again under the chairmanship of Prof. Kertes, who also became Editor-in-Chief of the Series. The Series has as its goal the preparation of a comprehensive and critical compilation of data on solubilities in all physical systems, including gases, liquids and solids.

The motivation for the Series arose from the realization that, while solubility data are of importance in a wide range of fields in science and technology, the existing data had not been summarized in a form that was at the same time comprehensive and complete. Existing compilations of solubility data indeed existed, but they contained many errors, were in general uncritical, and were seriously out-of-date.

It was also realized that a new series of compilations of data gave educational opportunities, in that careful compilations of existing data could be used to demonstrate what constitutes data of high and lasting quality. As well, if the data were summarized in a sufficiently complete form, any individual could prepare his or her own evaluation, independently of the published evaluation. Thus, a special format was established for each volume, consisting of individual data sheets for each separate publication, and critical evaluations for each separate system, provided sufficient data from different sources were available for comparison. The compilations and, especially, the evaluation were to be prepared by active scientists who were either involved in producing new data, or were interested in using data of high quality. With minor modifications in format, this strategy has continued throughout the Series.

In the standard arrangement of each volume, the Critical Evaluation gives the following information:

(i) A text which discusses the numerical solubility information which has been abstracted from the primary sources in the form of compilation sheets. The text concerns primarily the quality of the data, after consideration of the purity of the materials and their characterization, the experimental method used, the uncertainties in the experimental values, the reproducibility, the agreement with accepted test values, and finally, the fitting of the data to suitable functions, along with statistical tests of the fitted data.

- (ii) A set of recommended data, whenever possible, including weighted averages and estimated standard deviations. If applicable, one or more smoothing equations which have been computed or verified by the evaluator are also given.
- (iii) A graphical plot of the recommended data, in the form of phase diagrams where appropriate.

The Compilation part consists of data sheets which summarize the experimental data from the primary literature. Here much effort is put into obtaining complete coverage; many good data have appeared in publications from the late nineteenth and early twentieth centuries, or in obscure journals. Data of demonstrably low precision are not compiled, but are mentioned in the Critical Evaluation. Similarly, graphical data, given the uncertainty of accurate conversion to numerical values, are compiled only where no better data are available. The documentation of data of low precision can serve to alert researchers to areas where more work is needed.

A typical data sheet contains the following information:

- (i) list of components: names, formulas, Chemical Abstracts Registry Numbers;
- (ii) primary source of the data;
- (iii) experimental variables;
- (iv) compiler's name;
- (v) experimental values as they appear in the primary source, in modern units with explanations if appropriate;
- (vi) experimental methods used;
- (vii) apparatus and procedure used;
- (viii) source and purity of materials used;
  - (ix) estimated error, either from the primary source or estimated by the compiler;
  - (x) references relevant to the generation of the data cited in the primary source.

Each volume also contains a general introduction to the particular type of system, such as solubility of gases, of solids in liquids, etc., which contains a discussion of the nomenclature used, the principle of accurate determination of solubilities, and related thermodynamic principles. This general introduction is followed by a specific introduction to the subject matter of the volume itself.

The Series embodies a new approach to the presentation of numerical data, and the details continue to be influenced strongly by the perceived needs of prospective users. The approach used will, it is hoped, encourage attention to the quality of new published work, as authors become more aware that their work will attain permanence only if it meets the standards set out in these volumes. If the Series succeeds in this respect, even partially, the Solubility Data Commission will have justified the labour expended by many scientists throughout the world in its production.

January, 1989

J. W. Lorimer, London, Canada

# **PREFACE**

This volume of The Solubility Data Series contains evaluated data for the solubility in non-aqueous solvents of carbon dioxide at a partial pressure not greater than 200 kPa. In some cases a compiler has extrapolated published data for higher pressures to obtain a value for a solubility at a pressure below 200 kPa. Two further volumes in the series will include data for aqueous systems at all pressures and data for non-aqueous systems at pressures above 200 kPa.

Measurements of the solubility of carbon dioxide have been carried out for over a hundred years. New techniques have been developed and old techniques modified during this time but some of the early measurements are in close agreement with recent measurements. Reliance may be placed on data when there is good agreement between the measurements of different groups of workers. Unfortunately there are sometimes inconsistencies between measurements by different groups. Judgements have then to be made of the relative reliability of different experimental methods. Difficulties in attaining equilibrium between the gas and liquid phase are an important cause of discrepancies.

In some cases it has been possible to recommend equations relating mole fraction solubility at a partial pressure of 101.3 kPa with temperature. These equations are based on the data which have been considered to be the most reliable. The use of these equations for extrapolation more than a few degrees outside the temperature range of the experimental measurements can lead to errors.

The editor is grateful for support, encouragement and help from fellow members of the IUPAC Commission on Solubility Data. He would like to acknowledge the help given by Dr Elena Gryzlova in obtaining copies of papers from the less accessible Russian journals. He would also like to thank Dr Sim-wan Annie Bligh for her assistance in translating Chinese and Japanese papers.

Peter Fogg

London

September 1991

# WILLIAM GERRARD 1900-1990

Members of the Solubility Data Commission of the International Union of Pure and Applied Chemistry were saddened by the death of Dr William Gerrard on 5th February 1990, shortly before his ninetieth birthday. William Gerrard was the oldest and one of the longest serving members of the Commission.

William Gerrard was born in Tyldesley, Lancashire, U.K. on 24th February, 1900. He studied part-time at a local technical college and eventually graduated as an external student of the University of London with first class honours in chemistry. Later he gained a PhD after part-time research at Battersea Polytechnic in London under the direction of Dr Joseph Kenyon, FRS. This gave him a life long interest in the mechanisms and stereochemistry of reactions of esters of phosphorus and sulfur. William Gerrard joined the staff of the Northern Polytechnic (now Polytechnic of North London) in 1934 after holding earlier academic posts. He became Head of the Department of Chemistry, Mathematics, Botany, Zoology, Biology and Geology in 1948, a post which he held until he retired in 1965.

During the Second World War he had responsibilities for a section of the London University Air Squadron training at the Northern Polytechnic and held the rank of Flight Lieutenant.

It is as an experimental organic chemist that he made his most important contribution to chemistry. He established a flourishing research school covering a wide range of organic chemistry and published over 200 research papers. He was awarded the degree of DSc in 1947. His monograph The Organic Chemistry of Boron was published in 1961. He also contributed a chapter on boron chemistry to Mellor's Inorganic Chemistry and a chapter on the organic chemistry of phosphorous and thiophosphorous acids to the Kosolapoff and Maier series Organic Compounds of Phosphorus. For many years after his retirement he continued to direct the studies of part time and full time research students and to work at the bench himself. His interest in solubility phenomena arose from his observations of the behaviour of gases such as hydrogen chloride and sulfur dioxide during organic reactions in the liquid phase. As his many research students and collaborators can testify, once William Gerrard's enthusiasm was roused he had the ability to transmit his enthusiasm to others.

He and his co-workers published many papers containing solubility data for the hydrogen halides and other gases. His book entitled Solubility of Gases and Liquids was published in 1976. Gas Solubilities - Widespread Applications followed in 1980. At the time of his death he was co-operating with Peter Fogg in the preparation of Solubility of Gases in Liquids which was published later in the year.

Publications on the solubility of gases led to an invitation to assist in the Solubility Data Project shortly after its inception and continued to serve when Commission status was achieved in 1979. He contributed to several of the volumes on gas solubilities and was co-editor of Hydrogen Halides in Non-aqueous Solvents. He was always fearless in his determination to maintain high standards. Not one of his colleagues working in the Solubility Data Commission could escape his criticism if things did not meet his approval. Eventually failing hearing and eyesight and general frailty made it impossible for him to attend annual meetings of the Solubility Data Commission. Until the last he took a keen interest in the affairs of the Commission and continued to provide detailed comments.

He was awarded an OBE for services to chemistry in 1981.

William Gerrard had an infectious delight in many aspects of chemistry and former colleagues and students have been inspired by his unforgettable enthusiasms, scholarship and devotion to hard and careful work. It is a privilege to have worked with him.

Peter Fogg

# THE SOLUBILITY OF GASES IN LIQUIDS

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

#### 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 recommended and in some cases a smoothing equation suggested 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.

#### 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, 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 and inevitably 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 Kelvin.

#### 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 measurement 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. For 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 gas-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 very 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:

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

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

here n is the number of moles of a substance (an amount 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

$$wt% = 100 W(g)/[W(g) + W(1)]$$

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,  $C_{\mathbf{w}}$ 

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

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

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

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

where  $v^{O}(1)$  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 is assumed to be obeyed,

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

where V(g) is the volume of gas absorbed and V(1) is the original (starting) volume of absorbing solvent. The mole fraction solubility is related to the Bunsen coefficient by

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

where  $v^{O}(g)$  and  $v^{O}(1)$  are the molar volumes of gas and solvent at a pressure of one atmosphere. If the gas is ideal,

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

Real gases do not follow the ideal gas law and it is important to establish the real gas law used for calculating  $\alpha$  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 at 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, is related to the Ostwald coefficient by

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

where P is the partial pressure of gas. The mole fraction solubility will be at a partial pressure of P(g).

#### 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.  $\beta$  is related to the Bunsen coefficient by

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

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

#### The Henry's Law Contant

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

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

where  $\mathbf{K}_{\mathbf{H}}$  is the Henry's Law constant and x the mole fraction solubility. Other formulations are

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

or

$$C(g) = K_C(1)$$

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 fraction 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.

TABLE 1. Interconversion of parameters used for reporting solubility.

 $L = \alpha(T/273.15)$ 

 $C_{xy} = \alpha/v_0 \rho$ 

 $K_{H} = \frac{17.033 \times 10^{6} \rho (soln)}{\alpha M(1)} + 760$ 

 $L = C_w v_{t,gas} \rho$ 

where  $v_o$  is the molal volume of the gas in cm³ mol<sup>-1</sup> at 0°C,  $\rho$  the density of the solvent at the temperature of the measurement,  $\rho_{soln}$  the density of the solution at the temperature of the measurement, and  $v_{t,gas}$  the molal volume of the gas (cm³ mol<sup>-1</sup>) at the temperature of the measurement.

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Revised: December 1984 (CLY)

APPENDIX I. Conversion Fact	ors	k a	ınd k	·- 1	•		
	1		k n-SI (SI		Jnit)	=	$k^{-1}$ 1 (SI Unit) = $k^{-1}$ (non-SI Unit)
LENGTH							SI Unit, m
A (angstrom cm (centimeter) in (inch) ft (foot)		3	1 254	×	10 <sup>-1</sup> 10 <sup>-2</sup> 10 <sup>-4</sup> 10 <sup>-4</sup>	(*) (*)	$ \begin{array}{c} 1 \times 10^{10} & (*) \\ 1 \times 10^{2} & (*) \\ 3 937 008 \times 10^{-5} \\ 3 280 840 \times 10^{-6} \end{array} $
AREA							SI Unit, m²
cm <sup>2</sup> in <sup>2</sup> ft <sup>2</sup>	9		516	×	10 <sup>-4</sup> 10 <sup>-8</sup> 10 <sup>-8</sup>		$\begin{array}{c} 1 \times 10^{4} & (*) \\ 1 550 003 \times 10^{-3} \\ 1 076 391 \times 10^{-5} \end{array}$
VOLUME					-		SI Unit, m <sup>3</sup>
cm <sup>3</sup> in <sup>3</sup> ft <sup>3</sup> 1 (litre) UKgal (UK gallon) USgal (US gallon)		831 45	064 685 1 461	× × ×	10 <sup>6</sup> 10 <sup>-1</sup> 10 <sup>-8</sup> 10 <sup>-3</sup> 10 <sup>-7</sup>	(*)	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
MASS							SI Unit, kg
g (gram) t (tonne) lb (pound)	45	359	1	×	10 <sup>-3</sup> 10 <sup>3</sup> 10 <sup>-8</sup>	(*) (*) (*)	$\begin{array}{c} 1 \times 10^{3} & (*) \\ 1 \times 10^{-3} & (*) \\ 2 204 623 \times 10^{-6} \end{array}$
DENSITY							SI Unit, kg m <sup>-3</sup>
g cm <sup>-3</sup> g l <sup>-1</sup> lb in <sup>-3</sup> lb ft <sup>-3</sup> lb UKgal <sup>-1</sup> lb USgal <sup>-1</sup>	1	601 99	1 991 847 776	× × ×	10 <sup>3</sup> 10 <sup>-2</sup> 10 <sup>-5</sup> 10 <sup>-3</sup> 10 <sup>-4</sup>	(*) (*)	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
PRESSURE			s	r ı	Unit,	Pa (p	pascal, kg $m^{-1}$ $s^{-2}$ )
3. C C2	6	101 894 47 386	665 325 1 757 880 388	× × × ×	10 <sup>-1</sup> 10 <sup>-1</sup> 10 <sup>5</sup> 10 <sup>-3</sup> 10 <sup>-3</sup> 10 <sup>-4</sup>	(*) (*) (*)	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
ENERGY			s	ן ז	Unit,	J (jo	oule, kg m² s <sup>-2</sup> )
erg cal <sub>IT</sub> (I.T. calorie) calth (thermochemical calorie kW h (kilowatt hour) l atm ft lbf hp h (horse power hour) Btu (British thermal unit)	1 2	4 101 355 684	868 184 36 325 818 519	× × × ×	10 <sup>-7</sup> 10 <sup>-4</sup> 10 <sup>-3</sup> 10 <sup>-3</sup> 10 <sup>-6</sup>	(*) (*)	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$
						tions	

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

#### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

Solubility of carbon dioxide in alkanes, cyclic alkanes and alkenes.

The solubility of solid carbon dioxide in methane, ethane, propane and butane was measured by Cheung and Zander (1) at temperatures between 87.4 K and 194.6 K. Solubility in methane at 126.4 K and 137.5 K was measured by Preston et al. (2). There is satisfactory agreement with Cheung's data. The concentration of carbon dioxide in solution in the presence of solid carbon dioxide increases with increase in temperature. The partial vapor pressure also increases with temperature and mole fraction solubilities corrected to the same partial vapor pressure show a decrease with increase in temperature in line with the behaviour of the gas in other solvents. Data indicate that there are insignificant differences between solubilities in methane, propane and butane under the conditions of the measurements but that solubility is greatest in ethane. (see table below)

alkane	T/K	mole% of $CO_2$ in solution
methane	183.2	6.60
	183.2	5.85
ethane	180.3	7.54
propane	180.2	5.7
butane	180.3	5.6

Solubility of solid carbon dioxide in liquid ethane was also measured by Clark and Din (3) from 130 K to 180 K. Clark's measurements are close to those of Cheung at lower temperatures. Clark found a solubility of 0.9 mol% at 150 K and Cheung a value of 0.85 mol% at 149 K. The agreement at higher temperatures is poor. Clark's value for 180 K is 6.7 mol% and Cheung's value at 180.3 K is 7.54 mol%

Nagahama et al. (4) studied phase equilibria between gaseous carbon dioxide and ethane, propane, butane or 2-methylpropane. Measurements were extended to high pressures over the whole concentration range. Approximate mole fraction solubilities for a partial pressure of 101.3 kPa show an increase with carbon number at constant temperature. These have been estimated by the evaluator from data for partial pressures of carbon dioxide from 71 to 214 kPa, assuming that mole fraction solubility is proportional to pressure, and are given below.

alkane	T/K	<sup>x</sup> co₂
ethane	252.95	0.026
propane	252.95	0.029
butane	273.15 273.15	0.019 0.021
2-methylpropane	273.15	0.019

Makranczy et al. (5) measured the solubility of carbon dioxide in straight chain alkanes from pentane to hexadecane at 298.2 K and 313.2 K. These measurements show a decrease in mole fraction solubility with increase in chain length at a partial pressure of gas of 101.3 kPa. This is not in accord with measurements reported by other workers and the bulk of evidence indicates that mole fraction solubility increases with chain length.

Solubility in pentane has been reported by Makranczy et al. (5) and by Cheng et al. (6). Cheng's data indicate a mole fraction solubility of approximately 0.0138 at 298.2 K and a partial pressure of carbon dioxide of 101.3 kPa. The mole fraction solubility from Makranczy's measurements under these conditions is 0.01258. The following equation for mole

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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#### CRITICAL EVALUATION:

fraction solubility at a partial pressure of carbon dioxide of 101.3 kPa is based upon data from the two sources.

$$\ln x_{CO_2} = 83.727 - 2635.9/(T/K) - 13.906\ln(T/K)$$

temperature range = 252.7-313.2 Kstandard deviation in  $x_{CO_2} = 0.00033$ 

Solubility in 2,2-dimethylpropane (neopentane) was measured by Stead and Williams (7) at pressures below 516 kPa from 250 K to 300 K. The data are self-consistent. Mole fraction solubility at a partial pressure of 101.3 kPa estimated from these data fit the following equation

$$\ln x_{CO_2} = 85.021 - 2788.0/(T/K) - 14.006\ln(T/K)$$

temperature range = 250-300 Kstandard deviation in  $x_{CO_2} = 0.00071$ 

The mole fraction solubility at 298.2 K from this equation is 0.0161 compared with a value of 0.0130 from the equation for pentane.

Mole fraction solubilities of gas in hexane at a partial pressure of  $101.3~\mathrm{kPa}$  from work by various authors (5,8-13) show good agreement (Fig 1) and fit the equation

$$\ln x_{CO_2} = 26.213 - 429.93/(T/K) - 5.1244ln(T/K)$$

temperature range 238.2-313.2 K standard deviation in  $x_{CO_2} = 0.00018$ 

Data published by Tong  $et\ al.$  (14) appear to be inconsistent with other data and have not been used to derive the above equation.

Solubility of solid carbon dioxide at 177-216 K was measured by Im and Kurata (13). The data are self-consistent and may be accepted as reliable. Mole fraction solubilities for a partial pressure of carbon dioxide of 101.3 kPa estimated from these data for low temperatures are higher than values estimated from the equation given above.

Most of the data from various sources (5,10,11,15,16) for solubilities in heptane show a similar consistency. The following equation fits values of mole fraction solubilities at a partial pressure of gas of 101.3 kPa.

$$\ln x_{CO_2} = 18.584 - 61.706/(T/K) - 4.0034 \ln(T/K)$$

temperature range = 238.2-313.2 Kstandard deviation in  $x_{CO_2} = 0.00035$ 

Data published by Tong  $et\ al.$  (14) appear to be inconsistent with data published by other authors and have not been included in the evaluation of the constants in this equation.

Im and Kurata (13) also measured the solubility of solid carbon dioxide in heptane over the temperature range 182-216 K. Data for this system are self consistent. Mole fraction solubilities of solid carbon dioxide in heptane are lower than solubilities in hexane. The equation given above is not applicable to the solubility of solid carbon dioxide in heptane.

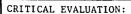
Data for the solubility of carbon dioxide in octane published by Wilcock  $et\ al.$  (17), Shenderei and Ivanovsky (11), King and Al-Najjar (10) are consistent with each other. Mole fraction solubilities at a partial

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alkanes, Cyclic Alkanes and Alkenes

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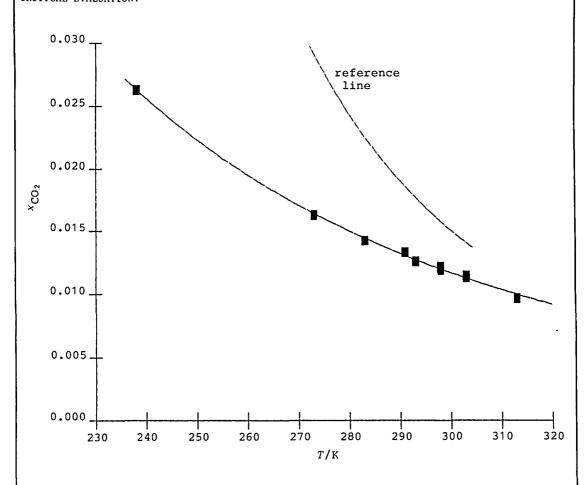


Fig. 1 Variation with temperature of the mole fraction solubility of carbon dioxide in hexane at a partial pressure of gas of 101.3 kPa.

Points based upon experiemntal measurements by various authors (5,8-13) have been superimposed on a curve corresponding to the equation

$$\ln x_{CO_2} = 26.213 - 429.93/(T/K) - 5.1244ln(T/K)$$

A reference line corresponding to values from the Raoult's law equation is also shown.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
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CRITICAL EVALUATION:

pressure of gas of 101.2 kPa from these three sets of data fit the equation  $\ \ \,$ 

 $\ln x_{CO_2} = -9.6225 + 1063.4/(T/K) + 0.2883\ln(T/K)$ 

temperature range = 238.2-313.4 K standard deviation in  $x_{\rm CO_2}$  = 6.2 × 10<sup>-5</sup>

The mole fraction solubility at 298.15 K published by Tong  $et\ al.$  (14) is close to the value from this equation (Tong 0.0119; eqn. 0.0121). Mole fraction solubilities at 298.15 and 313.15 K calculated from data given by Makranczy  $et\ al.$ (5), fall below values given by the equation.

Asano et al. (18) used a chromatographic method to measure K-values for dissolution of carbon dioxide in solutions of methane in octane. The K-values were defined as the ratio of mole fractions of  $CO_2$  in the vapor and in the liquid phases and correspond to very low concentrations of carbon dioxide. The data are self-consistent but no other data on this system are available for comparison.

Hiraoka and Hildebrand (19) measured solubility in the non-linear 2,2,4-trimethylpentane. The mole fraction solubility at 298.15 and a partial pressure of 101.3 kPa estimated from these data is 0.0139 compared with a value for solubility in octane from the above equation of 0.0121. This difference may be compared with that between solubilities in pentane and 2,2-dimethylpropane which has been noted above.

Solubility in nonane was measured by Makranczy  $et\ al.$  (5). Measurements of solubilities of carbon dioxide in the higher alkanes by this group do not conform to the general trend indicated by other workers. A value for 298.15 K has also been published by Tong  $et\ al.$ (14). The data for nonane cannot be recommended until they are substantiated by other measurements on this system.

Solubility in decane has been measured by Wilcock  $et\ al.(17)$ , King and Al-Najjar (10), Horvath  $et\ al.(20)$ , Makranczy  $et\ al.(5)$ , and Tong  $et\ al.(14)$ . The following equation for mole fraction solubility at a partial pressure of 101.3 kPa is based upon data from the first three groups of workers.

 $\ln x_{CO_2} = 14.481 - 114.51/(T/K) - 3.2438\ln(T/K)$ 

temperature range = 283.2-313.5 K. standard deviation in  $x_{CO_2} = 0.00016$ 

Data published by Makranczy and by Tong are not consistent with this equation.

Values of the solubility in undecane, tridecane and pentadecane reported by Makranczy  $et\ al.$  appear to be too low and cannot be recommended until the measurements have been repeated by other workers. The mole fraction solubility in undecane at 298.15 K has been published by Tong  $et\ al.$  In contrast this value appears to be too high in comparison with data for other alkanes.

Solubility in dodecane has been measured by Hayduk  $et\ al.(16)$ , by King and Al-Najjar (10) and by Makranczy  $et\ al.(5)$ . Measurements by Hayduk are consistent with those by King. Mole fraction solubilities at a partial pressure of 101.3 kPa from these two sources fit the equation

 $\ln x_{CO_2} = 11.161 + 66.063/(T/K) -2.7623ln(T/K)$ 

temperature range = 283.15-323.15 K standard deviation in  $\times_{CO_2}$  = 0.00014

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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#### CRITICAL EVALUATION:

Solubilities measured by Macranczy et al. are about 14% lower than those reported by the other authors.

Mole fraction solubility in tetradecane at a partial pressure of 101.3 kPa from measurements by King and Al-Najjar (10) fit the equation

$$\ln x_{CO_2} = -49.650 + 2870.5/(T/K) + 6.2703\ln(T/K)$$

temperature range = 298.2-343.2 K standard deviation in  $x_{\rm CO_2}$  = 1.2 × 10<sup>-5</sup>

Measurements by Makranczy  $et\ al.(5)$  are about 20% lower and are less likely to be reliable.

Solubility in hexadecane has been measured by at least seven groups  $(5,10,16,\ 21-24)$ . Measurements by Macranczy et al. appear to be be too low and those by Lenoir et al.(21) to be too high. Values of mole fraction solubility from measurements by the other groups are mutually consistent and fit the equation

$$\ln x_{CO_2} = -26.045 + 1769.0/(T/K) + 2.7810\ln(T/K)$$

temperature range = 298.2-475.0 Kstandard deviation in  $x_{CO_2} = 0.00015$ 

The solubility in heptadecane at 313.2 K was measured by Lenoir et a1.(21) using a chromatographic method to find the limiting value of Henry's constant. The corresponding value of the mole fraction solubility at 101.3 kPa is 0.0139. This may be compared with the value of 0.01210 for solubility in hexadecane at this temperature and pressure from the equation given above.

Henry's law constants for dissolution of carbon dioxide in eicosane  $(C_{20}H_{+2})$  were measured by Chai and Paulaitis (24), Gasem and Robinson (25) and by Huang et al. The sets of data are mutually consistent. The corresponding mole fraction solubilities for a partial pressure of 101.3 kPa fit the equation

$$\ln x_{CO_2} = -23.875 + 1622.2/(T/K) + 2.5006 \ln(T/K)$$

temperature range = 313.2-573.4 Kstandard deviation in  $x_{CO_2} = 0.00044$ 

Solubility in octacosane ( $C_{28}H_{58}$ ) was reported by Huang et a1.(26), Gasem and Robinson (25) and by Lin and Parcher (22) with good agreement between the sets of data. Mole fraction solubilities at a partial pressure of 101.3 kPa fit the equation

$$\ln x_{CO_2} = -25.506 + 1747.4/(T/K) + 2.7523ln(T/K)$$

temperature range = 348.2-573.2 standard deviation in  $x_{\rm CO_2}$  = 4.2 × 10<sup>-5</sup>

Solubilities in hexatriacontane ( $C_{36}H_{74}$ ) have also been published by Gasem and Robinson (25) and by Lin and Parcher (22). There is again good agreement between sets of data. Mole fraction solubilities at a partial pressure of 101.3 kPa fit the equation

$$\ln x_{CO_2} = 5.2340 + 123.53/(T/K) - 1.6712ln(T/K)$$

temperature range = 353.2-423.2 Kstandard deviation in  $x_{CO_2} = 0.00014$ 

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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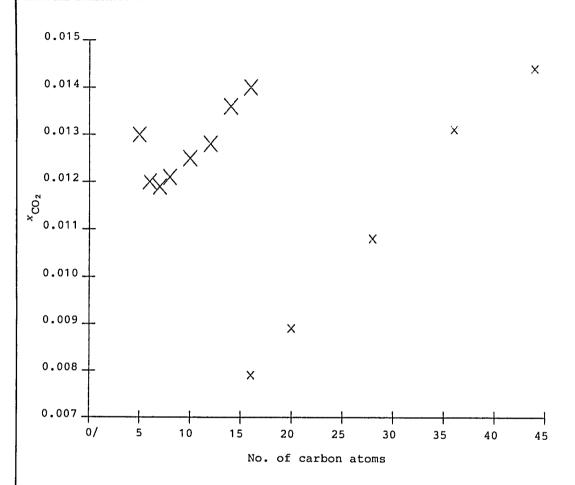


Fig. 2 Selected values of the mole fraction solubility of carbon dioxide in straight chain alkanes at 298.15 K or 373.15 K and a partial pressure of gas of 101.3 kPa.

large crosses 298.15 K small crosses 373.15 K

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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Gasem and Robinson (25) measured solubility in tetratetracontane ( $C_{4\,4}H_{9\,0}$ ) at 373.2 and 423.2 K. Mole fraction solubilities for a partial pressure of 101.3 kPa are in accord with the general trend of values with increase in chain length (see fig 2).

Chai and Paulaitis (24) have published Henry's constants at infinite dilution for the carbon dioxide - squalane ( $C_{30}H_{62}$ ) system for 298.6-330.2 K. Mole fraction solubilities at a partial pressure of 101.3 kPa estimated from these constants fit the equation

$$\ln x_{CO_2} = -16.170 + 1354.4/(T/K) + 1.3729\ln(T/K)$$

temperature range = 298.6-330.2 Kstandard deviation in  $x_{CO_2} = 0.00011$ 

A plot of the mole fraction solubility at 101.3 kPa against temperature lies close to an extrapolation of a similar plot for hexatriacontane. Mole fraction solubilities are higher than extrapolated values for octacosane (Fig 3).

Phase equilibria between cyclopropane and carbon dioxide has been studied by Haselden and Snowden (27). They reported dew and bubble points from 179 K to 237 K. Data are self-consistent. The mole fraction solubility at 228.3 K and a partial pressure of carbon dioxide of approximately 99.51 kPa is 0.0489. This may be compared with the ideal solubility of 0.119 estimated from Raoult's law.

Mole fraction solubilities in cyclic alkanes are lower than in the corresponding straight chain compounds. Eckert and Sandler (28) studied equilibria between cyclopentane and carbon dioxide at 310.9 K to 333.2 K and pressures to 8263 kPa. The mole fraction solubility at 310.9 K and a partial pressure of carbon dioxide of 101.3 kPa from this work is 0.0065. The corresponding value for solubility in pentane from the smoothing equation given above is 0.0104. The ideal solubility from Raoult's law is 0.0118.

At least nine groups have measured solubility in cyclohexane (8,9,12,15, 29-33). Solubility at 293.2 K reported by Horsman-van den Dool and Warman (12) was measured by an unsatisfactory method and is not consistent with measurements by other workers. Mole fraction solubility at a partial pressure of 101.3 kPa from other sources fit the equation below.

$$\ln x_{CO_2} = 0.11850 + 454.47/(T/K) - 1.1454ln(T/K)$$

temperature range = 283.2-313.2 K standard deviation in  $x_{\text{CO}_2}$  = 0.00016

The mole fraction solubility at 298.15 from this equation is 0.00757. The corresponding smoothed value for solubility in hexane is 0.01196.

Field et a1.(34) measured solubility in methylcyclohexane at 283.9-313.3 K. Horsman-van den Dool (12) also reported a value at 294.3 which is about 5% lower than the corresponding value from data published by Field et a1. Field's value is the more reliable and can be recommended. The mole fraction solubility at 298.13 K and a partial pressure of 101.3 kPa from Field's work is 0.00928 compared with a smoothed value of 0.01188 for dissolution in heptane.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
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#### CRITICAL EVALUATION:

Wilcock et a1.(35) measured the solubility in cyclooctane at 289.1-313.5 K. No other data on this system are available for comparison but this work is likely to be reliable. The mole fraction solublity at a partial pressure of 101.3 kPa and 298.27 K is 0.006860 compared with a smoothed value of 0.01210 for dissolution in octane under these conditions.

Geller et al.(36) measured solubilities in various isomers of dimethylcyclohexane. The work is likely to be reliable but no other work on these systems is available for comparison. Mole fraction solubilities, corrected to 298.15 K and a partial pressure of 101.3 kPa are given below together with the smoothed value for octane.

(Z)-1,2-dimethylcyclohexane	0.00938
(E)-1,2-dimethylcyclohexane	0.01020
1,3-dimethylcyclohexane	
(59  mol & Z + 41  mol & E)	0.01021
1,4-dimethylcyclohexane	
(70  mol & Z + 30  mol & E)	0.01035
octane	0.01211

There is a significant difference between solubilities in (Z)- and (E)-1,2-dimethylcyclohexane.

Tremper and Prausnitz (23) published Henry's constants in 1,1'-bicyclohexyl from 300 K to 475 K. Horsman-van den Dool reported an Ostwald coefficient at 295.2 K. This corresponds to a mole fraction solubility at a partial pressure of 101.3 kPa of 0.00854. Extrapolation of Tremper's measurements indicates a mole fraction solubility of 0.00820 at 295.2 K and 101.3 K. Horsman-van den Dool used very simple apparatus and Tremper's data are likely to be the more reliable.

Solubility in decahydronaphthalene (decalin) was measured by Luhring and Schumpe (33) and by Horsman-van den Dool and Warman (12). The former group used a mixture of isomers and the latter made separate measurements on the two isomers. Lenoir et al.(21) measured limiting values of Henry's constant for a mixture of isomers by gas-liquid chromatography. Mole fraction solubilities at a partial pressure of 101.3 kPa from the available data are as follows

293.2 K	0.00790	(33)
298.2	0.00909	(21)
323.2	0.00735	(21)
296.6 K	0.00697	(12)
296.6 K	0.00816	(12)
	323.2 296.6 K	298.2 0.00909 323.2 0.00735 296.6 K 0.00697

Further measurements on this system need to be made before solubility data can be recommended.

Nagahama et al.(4) have studied phase equilibria between ethene and carbon dioxide to high pressures. At 252.95 K the mole fraction solubility in ethene at a partial pressure of carbon dioxide of 183 kPa is 0.071. This may be compared with their value of 0.055 for the mole fraction solubility in ethane at 252.95 K and a partial pressure of carbon dioxide of 214 kPa. Clark and Din (3) measured the solubility of solid carbon dioxide in liquid ethene and in various mixtures with ethane at 130-180 K. Under these conditions carbon dioxide was again more soluble in ethene than in ethane.

Haselden and Snowden (27) have reported dew points and bubble points for mixtures of carbon dioxide and propene at 116-225 K. Phase equilibria in

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alkanes, Cyclic Alkanes and Alkenes

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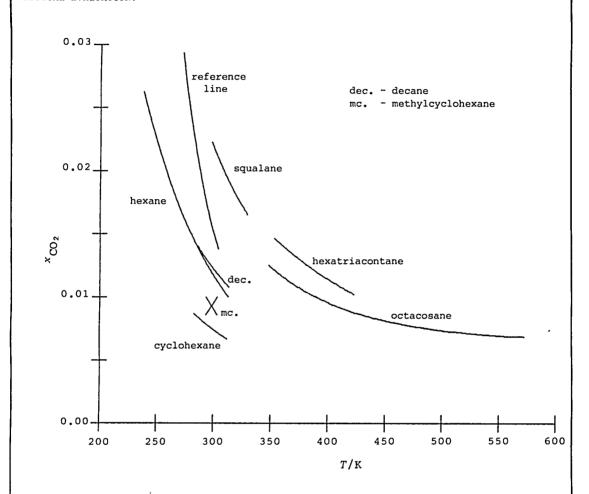


Fig. 3 Mole fraction solubility of carbon dioxide in various alkanes and cyclic alkanes at a partial pressure of gas of 101.3 kPa.

The curves showing the variation of solubility with temperature correspond to equations derived by the evaluator. The solubilility of methylcyclohexane is from ref. (34).

A reference line corresponding to values from the Raoult's law equation is also shown.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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#### CRITICAL EVALUATION:

this system have also been studied to high pressure by Nagahama *et al.*(4) Cheung and Zander (1) have measured solubilities of solid carbon dioxide in propene. There is no obvious incompatibility between the three sets of measurements. Nagahama's measurements indicate a mole fraction solubility of 0.076 at 252.95 K and a partial pressure of carbon dioxide of 184 kPa and a solubility of 0.014 at 273.15 and a partial pressure of 81 kPa. The corresponding ideal solubilities from Raoult's law are 0.094 and 0.023

Nagahama  $et\ al.(4)$  also studied phase equilibria between carbon dioxide and 1-butene to high pressures. The mole fraction solubilities of carbon dioxide given below are based upon their data and show an increase from ethene to 1-butene.

Hydrocarbon	T/K	P/kPa	<sup>x</sup> CO₂
ethene	252.95	183	0.071
propene	252.95	184	0.076
	273.15	219	0.050
1-butene	273.15	193	0.059

Luhring and Schumpe (33) have published Henry's constant for dissolution in 1-tetradecene at 293.2 K. This corresponds to a mole fraction solubility of 0.001654 at a partial pressure of 101.3 kPa. The corresponding value for dissolution in tetradecane is 0.01442.

Solubility in tetrahydronaphthalene has been measured by Luhring and Schumpe (33), by Horvath  $et\ al.(20)$ , by Krauss and Gestrich (32) and by Bratzler  $et\ al.(37)$ . The seven data points for mole fraction solubility at a partial pressure of 101.3 kPa fit the equation below.

$$\ln x_{CO_2} = 22.419 - 306.70/(T/K) - 4.6125ln(T/K)$$

temperature range = 283.15-313.15 K. standard deviation in values of  $x_{\rm CO_2}$  = 0.00031

The mole fraction solubility at 293.15 K from this equation is  $0.00799 \pm 0.00034$ . The value for 296.6 K is  $0.00766 \pm 0.00034$ . These may be compared with solubility data for decahydronaphthalene given above. Further measurements are needed to determine the relative solubilities in the two solvents.

Just (38) measured solubility in 1-methyl-4-(1-methylethenyl)cyclohexene (d-limonene, carvene). No other measurements on this compound are available for comparison.

Selected values of mole fraction solubilities in non-aromatic hydrocarbons are shown in Table 1 and Fig 3.

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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

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- 34. Field, L.R.; Wilhelm, E.; Battino, R. *J. Chem. Thermodyn.* <u>1974</u>, 6, 237-243.
- 35. Wilcock, R.J.; Battino, R.; Wilhelm, E. *J. Chem. Thermodyn.* <u>1977</u>, 9, 111-115.
- Geller, E.B.; Battino, R.; Wilhelm, E. J. Chem. Thermodyn. <u>1976</u>, 8, 197-202.
- 37. Bratzler, K.D.; Doerges, A.; Herbert, W. German Patent No. 1 769 197 to Metallgesellschaft AG 1971.
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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Alkanes, Cyclic Alkanes and Alkenes

#### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

Table 1. Mole fraction solubilities of carbon dioxide at a partial pressure of 101.3 kPa in alkanes and alkenes.

Solvent	<i>T</i> /K	<sup>X</sup> CO₂	Reference
Propane	273.15	0.019	4
Butane	273.15	0.021	4
2-Methylpropane	273.15	0.019	4
Pentane	273.15	0.01953 ±0.00033	*
	298.15	0.01298 ±0.00033	*
2,2-Dimethylpropane			
	298.15	0.01607 ±0.00071	*
Hexane	298.15	0.01197 ±0.00018	*
Heptane	298.15	0.01188 ±0.00035	*
Octane	298.15	0.01212 ±0.00006	*
2,2,4-Trimethylpenta	ne		
	298.15	0.01387	19
Decane	298.15	0.01246 ±0.00016	*
Dodecane	298.15	0.01283 ±0.00014	*
Tetradecane	298.15	0.01361 ±0.00001	*
Hexadecane	298.15	0.01403 ±0.00015	*
	373.15	0.00794 ±0.00015	*
Eicosane	373.15	0.00892 ±0.00044	*
2,6,10,15,19,23-Hexa			
	298.6	0.02205	24
	330.2	0.01655	24
	348.2	0.01434	24
Octacosane	348.15	0.01254 ±0.00004	*
	373.15		*
Hexatriacontane	373.15	0.01314 ±0.00014	*
Tetratetracontane	373.15	0.0144	25
Cyclohexane	298.15	0.00757 ±0.00016	*
Methylcyclohexane	298.13	0.00928	34
(Z)-1,2-Dimethylcycle			
	297.88	0.009408	36
(E)-1,2-Dimethylcycle			
	298.19	0.010197	36
Cyclooctane	298.27	0.006860	35
,1'-Bicyclohexyl	298.15	0.007979	23
-Tetradecene	293.15	0.00165	33
Tetrahydronaphthalen			
	298.15	0.00752 ±0.00031	*
-Methyl-4-(methylet		lohexene (d-limonene)	
	298.15	0.0118	38

<sup>¶</sup> interpolated; † extrapolated

<sup>\*</sup> from the equation given by the evaluator on a previous page

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Methane;  $CH_4$ ; [74-82-8]Ethane;  $C_2H_6$ ; [74-84-0]Propane;  $C_3H_8$ ; [74-98-6]Propene;  $C_3H_6$ ; [115-07-1]Butane;  $C_4H_{10}$ ; [106-97-8]

#### ORIGINAL MEASUREMENTS:

Cheung, H.; Zander, E.H.

Chem. Eng. Prog. Symp. Ser. 1968, 64(88), 34-43.

#### VARIABLES:

T/K = 87.4-194.6 $P_{CO_2}/kPa = 0-100$ 

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

Compositions of solutions of carbon dioxide in liquid hydrocarbons in equilibrium with solid carbon dioxide at various temperatures.

Solvent	T/K	P <sub>CO2</sub> /kPa <sup>†</sup> M	ole% of carb	on dioxide
Methane	110.70 124.90 125.20	0.00043 0.0119 0.0127	0.03 0.08 0.08	
	138.70 151.40 167.20	0.154 1.04 7.31	0.29 0.99 3.14	(0.99; 0.90)*
	183.20 183.20 183.20 194.60	37.3 37.3 100.7	6.60	(5.9; 5.8)* (12.6: 12.6)*

 $<sup>^{*}</sup>$  mole% of CO $_{2}$  measured by mass spectrometry and chromatography respectively.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Mixtures of carbon dioxide and the hydrocarbon gas under test flowed through a cell held in a cryostat. The carbon dioxide was in excess so that a solution of carbon dioxide and solid carbon dioxide condensed in the cell. Samples of the solution were withdrawn into a sample bulb through a fritted disc of fine porosity so that particles of solid were held back. samples were then vaporized and analysed by gas chromatography. Some samples were also analysed by mass spectrometry. The authors claim good agreement between the two methods of analysis. Typical values given by the authors are within about 2% except at low concentration. Most of the measurements on solvents other than methane were made at a pressure less than 101.3 kPa using glass apparatus. Stainless steel apparatus was used for higher pressures.

#### SOURCE AND PURITY OF MATERIALS:

No information

#### ESTIMATED ERROR:

 $\delta(\text{mole% CO}_2) = \pm 2\%$ 

#### REFERENCES:

- Meyers, C.H.; van Dusen, M.S. Bur. Std. J. Res. 1933, 10, 381.
- Giauque, W.F.; Egan, C.J.
   J. Chem. Phys. 1937, 5, 45.

<sup>&</sup>lt;sup>†</sup> calculated by the compiler from equations given in ref.(1) for T/K = 87-150 and ref.(2) for T/K = 150-194.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Methane;  $CH_4$ ; [74-82-8]Ethane;  $C_2H_6$ ; [74-84-0]Propane;  $C_3H_8$ ; [74-98-6]Propene;  $C_3H_6$ ; [115-07-1]Butane;  $C_4H_{10}$ ; [106-97-8]

#### ORIGINAL MEASUREMENTS:

Cheung, H.; Zander, E.H.

Chem. Eng. Prog. Symp. Ser.  $\underline{1968}$ , 64(88), 34-43.

#### EXPERIMENTAL VALUES:

Compositions of solutions of carbon dioxide in liquid hydrocarbons in equilibrium with solid carbon dioxide at various temperatures.

Solvent	T/K	P <sub>CO₂</sub> /kPa <sup>†</sup> Mol	e% of carbon dioxide
Ethane	137.80 149.00 161.20 164.20 167.30 172.90 175.40 180.30	0.132 0.750 3.65 5.20 7.39 13.5 17.5	0.40 0.85 2.06 2.50 (2.50; 2.48)* 3.33 (3.33; 3.36)* 4.88 (4.88; 5.07)* 5.62 7.54 (7.54; 7.60)*
Propane	87.40	0.0000002	<0.00001
	105.00	0.0009	0.009
	106.70	0.0014	0.010
	123.30	0.0085	0.07
	149.70	0.829	0.80
	180.10	27.8	5.8
	180.20	28.1	5.7
Butane	139.80	0.184	0.35
	150.20	0.880	0.66
	160.00	3.15	1.71
	160.20	3.23	1.58
	180.20	28.1	6.1
	180.30	28.4	5.6
Propene	120.40	0.0045	0.68
	140.00	0.190	2.4
	140.00	0.190	2.1

<sup>\*</sup> mole% of CO<sub>2</sub> measured by mass spectrometry and chromatography respectively.

<sup>&</sup>lt;sup>†</sup> calculated by the compiler from equations given in ref.(1) for T/K = 87-150 and ref.(2) for T/K = 150-194.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Ethane; C<sub>2</sub>H<sub>6</sub>; [74-84-0]
  Propane; C<sub>3</sub>H<sub>8</sub>; [74-98-6]
  Butane; C<sub>4</sub>H<sub>10</sub>; [106-97-8]
  2-Methylpropane; C<sub>4</sub>H<sub>10</sub>;
  [75-28-5]

#### ORIGINAL MEASUREMENTS:

Nagahama, K.; Konishi, H. Hoshino, D.; Hirata, M.

J. Chem. Eng. Japan 1974, 7(5), 323-328.

#### VARIABLES:

T/K = 252.95-273.15 $P_{CO_2} = 71-214 \text{ kPa}$ 

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

Solvent	T/K	P <sub>total</sub>	<sup>x</sup> co₂	<sup>y</sup> CO₂	P <sub>CO2</sub> /atm	P <sub>CO2</sub> /kPa
ethane	252.95	15.9	0.055	0.133	2.11	214
propane	273.15 252.95	5.5 3.3	0.013 0.030	0.127 0.313	0.70 1.03	71 105
butane	273.15	2.4	0.030	0.588	1.41	143
2-methylpropane	273.15 273.15	2.7 3.5	0.022 0.037	0.422 0.541	1.14 1.89	115 192

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The data given above were obtained during studies of the systems to higher pressures over the whole of each composition range. The apparatus has been described previously (1). The components were charged into a glass-windowed equilibrium cell. A magnetic piston pump recirculated vapor, removed it from the top of the liquid and reintroduced it into the bottom of the liquid. After equilibrium was reached (c. 0.5 h) samples of the gas phase and of the liquid phase were analysed by gas chromatography.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Purity at least 99.8%
- 2. Ethane; purity at least 99.0% Propane; purity at least 99.85% Butane; purity at least 99.35% 2-Methylpropane; purity at least 99.2%

#### EXPERIMENTAL ERROR:

 $\delta T/K = \pm 0.05$  (authors)

#### REFERENCES:

1. Hakuta, T.; Nagahama, K.; Hirata, M. Bull. Japan Petrol. Inst. 1969, 11, 10.

## 

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $\frac{10^2 x_1}{}$	Bunsen Coefficient α/cm³(STP)cm-3atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	1.258	2.460	2.685
313.15	0.999	1.897	2.175

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

# SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

#### REFERENCES:

 Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Cheng, H.; Fernandez, M.E.P.; Zollweg, J.A.; Streett, W.B.
2. Pentane; C <sub>5</sub> H <sub>12</sub> ; [109-66-0]	J. Chem. Eng. Data <u>1989</u> , 34, 319-323.
VARIABLES:	PREPARED BY:
T/K = 252-458 P/MPa = 0.16-9.62	P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/K	<sup>P</sup> total /MPa	Mole fraction of CO <sub>2</sub> in the liquid phase,  *CO <sub>2</sub>	Mole fraction of CO <sub>2</sub> in the gas phase,  yCO <sub>2</sub>	P <sub>CO2</sub> /kPa*
252.67	0.159	0.0388	0.9375	149
273.41	0.269	0.0451	0.8798	237
294.09	0.172	0.0165	0.6769	116

(other measurements extend to higher pressures)

calculated by the compiler on the assumption that  $P_{\text{CO}_2}$  =  $P_{\text{total}}$  ×  $y_{\text{CO}_2}$ 

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A vapor-recirculating equilibrium apparatus described in ref. (1) was used. Gas and liquid phases were analysed by gas chromatography.

#### SOURCE AND PURITY OF MATERIALS:

- Supplied by Air Products and Chemicals Inc.; purity 99.99%
   Fisher Infra-red Spectranalyzed
- Fisher Infra-red Spectranalyzed grade.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$  $\delta P/kPa = \pm 7$  (authors)

#### REFERENCES:

 Pozo, M.E.; Streett, W.B.
 J. Chem. Eng. Data 1984, 29, 324.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2,2-Dimethylpropane, (neopentane); C<sub>5</sub>H<sub>12</sub>; [463-82-1]

#### ORIGINAL MEASUREMENTS:

Stead, K.; Williams, J.M.

J. Chem. Thermodynamics 1980, 12, 265-275

## VARIABLES:

T/K = 250-300P/kPa = 43-516 PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

THE THETHER.	TAL VALUES.			
т/к	Total Pressure /kPa	<sup>x</sup> CO₂	<sup>y</sup> CO₂	P <sub>CO₂</sub> /kPa*
250	154.0	0.039	0.822	126.59
	201.6	0.055	0.865	174.38
	378.6	0.120	0.930	352.10
260	42.8	0.000	0.000	0.00
	54.2	0.003	0.213	11.54
	63.8	0.006	0.330	21.05
	86.8	0.012	0.516	44.79
	159.0	0.032	0.735	116.87
270	275.2	0.064	0.842	231.72
	64.4	0.000	0.000	0.00
	78.2	0.003	0.186	14.55
	93.2	0.007	0.308	28.71
	122.2	0.014	0.478	58.41
280	218.4	0.036	0.697	152.22
	374.6	0.074	0.820	307.17
	93.6	0.000	0.000	0.00
	112.2	0.004	0.171	19.19
	132.8	0.008	0.289	38.38
	172.6	0.016	0.454	78.36
290	293.8	0.039	0.667	195.96
	132.8	0.000	0.000	0.00
	156.2	0.005	0.150	23.43
	181.6	0.010	0.262	47.58
	234.2	0.019	0.422	98.83
300	388.4	0.045	0.643	249.74
	184.0	0.000	0.000	0.00
	218.2	0.005	0.155	33.82
	248.6	0.011	0.252	62.65
	316.0	0.019	0.407	128.61
	516.0	0.050	0.634	327.14

 $\mathbf{x}_{\mathrm{CO_2}}$  is the mole fraction of  $\mathrm{CO_2}$  in the liquid phase.

 $\boldsymbol{y}_{\text{CO}_2}$  is the mole fraction of  $\text{CO}_2$  in the gas phase

\* calculated by the compiler and taken to be  $y_{CO}$ , × total pressure

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A mixture of carbon dioxide and 2,2-dimethylpropane was circulated through a thermostatted equilibrium cell. The rest of the apparatus was at a higher temperature so that condensation ocurred only in the cell. Samples of liquid in the cell and vapor circulating through the system were analysed by gas chromatography.

#### SOURCE AND PURITY OF MATERIALS:

- 1 Supplied by The Distillers Company; purity stated to be better than British Standard 4105 (1967).
- 2 Supplied by Fisons Scientific Apparatus Ltd; purity at least 99%.

# ESTIMATED ERROR:

- $\delta P/kPa = \pm 1.4$ ;  $\delta T/K = \pm 0.008$  (T/K<273);  $\delta T/K = \pm 0.010$  (T/K>273)
- $\delta$ (mole fraction) = ±0.01 at mole fractions close to 0.5
- $\delta$  (mole fraction) =  $\pm 0.003$  at mole fractions close to 0.01 or 0.99

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]
   Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5]
   Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]

#### ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Ivanovsky, F.P.

Khim. Prom. 1964, No 7, 506-508.

#### VARIABLES:

T/K = 238.15P/kPa = 202-1013

## PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

Solvent	T/K	P/atm	P/kPa	<sup>x</sup> CO₂	Henry's constant /kPa
Hexane	238.15	2 1	202.65 101.32	0.0580 0.0263*	4039*
Heptane	238.15	2 1	202.65 101.32	0.0600 0.0277*	3819 <sup>*</sup>
Octane	238.15	2 1	202.65 101.32	0.0600 0.0279*	3797*

<sup>\*</sup> Estimated by the compiler by use of a Krichevsky-Il'inskaya equation from the solubility data for 2-10 atm given in the paper.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Details of method given in ref. (1). A static method was used. A glass (low pressure) section of the apparatus was connected to a high pressure section made of metal. Carbon dioxide in the low pressure section was allowed to condense in a cooled metal bulb in the high pressure section. The quantity of gas collected was found from pressure changes in the glass section. The valve connecting the two section was then closed and the condensed gas allowed to evaporate to generate the required pressure and to come in contact with the solvent under test which was held in an absorption cell in a thermostat bath. The cell was stirred magnetically. The quantity of unabsorbed gas when equilibrium was reached was calculated from the final pressure and volume of the gas in the high pressure section.

#### SOURCE AND PURITY OF MATERIALS:

No information

#### ESTIMATED ERROR

 $\delta x_{\text{CO}_2} = \pm 5\% \text{ (compiler)}$ 

#### REFERENCES:

Shenderei, Zel'vensky, Ya.D.;
 Ivanovsky, F.P.

Khim. Prom. 1960, No 5, 370.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Hexane;  $C_6H_{14}$ ; [110-54-3]

#### ORIGINAL MEASUREMENTS:

Im, U.K.; Kurata, F.

J. Amer. Chem. Soc. 1971, 16, 412-415.

#### VARIABLES:

T/K = 177.2-215.7 $P_{CO_2}/kPa = 34-474$ 

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/K	P <sub>total</sub> /atm	P <sub>total</sub> /kPa	P <sub>CO2</sub> /kPa*	<sup>X</sup> CO₂
215.7 215.2 215.0 214.9 214.7	4.73 4.63 4.49	479 469 455	476.9 461.3 455.2 452.2 446.2	0.9723 0.9526 0.9514 0.7506 0.7252
214.2 213.2 211.7 210.2 207.7	4.32 4.02 3.78 3.46 2.86 2.18	438 407 383 351 290 221	431.5 403.3 364.0 328.1 274.9 213.0	0.6510 0.5722 0.4627 0.3593 0.2662 0.1990
204.2 200.2 195.2 190.2 186.2 183.2 180.2 178.2	1.16 1.11 0.74 0.48 0.37 0.28 0.23	118 112 75 49 37 28	157.3 105.8 69.6 49.0 37.3 28.1 23.1	0.1544 0.1177 0.0905 0.0681 0.0569 0.0457
178.2 177.2	0.23 0.21	23 21	21.0	0.0382

<sup>\*</sup> vapor pressure of solid CO2 from ref. (1).

#### AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

The solubility of solid carbon dioxide was measured as described earlier (2). The components were introduced into the glass cell and 1 to 2 hr allowed for equilibrium to be reached. Samples of liquid were withdrawn at various temperatures from the glass equilibrium cell for analysis by gas chromatography. Alternatively the equilibrium temperature of mixtures of known composition were measured. Temperatures were controlled by an air bath cooled by liquid nitrogen and measured by a calibrated platinum resistance thermometer. Pressures were measured by a calibrated Heise gage.

# SOURCE AND PURITY OF MATERIALS:

- Coleman Instrument grade obtained from Matheson Gas Products. Analysis showed that the purity was better than 99.9%
- Supplied by Phillips Petroleum Co. Analysis showed that the purity was better than 99.9%

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$  $\delta P/\text{atm} = \pm 0.03$ 

#### REFERENCES:

- Giauque, W.F.; Egan, C.J.;
   J. Chem. Phys. 1937, 5, 45.
- Im, U.K. PhD thesis, University of Kansas, Lawrence, Kan., 1969.

- (1) Carbon dioxide; CO2; [124-38-9]
- (2) Hexane;  $C_{6}H_{14}$ ; [110-54-3]

#### ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm³cm-3
298.15	1.207	2.080	2.270
313.15	0.963	1.621	1.858

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

#### SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

## ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

#### REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; $CO_2$ ; [124-38-9] King, M. B.; Al-Najjar, H. 2. Hexane; $C_6H_{14}$ ; [110-54-3] Chem. Eng. Sci. 1977, 32, 1241-1246. VARIABLES: PREPARED BY: C. L. Young Temperature

#### EXPERIMENTAL VALUES:

T/K	Mole fraction of carbon dioxide at a partial pressure of 101.3 kPa
293.2	0.0126
298.2	0.0119
303.2	0.0113

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Solvent degassed by spraying into a continuously evacuated chamber. Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved. Flow rates may be varied over a wide range without affecting the solubility.

Similar to the apparatus of Morrison and Billett.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$   $\delta x_{CO_2} = \pm 2\%$ 

(estimated by compiler).

#### REFERENCES:

1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819.

allowance was made for the non-ideal gas behaviour of carbon dioxide.

24 COMPONENTS: ORIGINAL MEASUREMENTS: Patyi, L.; Furmer, I. E.; Makranczy, J.; Sadilenko, A. S.; 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Stepanova, Z. G.; Berengarten, 2. Hexane;  $C_6H_{14}$ ; [110-54-3] Zh. Prikl. Khim. 1978, 51, 1296-1300. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: Mole fraction of carbon dioxide α<sup>†</sup> T/K at a partial pressure of 101.325 kPa xco2 2.08 0.01215 298.15 † volume of gas (measured at 101.325 kPa and 273.15 K) dissolved by one volume of hexane. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Purity better than 99 mole per Volumetric method. Pressure cent as determined by gas measured when known amounts of gas were added, in increments, to a chromatography. known amount of liquid in a vessel of known dimensions. Corrections were made for the partial pressure of solvent. Details in ref. (1).

# 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.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Hexane; C<sub>6</sub>H<sub>14</sub>; [110-54-3]

# ORIGINAL MEASUREMENTS:

Horsman-van den Dool, L. E. W.; Warman, J. W.

Interuniversity Reactor Institute (IRI)-Report 134-81-01

#### VARIABLES:

$$T/K = 291.1$$
  
 $p_1/kPa = not given$ 

#### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

Temperature		Ostwald Coefficient	Number of Runs	
t/°C	<i>T</i> /K	L/cm <sup>3</sup> cm <sup>-3</sup>		
17.9	291.1	2.46	1	

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A cylindrical glass container of approximately 15 cm³ volume is partly filled with solvent and closed with a half-hole septum. An amount of the gaseous solute is added to the container. The closed container is shaken for 30 minutes. Samples of both the vapor and liquid phases are taken in a calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.

The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 200 cm Porapak Q column is used for the separation.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Baker Chemical Co. Instrument grade, 99.99 percent. Used as received.
- (2) Hexane. Merck, Uvasol Spektroskopie grade. Impurities which give the same retention time as the gas are removed before the experiment by adsorption or distillation.

ESTIMATED ERROR:

$$\delta L/L = \pm 0.05$$

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Hexane, C<sub>6</sub>H<sub>1</sub>4; [110-54-3] VARIABLES: T/K = 273.15-303.15 P/MPa = 1.066-6.109 ORIGINAL MEASUREMENTS: Kaminishi, G-I.; Yokoyama, C.; Takahashi, S. Fluid Phase Equilibria, 1987, 34, 83-99. PREPARED BY: PREPARED BY: P.G.T. Fogg

#### EXPERIMENTAL VALUES:

т/к	Henry's la H/MPa	w constant H/kPa	Mole fraction $x_{\text{CO}_2}$ at $P_{\text{CO}_2}$ = 101.3kPa*
273.15	6.22	6220	0.01629
283.15	7.12	7120	0.01423
298.15	8.42	8420	0.01203
303.15	8.86	8860	0.01144

$$H = \begin{bmatrix} f_1 \\ \bar{x}_1 \end{bmatrix}$$

$$x_1 = x_{CO_2}$$
;  $f_1 = \text{fugacity of } CO_2$ 

#### AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Apparatus able to withstand pressures to 20 MPa was used to determine phase equilibria by the bubble point method. Henry's constants at zero pressure were obtained from the experimental data by using the method described by Prausnitz and Chueh (1)

#### SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Showa Tansan Industry Co., Ltd; purity better than 99.9%
- 2. Supplied by Dojin Yakugaku Research Institute; purity better than 99.8%

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$  (authors)  $\delta P/kPa = \pm 0.1$ 

#### REFERENCES:

 Prausnitz, J.M.; Chueh, P.L. Computer Calculations for High Pressure Vapor-Liquid Equilibria, Prentice-Hall, Englewood Cliffs, USA, 1968.

<sup>\*</sup> taken by the compiler to be given approximately by  $P_{\rm CO_2}/H$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> </ol>	Tong Jingshan; Gao Guanghua; Wang Xiagong
2. Alkanes	Qinghua Dazue Xuebao <u>1988</u> , 28(3), 28-32.
VARIABLES:	PREPARED BY:
T/K = 298.15 $P_{CO_2}/kPa = 101$	P.G.T. Fogg

# EXPERIMENTAL VALUES:

	Solvent	P/kPa	T/K	x <sub>CO<sub>2</sub></sub>
_	Hexane; C <sub>6</sub> H <sub>14</sub> ; [110-54-3]	101	298.15	0.0089104
	Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]	101	298.15	0.011382
	Octane; C <sub>8</sub> H <sub>18</sub> ; [111-65-9]	101	298.15	0.011900
	Nonane; C <sub>9</sub> H <sub>20</sub> ; [111-84-2]	101	298.15	0.013888
	Decane; C <sub>10</sub> H <sub>22</sub> ; [124-18-5]	101	298.15	0.017645
	Undecane; C <sub>11</sub> H <sub>24</sub> ; [1120-21-4]	101	298.15	0.019997

#### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Gas circulated through the solvent	1. No information
with provision to sample the gas and liquid phases.	2. Purity of nonane and decane > 99%
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1  (authors)$
	REFERENCES:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Heptane; C<sub>7</sub>H<sub>16</sub>;[142-82-5]

#### ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.

Acta Chem. Scand. 1953, 7, 537 - 544.

VARIABLES:

: 
$$T/K = 293.65 - 307.65$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

J. Chr. Gjaldbaek

EXPERIMEN	TAL	VALUES:	ì

T/K	Carbon Dioxide Pressure p <sub>1</sub> /mmHg	Mol Fraction <sup>1</sup> 10 <sup>2</sup> x <sub>1</sub>	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
293.65 298.25 298.25 307.65	718.6 712.4 710.3 727.7	1.33 1.21 1.22 1.08	1.98 1.84 1.85 1.62	2.13 2.01 2.02 1.82

Mole fraction solubility values adjusted to a gas partial pressure of 101.325 kPa (1 atm) by the compiler.

Smoothed Data: For use between 293.65 and 307.65 K.

 $\ln x_1 = -8.7743 + 13.0435/(T/100 K)$ 

The standard error about the regression line is  $1.78 \times 10^{-4}$ 

<i>T</i> /K	Mol Fraction $10^2x_{ ilde{1}}$
293.15	1.32
298.15	1.23
303.15	1.14
308.15	1.07

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as confining liquid. The solventwas degassed in the apparatus.

The absorbed volume of gas is calculated from the initial and final amounts, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury.

The mole fraction solubility values are at 1 atm assuming Henry's law is obeyed.

Details of the apparatus and procedure are given in ref. 1 and 2.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate (analytical reagent) and concentrated sulfuric acid. 99.9 per cent CO<sub>2</sub>.
- (2) Heptane. Phillips Petroleum Co. Pure grade. B.p.  $(760 \text{ mmHg})/^{\circ}\text{C} = 98.3 98.4. n_{D}(25 ^{\circ}\text{C}) = 1.3855.$

#### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- Gjaldbaek, J. C.
   Acta Chem. Scand. 1952, 6, 623.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5]

#### ORIGINAL MEASUREMENTS:

Im, U.K.; Kurata, F.

J. Amer. Chem. Soc. <u>1971</u>, 16, 412-415.

#### VARIABLES:

T/K = 182.2-215.6 $P_{CO_2}/kPa = 34-474$ 

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/K	P <sub>total</sub> /atm	P <sub>total</sub> /kPa	P <sub>CO2</sub> /kPa*	x <sub>CO2</sub>
215.6 215.2 214.2 211.7 210.2 207.2 204.2 200.2 195.2 190.2 185.2 183.2 182.2	4.70 4.32 3.78 3.33 2.65 2.14 1.57 1.11 0.72	476 438 383 337 269 217 159 112 73	473.7 461.3 431.5 364.0 328.1 265.2 213.0 157.3 105.8 69.6 44.8 37.3 34.0	0.6801 0.5810 0.4440 0.2908 0.2592 0.2152 0.1737 0.1544 0.1108 0.0798 0.0608 0.0550 0.0519

<sup>\*</sup> vapor pressure of solid CO<sub>2</sub> from ref. (1).

#### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

The solubility of solid carbon dioxide was measured as described earlier (2). The components were introduced into the glass cell and 1 to 2 hr allowed for equilibrium to  $\,$ be reached. Samples of liquid were withdrawn at various temperatures from the glass equilibrium cell for analysis by gas chromatography. Alternatively the equilibrium temperatures of mixtures of known composition were measured. Temperatures were controlled by an air bath cooled by liquid nitrogen and measured by a calibrated platinum resistance thermometer. Pressures were measured by a calibrated Heise gage.

# SOURCE AND PURITY OF MATERIALS:

- Coleman Instrument grade obtained from Matheson Gas Products. Analysis showed that the purity was better than 99.9%
- Supplied by Phillips Petroleum Co. Analysis showed that the purity was better than 99.9%

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$  $\delta P/atm = \pm 0.03$ 

- Giauque, W.F.; Egan, C.J.;
   J. Chem. Phys. 1937, 5, 45.
- Im, U.K. PhD thesis, University of Kansas, Lawrence, Kan., 1969.

COMPONENTS:		ORIGINAL MEA	SUREMENTS:	
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]		Hayduk, W.; Walter, E.B.; Simpson, P.		
2. Alkanes		J. Chem.	Eng. Data <u>1972</u> , 17, 59-61	
VARIABLES:		PREPARED BY:		
P/kPa = 101.3 T/K = 293.15-323.15		P.	G.T. Fogg	
EXPERIMENTAL VALUES:				
Solvent	T/K	Ostwald	*CO2 at	
		coeff. L	$P_{\text{CO}_2} = 101.3 \text{ kPa}$	
Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]		2.24		
		1.95		
	313.15	1.71	0.00995	
Dodecane; C <sub>12</sub> H <sub>26</sub> ; [112-40-3]	283.15	1.55	0.01490	
12 20, 1		1.37	0.01270	
	313.15	1.22	0.01090	
Hexadecane; C <sub>16</sub> H <sub>34</sub> ; [544-76-3]	298.15	1.16	0.01380	
	313.15	1.05 5 1.00	0.01210	
AU	JXI LI ARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:		SOURCE AND I	PURITY OF MATERIALS:	
The apparatus was described in earlier paper (1). Deaerated			n Instrument Grade; minimum 99.99%.	
solvent slowly flowed down a sp tube in contact with the gas un test. The gas was maintained a constant pressure close to barometric. The rate of absorp of gas was measured by the rate decrease of volume of gas. The concentration of gas in the liq could then be calculated from t	der t otion of guid		ed by Canadian Laboratory es; minimum purity 99.0 mol	
rate of flow of liquid.		ESTIMATED E	RROR:	
		$\delta T/K = \pm$	0.05 (authors)	
		REFERENCES:		
			nk, W.; Cheng, S.C. J. Chem. Eng. <u>1970</u> , 48, 93.	

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Heptane; C<sub>7</sub>H<sub>16</sub>; [142-82-5]

#### ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 269 - 280.

#### VARIABLES:

#### PREPARED BY:

T/K: 298.15, 313.15 p/kPa: 101.325 (1 atm)

S. A. Johnson H. L. Clever

#### EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3	
298.15	1.177	1.810	1.976	
313.15	0.978	1.397	1.602	

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

#### SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

#### REFERENCES:

Bodor, E.; Bor, Gy.;
 Mohai, B.; Sipos, G.
 Veszpremi Vegyip. Egy. Kozl.
 1957, 1, 55.
 Chem. Abstr. 1961, 55, 3175h.

COMPONENTS:  1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]  2. Heptane; C <sub>7</sub> H <sub>16</sub> ; [142-82-5]	ORIGINAL MEASUREMENTS:  King, M. B.; Al-Najjar, H.  Chem. Eng. Sci.  1977, 32, 1241-1246.
VARIABLES: Temperature	PREPARED BY:  C. L. Young
EXPERIMENTAL VALUES:  T/K Mole fraction* of car	bon dioxide at a partial pressure of 101.3 kPa
293.2 298.2 303.2	0.0126 0.0119 0.0113
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]

#### ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3	
298.15	1.153	1.600	1.746	
313.15	0.911	1.239	1.420	

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

# SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

#### REFERENCES:

Bodor, E.; Bor, Gy.;
 Mohai, B.; Sipos, G.
 Veszpremi Vegyip. Egy. Kozl.
 1957, 1, 55.
 Chem. Abstr. 1961, 55, 3175h.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]</li> </ol>	King, M. B.; Al-Najjar, H.  Chem. Eng. Sci.  1977, 32, 1241-1246.
VARIABLES: T/K = 293.2 - 303.2 P/kPa = 101.3	PREPARED BY:  C. L. Young

T/K Mole fraction of carbon dioxide at a partial pressure of 101.3 kPa

293.2	0.0128
298.2	0.0121
303.2	0.0115

<sup>\*</sup> allowance was made for the non-ideal gas behaviour of carbon dioxide.

#### AUXILIARY INFORMATION

Solvent degassed by spraying into a
continuously evacuated chamber.
Solvent flows in a thin film down a
glass spiral into a buret system
containing the gas to be dissolved.
Flow rates may be varied over a wide
range without affecting the solu-
tion.

Similar to the apparatus of Morrison and Billett.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given.

#### ESTIMATED ERROR:

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

# REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]

#### ORIGINAL MEASUREMENTS:

Wilcock, R. J.; Battino, R.; Danforth, W. F.; Wilhelm, E.

J. Chem. Thermodyn. 1978, 10, 817 - 822.

#### VARIABLES:

T/K: 283.44 - 313.43 p/kPa: 101.325 (1 atm)

#### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^3 x_1$	Bunsen Coefficient α/cm³(STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³ cm-3
283.44	14.44	2.031	2.108
298.27	11.98	1.654	1.806
313.43	10.38	1.407	1.614

The Bunsen coefficients were calculated by the compiler.

It is assumed that the gas is ideal and that Henry's law is obeyed.

Smoothed Data: For use between 283.15 and 313.15 K

 $\ln x_1 = -7.6969 + 9.7909/(T/100K)$ 

The standard error about the regression line is  $1.51 \times 10^{-4}$ .

<i>T</i> /K	Mol Fraction 10 <sup>3</sup> x <sub>1</sub>
283.15	14.42
293.15	12.82
298.15	12.12
303.15	11.48
313.15	10.35

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum mole per cent purity stated to be 99.8.
- (2) Octane. Phillips Petroleum Co. 99 mole per cent, distilled, density at 298.15 K, ρ/g cm<sup>-3</sup> 0.6988.

#### ESTIMATED ERROR:

 $\delta T/K = 0.02$   $\delta P/\text{mmHg} = 0.5$   $\delta x_1/x_1 = 0.01$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.;
   Bogan, M.; Wilhelm, E.
   Anal. Chem. 1971, 43, 806.

- Carbon dioxide; CO2; [124-38-9]
- 2. Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
- 3. Methane; CH4; [74-82-8]

# PREPARED BY:

Kobayashi, R.

P.G.T. Fogg

ORIGINAL MEASUREMENTS:

Asano, K.; Nakahara, T.;

J. Chem. Eng. Data 1971, 16, 16-18.

#### VARIABLES:

T/K = 233-293 $P_{\text{CH}_{u}} = 138-10342 \text{ kPa}$ 

EXPERIMENTAL VALUES:

Т/К	P <sub>CH4</sub> /psia	P <sub>CH4</sub> /kPa	Mole fraction of CH4 in liquid phase*	K-value Exptl.	for CO <sub>2</sub> Smoothed <sup>†</sup>
233.15	20 100 200 400 600 800 1000 1250 1500	138 689 1379 2758 4137 5516 6895 8618 10342	0.0104 0.0515 0.1000 0.1923 0.2725 0.3509 0.4167 0.4902	16.5 3.78 2.06 1.16 0.88 0.79 0.74 0.73	16.5 3.80 2.11 1.20 0.88 0.80 0.74 0.71 0.80

The K-value for CO2 was defined as:

mole fraction of CO, in the vapor phase/mole fraction in the liquid phase These K-values correspond to essentially infinite dilution.

## AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

Retention volumes for small samples of carbon dioxide were measured by gas chromatography with octane as the stationary phase and methane as the carrier gas. Temperatures were maintained to  $\pm 0.1$  K and the pressure of methane measured to ±0.2%. Experimental details are given in refs (2)-(4).

# SOURCE AND PURITY OF MATERIALS:

- 1. At least 99.6% pure.
- 2. 99.88% pure.
- 3. 99.99% pure.

#### ESTIMATED ERROR:

 $\delta P_{\text{CH}_4} = \pm 2\%$  $\delta T/K = \pm 0.1;$ (authors)

- Kohn, J.P.; Bradish, W.F.
   J. Chem. Eng. Data 1964, 9, 5.
- 2. van Horn, L.D.; Kobayashi, R.
- J. Chem. Eng. Data 1967, 12, 294.3. Masukawa, S.; Kobayashi, R. J. Gas Chromatography 1968, 6, 257.
- 4. Koonce, K.T.; Kobayashi, R. J. Chem. Eng. Data 1964, 9, 494.

calculated by the compiler from K-values for methane in octane from ref. (1).

<sup>†</sup> given by the authors

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Octane; C<sub>8</sub>H<sub>18</sub>; [111-65-9]
- 3. Methane; CH4; [74-82-8]

#### ORIGINAL MEASUREMENTS:

Asano, K.; Nakahara, T.; Kobayashi, R.

J. Chem. Eng. Data 1971, 16, 16-18.

#### EXPERIMENTAL VALUES:

<i>T/</i> K	P <sub>CH4</sub> /psia	P <sub>CH4</sub> /kPa	Mole fraction of CH4 in liquid phase*	K-value Exptl.	for CO <sub>2</sub> Smoothed <sup>†</sup>
253.15	20	138	0.0090	28.1	25.4
	100	689	0.0429	6.17	5.87
	200	1379	0.5556	3.11	3.24
	400	2758	0.1639	1.77	1.75
	600	4137	0.2336	1.33	1.30
	800	5516	0.2985	1.11	1.11
	1000	6895	0.3546	0.99	1.00
	1250	8618	0.4149	0.95	0.95
	1500	10342	0.4695	0.95	0.95
273.15	20	138	0.0078	37.2	37.2
	100	689	0.0376	8.45	8.60
	200	1379	0.0746	4.46	4.71
	400	2758	0.1429	2.41	2.47
	600	4137	0.2075	1.80	1.80
	800	5516	0.2667	1.46	1.46
	1000	6895	0.3226	1.31	1.30
	1250	8618	0.3774	1.19	1.22
	1500	10342	0.4310	1.13	1.15
293.15	20	138	0.0070	57.7	51.0
	100	689	0.0336	12.3	11.9
	200	1379	0.0658	6.19	6.50
	400	2758	0.1282	3.35	3.32
	600	4137	0.1869	2.34	2.35
	800	5516	0.2410	1.88	1.88
	1000	6895	0.2882	1.62	1.64
	1250	8618	0.3367	1.51	1.51
	1500	10342	0.3774	1.41	1.41

The K-value for CO2 was defined as:

mole fraction of  ${\rm CO}_2$  in the vapor phase/mole fraction in the liquid phase These K-values correspond to essentially infinite dilution.

 $<sup>^{\</sup>uparrow}$  calculated by the compiler from K-values for methane in octane from ref. (1).

 $<sup>^{\</sup>dagger}$  given by the authors

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2,2,4-Trimethylpentane or isooctane; C<sub>8</sub>H<sub>18</sub>; [540-84-1]

#### ORIGINAL MEASUREMENTS:

Hiraoka, H.; Hildebrand, J. H.

J. Phys. Chem. 1964, 68, 213-214.

#### VARIABLES:

$$T/K = 277.63 - 308.20$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

 1 to the state of						
 Temperature		Mol Fraction	Bunsen	Ostwald		
t/°C	<i>T</i> /K	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm3cm-3		
4.48	277.63	1.838	2.59	2.63		
15.12	288.27	1.575	2.18	2.30		
24.97	298.12	1.385	1.90	2.07		
35.05	308.20	1.228	1.66	1.87		

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior.

Smoothed Data: For use between 277.63 and 308.20 K.

 $\ln x_1 = -8.0643 + 11.2899/(T/100 K)$ 

The standard error about the regression line is  $4.34 \times 10^{-5}$ .

T/K	Mol Fraction $10^2 x_{ extstyle{1}}$
278.15 288.15	1.820
298.15 308.15	1.387 1.226

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25°C, the pipet at any temperature from 5 to 30°C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, evacuating, then boiling with a heat lamp. degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that the sol-  $\delta$  T/Fvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the volume of mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by P-V measurements in the buret before and after

SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Western Gas Inc. Gas passed through a cold trap.
- (2) Isooctane. Source not given. Distilled, purity checked by ultraviolet absorbance.

$$\delta T/K = 0.02$$
  
 $\delta x_1/x_1 = 0.003$ 

#### REFERENCES:

1. Kobatake, Y.; Hildebrand, J. H. J. Phys. Chem. 1961, 65, 331.

introduction of the gas into the pipet. The stirrer is set in motion. Equilibrium is attained within 24 hours.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Nonane;  $C_9H_{20}$ ; [111-84-2]

# ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient a/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm³cm-3
298.15	1.126	1.420	1.550
313.15	0.898	1.112	1.275

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

#### SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

# REFERENCES:

Bodor, E.; Bor, Gy.;
 Mohai, B.; Sipos, G.
 Veszpremi Vegyip. Egy. Kozl.
 1957, 1, 55.
 Chem. Abstr. 1961, 55, 3175h.

- (1) Carbon dioxide; CO2; [124-38-9]
- (2) Decane; C<sub>10</sub>H<sub>22</sub>; [124-18-5]

# ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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	Mol Fraction $10^2x_1$	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm³cm-3	
298.15 313.15	1.106	1.280	1.397	

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

#### SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

# REFERENCES:

1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	King, M. B.; Al-Najjar, H.
2. Decane; C <sub>10</sub> H <sub>22</sub> ; [124-18-5]	Chem. Eng. Sci.
	<u>1977</u> , 32, 1241-1246.
VARIABLES:	PREPARED BY:
T/K = 293.2 - 323.2 P/kPa = 101.3	C. L. Young

T/K	Mole fraction to carbon dioxide at a partial pressure of 101.3 kPa
202.2	0.0122
293.2	0.0133
298.2	0.0125
303.2	0.0119
323.2	0.0099

<sup>\*</sup> allowance was made for the non-ideal gas behaviour of carbon dioxide.

#### AUXILIARY INFORMATION

# 4

METHOD/APPARATUS/PROCEDURE:

Solvent degassed by spraying into a continuously evacuated chamber.

Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved.

Flow rates may be varied over a wide range without affecting the solubility.

Similar to the apparatus of Morrison and Billett.

SOURCE AND PURITY OF MATERIALS:

No details given.

# ESTIMATED ERROR:

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

# REFERENCES:

Morrison, T. J.; Billett, F. J. Chem. Soc.
 1952, 3819.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Decane; C<sub>10</sub>H<sub>22</sub>; [124-18-5]

# ORIGINAL MEASUREMENTS:

Wilcock, R. J.; Battino, R.; Danforth, W. F.; Wilhelm, E.

J. Chem. Thermodyn. 1978, 10, 817 - 822.

VARIABLES:

T/K: 283.16 - 313.50 p/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^3 x_{1}$	Bunsen Coefficient α/cm³(STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
283.16	14.39	1.686	1.748
298.10	12.58	1.451	1.583
313.50	10.83	1.228	1.409

The Bunsen coefficients were calculated by the compiler.

It is assumed that the gas is ideal and that Henry's law is obeyed.

Smoothed Data: For use between 283.15 to 313.15 K

 $\ln x_1 = -7.1707 + 8.3068/(T/100K)$ 

The standard error about the regression line is  $1.31 \times 10^{-4}$ .

Т/К	Mol Fraction 10 3 x 1
283.15	14.45
293.15	13.07
298.15	12.47
303.15	11.91
313.15	10.91

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to  $500 \text{ cm}^3$  of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid  $N_2$  trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum mole per cent purity stated to be 99.8.
- (2) Decane. Phillips Petroleum Co. 99 mol %, distilled, density at 298.15 K, ρ/g cm<sup>-</sup> 0.7264.

ESTIMATED ERROR:

 $\delta T/K = 0.02$   $\delta p/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.01$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.;
   Bogan, M.; Wilhelm, E.
   Anal. Chem. 1971, 43, 806.

COMPONENTS:	ORIGINAL MEASUREMENTS:
	•
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Decane; C<sub>10</sub>H<sub>22</sub>; [124-18-5]</li> </ol>	Horvath, M. J.; Sebastian, H. M.; Chao, KC.  Ind. Eng. Chem. Fundam.
	<u>1981</u> , <i>20</i> , 394-396.
VARIABLES:	PREPARED BY:
T/K = 300 P/kPa = 101.3	C. L. Young
EXPERIMENTAL VALUES:	
T/K Henry's constan /atm	Mole fraction of at carbon dioxide in liquid, $^x{ m CO}_2$
300 83.4	0.0119
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
	<del></del>
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a	SOURCE AND PURITY OF MATERIALS:  1. No details given.
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants deter-	SOURCE AND PURITY OF MATERIALS:  1. No details given.
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula $H = (p - p_o)\phi(m + 1)/m$ where $p$ is the total pressure, $p_o$	SOURCE AND PURITY OF MATERIALS:  1. No details given.
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula $H = (p - p_o)\phi (m + 1)/m$ where $p$ is the total pressure, $p_o$ the vapor pressure of the solvent	SOURCE AND PURITY OF MATERIALS:  1. No details given.  2. Purity 99.56 mole per cent.
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula $H = (p - p_o)\phi(m + 1)/m$ where $p$ is the total pressure, $p_o$ the vapor pressure of the solvent and $\phi$ is the fugacity coefficient of	SOURCE AND PURITY OF MATERIALS:  1. No details given.  2. Purity 99.56 mole per cent.  ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula $H = (p - p_o)\phi(m + 1)/m$ where $p$ is the total pressure, $p_o$ the vapor pressure of the solvent and $\phi$ is the fugacity coefficient of the gas. The mole ratio, $m$ , is	SOURCE AND PURITY OF MATERIALS:  1. No details given.  2. Purity 99.56 mole per cent.  ESTIMATED ERROR: $\delta T/K = \pm 0.25;  \delta H/atm = \pm 3\%$
METHOD/APPARATUS/PROCEDURE:  Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula $H = (p - p_o)\phi(m + 1)/m$ where $p$ is the total pressure, $p_o$ the vapor pressure of the solvent and $\phi$ is the fugacity coefficient of	SOURCE AND PURITY OF MATERIALS:  1. No details given.  2. Purity 99.56 mole per cent.  ESTIMATED ERROR:

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] (2) Undecane; C<sub>11</sub>H<sub>24</sub>; [1120-21-4] VARIABLES: T/K: 298.15, 313.15 p/kPa: 101.325 (1 atm) CRIGINAL MEASUREMENTS: Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4, 269 - 280. PREPARED BY: S. A. Johnson H. L. Clever

EXPERIMENTAL	VALUES:			
	<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient _L/cm <sup>3</sup> cm <sup>-3</sup>
	298.15 313.15	1.053 0.874	1.124 0.917	1.227 1.051

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

# AUXILIARY INFORMATION

SOURCE AND PURITY OF MATERIALS:

METHOD/APPARATUS/PROCEDURE:

# Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1). Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information. ESTIMATED ERROR: $\delta L/L = \pm \ 0.03$ REFERENCES: 1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Dodecane; C<sub>12</sub>H<sub>26</sub>; [112-40-3]

# ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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	Mol Fraction $10^2 x_1$	Bunsen Coefficient a/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm³cm-3
298.15	1.089	1.080	1.179
313.15	0.867	0.845	0.969

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

Smoothed Data:  $\ln x_1 = -9.2793 + 14.1901/(T/100 \text{ K})$ 

The equation should be used with caution since it is based on only two experimental points.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

# SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

# ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

#### REFERENCES:

Bodor, E.; Bor, Gy.;
 Mohai, B.; Sipos, G.
 Veszpremi Vegyip. Egy. Kozl.
 1957, 1, 55.
 Chem. Abstr. 1961, 55, 3175h.

OMPONENTS:	ORIGINAL MEASUREMENTS:
l. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	King, M. B.; Al-Najjar, H.
2. Dodecane; C <sub>12</sub> H <sub>26</sub> ; [112-40-3]	Chem. Eng. Sci.
	<u>1977</u> , 32, 1241-1246.
ARIABLES:	PREPARED BY:
T/K = 293.2-323.2 P/kPa = 101.3	C. L. Young
XPERIMENTAL VALUES:	
T/K Mole fraction * of car	rbon dioxide at a partial pressure of 101.3 kPa
293.2	0.0137
298.2 303.2	0.0129 0.0122
323.2	0.0102
* allowance was made for the non carbon dioxide.	n-ideal gas behaviour of
	n-ideal gas behaviour of
carbon dioxide.	n-ideal gas behaviour of
carbon dioxide.	
AUXILIARY  ETHOD/APPARATUS/PROCEDURE:  Solvent degassed by spraying into a continuously evacuated chamber.  Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved.	INFORMATION
AUXILIARY  AUXILIARY	INFORMATION  SOURCE AND PURITY OF MATERIALS:
AUXILIARY  ETHOD/APPARATUS/PROCEDURE:  Solvent degassed by spraying into a continuously evacuated chamber.  Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved.	INFORMATION  SOURCE AND PURITY OF MATERIALS:  No details given.
AUXILIARY  GETHOD/APPARATUS/PROCEDURE:  Solvent degassed by spraying into a continuously evacuated chamber.  Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved. Flow rates may be varied over a wide cange without affecting the solu-	INFORMATION  SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR:
AUXILIARY  AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS: No details given. ESTIMATED ERROR: $\delta T/K = \pm 0.1;  \delta x_{\rm CO_2} = \pm 2\%$
AUXILIARY  GETHOD/APPARATUS/PROCEDURE:  Solvent degassed by spraying into a continuously evacuated chamber.  Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved. Flow rates may be varied over a wide range without affecting the solubility.  Similar to the apparatus of	INFORMATION  SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR: $\delta T/K = \pm 0.1;  \delta x_{\rm CO_2} = \pm 2\%$ (estimated by compiler).
AUXILIARY  GETHOD/APPARATUS/PROCEDURE:  Solvent degassed by spraying into a continuously evacuated chamber.  Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved. Flow rates may be varied over a wide range without affecting the solubility.  Similar to the apparatus of	INFORMATION  SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR: $\delta T/K = \pm 0.1;  \delta x_{\text{CO}_2} = \pm 2\%$ (estimated by compiler).  REFERENCES:

- (1) Carbon dioxide; CO2; [124-38-9]
- (2) Tridecane; C<sub>13</sub>H<sub>28</sub>; [629-50-5]

#### ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
298.15	1.080	1.000	1.091
313.15	0.855	0.778	0.892

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

#### SOURCE AND PURITY OF MATERIALS:

Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

## REFERENCES:

Bodor, E.; Bor, Gy.;
 Mohai, B.; Sipos, G.
 Veszpremi Vegyip. Egy. Kozl.
 1957, 1, 55.
 Chem. Abstr. 1961, 55, 3175h.

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] (2) Tetradecane; C<sub>14</sub>H<sub>30</sub>; [629-59-4] 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, 269 - 280.

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2 x_1$	Bunsen Coefficient \(\alpha/\text{cm}^3\)(STP)\(\text{cm}^{-3}\)atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
298.15	1.073	0.930	1.015
313.15	0.854	0.728	0.835

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

# AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).	Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.
	ESTIMATED ERROR:
	$\delta L/L = \pm 0.03$
	REFERENCES:
	1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>;</li> <li>Tetradecane; C<sub>14</sub>H<sub>30</sub>;</li> </ol>	King, M. B.; Al-Najjar, H.  Chem. Eng. Sci.  1977, 32, 1241-1246.
VARIABLES: T/K = 298.2-343.2 P/kPa = 101.3	 PREPARED BY:  C. L. Young

#### EXPERIMENTAL VALUES:

T/K	Mole fraction of carbon dioxide at a partial pressure of 101.3 kPa
298.2	0.0136
303.2	0.0129
323.2	0.0107
343.2	0.0093

<sup>\*</sup> allowance was made for the non-ideal gas behaviour of carbon dioxide.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Solvent degassed by spraying into a continuously evacuated chamber. Solvent flows in a thin film down a glass spiral into a buret system containing the gas to be dissolved. Flow rates may be varied over a wide range without affecting the solubility.

Similar to the apparatus of Morrison and Billett.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$   $\delta x_{CO_2} = \pm 2\%$  (estimated by compiler).

# REFERENCES:

Morrison, T. J.; Billett, F. J. Chem. Soc.
 1952, 3819.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Pentadecane; C<sub>15</sub>H<sub>32</sub>; [629-62-9]

# ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient _L/cm³cm-3
298.15	1.067	0.870	0.950
313.15	0.850	0.682	0.782

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

SOURCE AND PURITY OF MATERIALS:
Both the gas and the liquid were
analytical grade reagents of
Hungarian or foreign origin. No
further information.

# ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

#### REFERENCES:

 Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

COMPONENTS:	TS: ORIGINAL MEASUREMENTS:	
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Hexadecane; C<sub>16</sub>H<sub>34</sub>; [544-76-3] or Heptadecane; C<sub>17</sub>H<sub>36</sub>; [629-78-7]</li> </ol>	Lenoir, J-Y.; Renault, P.; Renon, H.  J. Chem. Eng. Data, 1971, 16, 340-2.	
VARIABLES:	PREPARED BY:	
T/K = 298.2  or  323.2	C. L. Young	

#### EXPERIMENTAL VALUES:

T/K	Henry's constant  HCO2/atm	Mole fraction at 1 atm*
	Hexadecane; C <sub>16</sub> H <sub>34</sub> ;	[544-76-3]
298.2	62.5	0.0160
	Heptadecane; C <sub>17</sub> H <sub>36</sub> ;	[629-78-7]
323.2	72.2	0.0139

\* Calculated by compiler assuming a linear function of  $^{P}_{\text{CO}_{2}}$  vs  $^{x}_{\text{CO}_{2}}$ , i.e.,  $^{x}_{\text{CO}_{2}}$  (1 atm) =  $^{1/H}_{\text{CO}_{2}}$ .

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

# SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Hexadecane; C<sub>16</sub>H<sub>34</sub>; [544-76-3]

#### ORIGINAL MEASUREMENTS:

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

Hung. J. Ind. Chem. 1976, 4, 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:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient _L/cm³cm-3
298.15	1.064	0.820	0.895
313.15	0.843	0.639	0.733

The Bunsen coefficient and mole fraction values were calculated by the compiler assuming that the gas is ideal and that Henry's law is obeyed.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus described by Bodor, Bor, Mohai and Sipos was used (1).

SOURCE AND PURITY OF MATERIALS:
Both the gas and the liquid were analytical grade reagents of Hungarian or foreign origin. No further information.

#### ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

# REFERENCES:

Bodor, E.; Bor, Gy.;
 Mohai, B.; Sipos, G.
 Veszpremi Vegyip. Egy. Kozl.
 1957, 1, 55.
 Chem. Abstr. 1961, 55, 3175h.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Tremper, K.K.; Prausnitz, J.M. 2. Hexadecane; $C_{16}H_{34}$ ; [544-76-3] J. Chem. Engng. Data 1976, 21,295-9 VARIABLES: PREPARED BY: T/K = 300 - 475C.L. Young EXPERIMENTAL VALUES: Mole fraction<sup>b</sup> of carbon dioxide at Henry's Constant<sup>a</sup> T/K /atm. latm partial pressure, <sup>x</sup>CO₂ 300 74.3 0.0135 93.2 0.0107 325 350 112.0 0.00893 375 129.0 0.00775 144.0 0.00694 400 425 157.0 0.00637 450 168.0 0.00595 176.0 0.00568 475 Authors stated measurements were made at several pressures and values of solubility used were all within the Henry's-Law region. AUXILIARY INFORMATION METHOD /APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS: Volumetric apparatus similar to that described by Dymond and Hildebrand (1) Solvent degassed, no other Pressure measured with a null detector and precision gauge. Details in ref. (2). details given. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta x_{CO_2} = \pm 1$ %. REFERENCES: 1. Dymond, J.; Hildebrand, J.H. Ind. Eng. Chem. Fundam. 1967, 6, 130. 2. Cukor, P.M.; Prausnitz, J.M. Ind. Eng. Chem. Fundam. 1971, 10, 638.

# 54 COMPONENTS: ORIGINAL MEASUREMENTS: King, M. E.; Al-Najjar, H. 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Chem. Eng. Sci. 2. Hexadecane; $C_{16}H_{34}$ ; [544-76-3] 1977, 32, 1241-1246. VARIABLES: PREPARED BY: C. L. Young T/K = 298.2 - 343.2P/kPa = 101.3EXPERIMENTAL VALUES: Mole fraction \* of carbon dioxide at a partial pressure T/K of 101.3 kPa 298.2 0.0142 0.0135 303.2 323.2 0.0113 343.2 0.0097 $^{\star}$ allowance was made for the non-ideal gas behaviour of carbon dioxide.

Solvent degassed by spraying into a
continuously evacuated chamber.
Solvent flows in a thin film down a
glass spiral into a buret system
containing the gas to be dissolved.
Flow rates may be varied over a wide
range without affecting the solu-
bility.
Similar to the apparatus of

METHOD/APPARATUS/PROCEDURE:

Morrison and Billett.

ESTIMATED ERROR:  $\delta T/K = +0.1$ 

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

SOURCE AND PURITY OF MATERIALS:

REFERENCES:

Morrison, T. J.; Billett, F. J. Chem. Soc.
 1952, 3819.

No details given.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Hexadecane; C<sub>16</sub>H<sub>34</sub>; [544-76-3] VARIABLES: T/K = 298.6 - 330.2 CRIGINAL MEASUREMENTS: Chai, C-P.; Paulaitis, M. E.; J. Chem. Eng. Data, 1981, 26, 277-279. PREPARED BY: C. L. Young

#### EXPERIMENTAL VALUES:

T/K	Henry´s constant /atm	Mole fraction of carbon dioxide
298.6	71.42	0.01400
298.6	71.92	0.01390
304.3	75.78	0.01320
304.3	75.98	0.01316
311.0	80.77	0.01238
311.0	81.40	0.01229
316.2	84.57	0.01182
316.2	85.66	0.01167
323.6	89.46	0.01118
323.6	91.13	0.01097
330.2	95.11	0.01051
330.2	95.47	0.01047

a Calculated by compiler for a partial pressure of 1 atm.

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Volumetric apparatus similar to that described in ref.(1). Known amount of carbon dioxide brought into contact with known amount of solvent. Reduction in pressure measured.

# SOURCE AND PURITY OF MATERIALS:

- 1. Linde "bone dry" grade.
- 2. Fisher certified grade.

#### ESTIMATED ERROR:

# REFERENCES:

 Dymond, J. H.; Hildebrand, J. H.; Ind. Eng. Chem. Fundam., 1967, 6, 130.

COMPONENTS:		ORIGINAL MEASUREMENTS:
1. Carbon d	ioxide; CO <sub>2</sub> ; [124-38-9]	Lin, P. J.; Parcher, J. F.
2. Alkanes		J. Chromatog. Sci.
		<u>1982</u> , 20, 33-38.
ļ		
VARIABLES:		PREPARED BY:
T/K = 298.	2 _ 413 2	C. L. Young
1/K = 290.	2 - 413.2	C. B. Toung
EXPERIMENTAL VAL	UES:	
	Van1 - 1	Mala Suastian at a mantial
T/K	constant, H	Mole fraction at a partial pressure of 1 atmosphere
	/atm	• <sup>∞</sup> CO₂
]	Hexadecane; C <sub>16</sub> H <sub>34</sub> ;	[544-76-3]
298.2	72.8	0.0138
313.2 328.2	82.7 91.6	0.0121 0.0109
320.2	J • 0	0.0103
	Octacosane; C28H58;	[630-02-4]
353.2	82.0	0.0122
373.2 393.2	92.4 101	0.0108 0.00990
<b>\</b>		
	Hexatriacontane; C <sub>36</sub>	H <sub>74</sub> ; [630-06-8]
353.2 373.2	68.6 74.8	0.0146 0.0134
393.2	85.2	0.0117
413.2	93.1	0.0107
	AUXILIARY	INFORMATION
METHOD/APPARATUS	/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	constant determined	
a chromatogr	on volume of gas on caphic column. Helium	No details given.
was used as	a carrier gas and a ometer was used as a	
detector.	The measured Henry's	
	s were independent of flow rate and composi-	
tion of inje	ected sample. The dead letermined by two	ESTIMATED ERROR:
independent	methods and the values	$\delta T/K = \pm 0.1;  \delta x_{CO_2} = \pm 5\%$
agreed withi	n experimental error.	(estimated by compiler).
<b>.</b>		
		REFERENCES:

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Eicosane; C<sub>20</sub>H<sub>42</sub>; [112-95-8]

# ORIGINAL MEASUREMENTS:

Chai, C-P.; Paulaitis, M. E.;

J. Chem. Eng. Data, 1981, 26,

277-279.

#### VARIABLES:

T/K = 314.3-330.2

#### PREPARED BY:

C. L. Young

#### EXPERIMENTAL VALUES:

T/K	Henry's constant /atm	Mole fraction of a carbon dioxide
314.3	75.58	0.01323
321.0	80.62	0.01240
321.0	80.24	0.01246
325.3	83.03	0.01204
325.3	82.75	0.01208
330.2	86.20	0.01160
330.2	86.21	0.01160

a Calculated by compiler for a partial pressure of 1 atm.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus similar to that described in ref.(1). Known amount of carbon dioxide brought into contact with known amount of solvent. Reduction in pressure measured.

# SOURCE AND PURITY OF MATERIALS:

- 1. Linde "bone dry" grade.
- 2. Fisher certified grade.

# ESTIMATED ERROR:

#### REFERENCES:

 Dymond, J. H.; Hildebrand, J. H.; Ind. Eng. Chem. Fundam., 1967, 6, 130.

- Carbon dioxide; CO2; [124-38-9]
- 2. Eicosane; C<sub>20</sub>H<sub>42</sub>; [112-95-8]

### ORIGINAL MEASUREMENTS:

Huang, S.H.; Lin, H.M.; Chao, K.C.

J. Chem. Eng. Data. 1988, 33, 145-147.

### VARIABLES:

T/K = 323.2-573.2P/kPa = 992-5063

### PREPARED BY:

P.G.T. Fogq

### **EXPERIMENTAL VALUES:**

T/K	Henry's law constant /atm	Henry's law constant <sup>*</sup> /kPa	Mole fraction solubility at 101.3 kPa*
323.3	(75) <sup>†</sup>	7646	0.0131
373.5	114	11551	0.0088
473.2	160	16212	0.0063
573.4	171	17327	0.0058

The Henry's law constant, H, is here defined as

$$H = \prod_{P \to 0} \left[ \frac{f}{x} \right]$$

where

x = mole fraction solubility of carbon dioxide

f = fugacity of carbon dioxide
P = pressure of carbon dioxide

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility of carbon dioxide in eicosane was measured at four temperatures at pressures from 992 to 5063 kPa. Apparatus and procedure are described in an earlier paper (1). Gas was passed through the liquid in a thermostatted cell until saturation was achieved. Samples of solution were then withdrawn. The volume of the gas evolved when the pressure was reduced was measured and the eicosane weighed when it had cooled and solidified. The fugacity, f, of the carbon dioxide at various pressures was estimated by the method described by Lee and Kesler (2). The variation of  $\ln(f/x)$  with pressure was linear to within a deviation of less than 0.8% The value of f/x at zero pressure was taken to be the limiting value of the Henry's law constant.

### SOURCE AND PURITY OF MATERIALS:

- Supplied by Matheson Gas Products. Minimum purity 99.8%
- 2. Supplied by Alfa Products, Morton Thiokol Inc. Minimum purity 99%. Gas chromatographic analysis showed no thermal degradation after the solubility measurements were carried out.

### ESTIMATED ERROR:

 $\delta H = \pm 3\%$  (authors)

- Huang, S.H.; Lin, H.M.; Chao, K.C. Fluid Phase Equilib. 1. 1987, 36, 141.
- Lee, B.I.; Kesler, M.G. AIChE J. 1975, 21, 510. 2.

<sup>†</sup> estimated by the compiler from data given in the paper.

calculated by the compiler.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Octacosane; C28H58; [630-02-4]

### ORIGINAL MEASUREMENTS:

Huang, S.H.; Lin, H.M.; Chao, K.C.

J. Chem. Eng. Data. 1988, 33, 143-145.

### VARIABLES:

T/K = 373.2-573.2P/kPa = 1013-5066

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Henry's law constant /atm	Henry's law constant * /kPa	Mole fraction solubility at 101.3 kPa
373.2	94 ± 2	9530 ± 200	0.0106
473.2	137 ± 1	13880 ± 100	0.0073
573.2	156 ± 2	15810 ± 200	0.0064

The Henry's law constant, H, is here defined as

$$H = \prod_{P \to 0} \left[ \frac{f}{x} \right]$$

where

x = mole fraction solubility of carbon dioxide

f = fugacity of carbon dioxide
P = pressure of carbon dioxide

\* calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

The solubility of carbon dioxide in octacosane was measured at three temperatures at pressures from 1013 to 5066 kPa. Apparatus and procedure are described in an earlier paper (1). Gas was passed through the liquid in a thermostatted cell until saturation was achieved. Samples of solution were then withdrawn. The volume of the gas evolved when the pressure was reduced was measured and the octacosane weighed when it had cooled and solidified. The fugacity, f, of the carbon dioxide at various pressures was estimated by the method described by Lee and Kesler (2). The variation of ln(f/x) with pressure was linear to within a deviation of less than 0.8% The value of f/x at zero pressure was taken to be the limiting value of the Henry's law constant.

# SOURCE AND PURITY OF MATERIALS:

- Supplied by Matheson Gas Products. Minimum purity 99.8%
- 2. Supplied by Alfa Products, Morton Thiokol Inc. Minimum purity 99%. Gas chromatographic analysis showed no thermal degradation after the solubility measurements were carried out.

### ESTIMATED ERROR:

 $\delta H = \pm 2\%$  (authors)

- Huang, S.H.; Lin, H.M.; Chao, K.C. Fluid Phase Equilib. 1987, 36, 141.
- Lee, B.I.; Kesler, M.G. AIChE J. 1975, 21, 510.

- 1. Carbon dioxide; CO2; [124-38-9]
- Alkanes

# ORIGINAL MEASUREMENTS:

Gasem, K.A.M.; Robinson, R.L.

J. Chem. Eng. Data 1985, 30, 53-56

# VARIABLES:

P/kPa = 524-8632T/K = 313.2-423.2

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	т/к	Henry's constant /kPa	$\overline{V}_{\text{CO}_2}^{\infty}$	x <sub>CO2</sub> at P <sub>CO2</sub> = 101.3kPa*
Eicosane; C <sub>20</sub> H <sub>42</sub> ;	323.2	8230±30	48±3	0.0123
[112-95-8]	373.2	11290±30	79±1	0.0090
Octacosane; C <sub>28</sub> H <sub>58</sub> ; [630-02-4]	348.2 373.2 423.2	8120±120 9380±90 11560±170	131±8 139±6 151±11	0.0125 0.0108 0.0088
Hexatriacontane; C <sub>36</sub> H <sub>74</sub> ; [630-06-8]	373.2	7740±30	170±4	0.0131
	423.2	9850±70	189±5	0.0103
Tetratetracontane; C <sub>44</sub> H <sub>90</sub> ; [7098-22-8]	373.2	7060±80	211±11	0.0144
	423.2	8520±80	226±8	0.0119

The authors found that, at mole fractions of carbon dioxide less than 0.45, the variation in mole fraction solubilities with variation in pressure could be represented by the Krichevsky-Kasarnovsky equation (1) in the form:

$$\ln(f_{\text{CO}_2}/x_{\text{CO}_2}) = \ln H + (\overline{V}_{\text{CO}_2}^{\infty}/RT)(P_{\text{b}} - P_{\text{hc}})$$

where  $f_{CO_2}$  = fugacity of  $CO_2$  in the mixture

H = Henry's constant

 $\overline{V}_{\text{CO}_2}$  = partial molar volume at infinite dilution of  $\text{CO}_2$  in the liquid phase

 $P_{\rm b}$  = bubble point pressure

 $P_{hc}$  = hydrocarbon vapor pressure

The authors found values of H by plotting  $\ln(f_{\text{CO}_2}/x_{\text{CO}_2})$  against  $P_{\text{b}}$  and extrapolating to zero pressure. Values of  $\overline{V}_{\text{CO}_2}^{\infty}$  were found from the slope of the line.

 $^*$  calculated by the compiler from values of H and of  $\overline{V}_{ extsf{CO}_2}^{\infty}$  given in the paper

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The authors used a static equilibrium cell capable of handling solvents which were solid at room temperature. Bubble point pressures for various quantities of CO2 were found by decreasing the volume of the mixture and observing the break in the volume-pressure curve as the system changed from two phase to one phase. Mole fraction solubilities of CO<sub>2</sub> for various pressures are given in the paper.

# SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Linde Speciality Gases; purity stated to be 99.99 mol%
- 2. Supplied by Alfa Products; purity stated to be 99 mol%

# ESTIMATED ERROR;

See above.

- Krichevsky, I.R.; Kasarnovsky, J.S.
- J. Amer. Chem. Soc. 1935, 57, 2168.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Tetracosane, 2,6,10,15,19,23-hexamethyl-, (squalane); C<sub>30</sub>H<sub>62</sub>;
  [111-01-3]

# ORIGINAL MEASUREMENTS:

Chai, C-P.; Paulaitis, M. E.; J. Chem. Eng. Data, 1981, 26, 277-279.

### VARIABLES:

T/K = 298.6-330.2

# PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

T/K	Henry's constant /atm	Mole fraction of <sup>a</sup> carbon dioxide
298.6	45.35	0.02205
298.6	44.92	0.02226
304.3	48.16	0.02076
304.3	47.75	0.02094
311.0	51.33	0.01948
311.0	50.94	0.01963
316.2	53.92	0.01855
316.2	53.22	0.01879
323.6	57.85	0.01729
323.6	57.56	0.01737
330.2	60.43	0.01655

a Calculated by compiler for a partial pressure of 1 atm.

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Volumetric apparatus similar to that described in ref.(1). Known amount of carbon dioxide brought into contact with known amount of solvent. Reduction in pressure measured.

### SOURCE AND PURITY OF MATERIALS:

- 1. Linde "bone dry" grade.
- 2. Fisher certified grade.

# ESTIMATED ERROR:

### REFERENCES:

 Dymond, J. H.; Hildebrand, J. H.; Ind. Eng. Chem. Fundam., 1967, 6, 130.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Cyclopropane; C<sub>3</sub>H<sub>6</sub>; [75-19-4]

ORIGINAL MEASUREMENTS: Haselden, G.G.; Snowden, P.

Trans. Faraday Soc. 1962, 58, 1515-1528.

VARIABLES:

T/K = 178.8-236.8 $P_{total}/kPa = 27-210$  PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

EXPERIMENT			of dew po	oints			
<sup>y</sup> CO₂	Total P/atm	Total P/kPa*	т/к	<sup>y</sup> CO₂	Total P/atm	Total* P/kPa*	<i>T</i> /K
0.2255 0.4008 0.6200	0.2862 0.4484 1.0191 1.4535 1.9195 0.2506 0.5606 0.8776 1.4396 1.8298 0.2191 0.4497	29.00 45.43 103.26 147.28 194.49 25.39 56.80 88.92 145.87 185.40 22.20 45.57	208.7 219.0 234.2 242.6 249.8 203.8 216.8 225.2 236.4 242.4 193.7 205.5	0.8454 0.9066	1.4602 1.9145 0.2182 0.4794 0.9695 1.4890 1.9354 0.2243 0.5025 0.9663 1.5050 1.8988	147.95 193.99 22.11 48.58 98.23 150.87 196.10 22.73 50.92 97.91 152.49 192.40	226.6 232.8 184.3 192.7 203.1 210.3 215.8 173.9 184.2 194.9 203.7 207.1
	0.9789 99.19 219.0  Measurement of bubble points						
<sup>×</sup> CO₂	Total P/atm	Total P/kPa*	Т/К	<sup>X</sup> CO₂	Total P/atm*	Total P/kPa	T/K
0.048	2.0741 1.6788 1.4995 1.2410 1.0856 0.9723 0.7835 0.6354 0.4937 0.3533 0.2649 1.9017 1.6101 1.2413 0.9555 0.8946 0.5721	210.16 170.10 151.94 125.74 110.00 98.52 79.39 64.38 50.02 35.80 26.84 192.69 163.14 125.77 96.82 90.65 57.97	236.8 230.1 226.5 221.0 217.6 214.4 208.4 203.0 196.6 188.6 182.1 223.8 219.2 212.1 205.2 203.7 198.1	0.195 0.299 0.391	0.5480 0.4066 0.3258 0.2694 1.8600 1.6749 1.4083 1.1559 0.9007 0.7907 0.7187 2.0577 1.7874 1.3730 2.0382 1.8213	55.53 41.20 33.01 27.30 188.46 169.71 142.70 117.12 91.26 80.12 72.82 208.50 181.11 139.12 206.52 184.54	192.7 186.6 182.3 178.8 208.8 206.2 202.0 197.5 192.3 189.5 187.6 205.3 202.0 195.9 202.7

 $x_{\rm CO_2}$  = mole fraction of carbon dioxide in the liquid phase  $y_{\rm CO_2}$  = mole fraction of carbon dioxide in the gas phase \* calculated by the compiler

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Dew points and bubble points of various mixtures of carbon dioxide and cyclopropane were measured. The dew and bubble point cells were immersed in a cryostat. Full details of the apparatus are described in the paper.

### SOURCE AND PURITY OF MATERIALS:

No information

ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$  (authors)

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Cyclopentane; C<sub>5</sub>H<sub>10</sub>; [287-92-3]

# ORIGINAL MEASUREMENTS:

Eckert, C.J.; Sandler, S.I.

J. Chem. Eng. Data 1986, 31, 26-28.

### VARIABLES:

T/K = 310.9-333.2P/kPa = 175-8263

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	P <sub>total</sub> /kPa	<sup>x</sup> co₂	<sup>y</sup> CO₂	P <sub>CO2</sub> /kPa*
310.86	175	0.0067	0.600	105

 $^*$ calculated by the compiler and taken to be  $^{y}_{ exttt{CO}_2}$   $^{ exttt{ iny P}}$ total

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Measurements on the vapor-liquid equilibria for the carbon dioxide-cyclopentane system were made at 310.9 K, 318.2 K and 333.2 K and total pressures to a maximum of 8263 kPa. The measurements reported above were the only ones at a pressure below 200 kPa. The apparatus and procedure were similar to that used previously by one of the authors (1). Mixtures were analysed by gas chromatography.

# SOURCE AND PURITY OF MATERIALS:

- Research grade (99.99%) supplied by the Linde Division of Union Carbide.
- 2. Supplied by Aldrich; purified by distillation under nitrogen with only the middle 50% cut used.

### ESTIMATED ERROR:

### REFERENCES:

Behrens, P.K.; Sandler, S.I.
 J. Chem. Eng. Data 1983, 28, 52.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cyclohexane;  $C_6H_{12}$ ; [110-82-7]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.

Acta Chem. Scand. 1953, 7, 537 - 544.

### VARIABLES:

T/K = 298.15 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

J. Chr. Gjaldbaek

## EXPERIMENTAL VALUES:

<i>T/</i> K	Carbon Dioxide Pressure P <sub>1</sub> /mmHg	Mol Fraction <sup>1</sup> 10 <sup>3</sup> x <sub>1</sub>	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	700.3	7.67	1.57	1.71
	814.1	7.77	1.59	1.73

Mole fraction solubility values adjusted to a gas partial pressure of 101.325 kPa (1 atm) by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as confining liquid. The solvent was degassed in the apparatus.

The absorbed volume of gas is calculated from the initial and final amounts, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury.

The mole fraction solubility values are at 1 atm assuming Henry's law is obeyed.

Details of the apparatus and procedure are given in ref. 1 and 2.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate (analytical reagent) and concentrated sulfuric acid. 99.9 per cent CO<sub>2</sub>.
- (2) Cyclohexane. Purified by fractional freezing, dried, and distilled. F.p./°C = 6.2 6.4, b.p./°C = 80.69 80.71.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- Gjaldbaek, J. C.
   Acta Chem. Scand. <u>1952</u>, 6, 623.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]

# ORIGINAL MEASUREMENTS:

Dymond, J.; Hildebrand, J. H.

Ind. Eng. Chem., Fundam. 1967, 6, 130 - 131.

### VARIABLES:

T/K: 298.15 Total P/kPa: 101.325

### PREPARED BY:

A. L. Cramer H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
298.15	77.1	1.601	1.748

The Bunsen and Ostwald coefficients were calculated by the compiler.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of an allglass buret system and a two bulb absorption vessel.

A magnetic pump forces solvent from the lower bulb over the wall of the upper bulb which contains the gas. The solvent flow back to the lower bulb. Pumping is continued until there is no further pressure change.

The amount of gas absorbed is calculated from the initial and final gas pressure.

# SOURCE AND PURITY OF MATERIALS:

No information.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.01$  or less.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]

# ORIGINAL MEASUREMENTS:

Dymond, J. H.

J. Phys. Chem. 1967, 71, 1829-1831.

### VARIABLES:

T/K: 293.39 - 310.55 p/kPa: 101.325 (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	rature T/K	Mol Fraction $10^3 x_1$	Bunsen Coefficient	Ostwald Coefficient
			$\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	$L/\text{cm}^3\text{cm}^{-3}$
20.24	293.39	8.02	1.68	1.80
26.60	299.75	7.58	1.57	1.72
31.08	304.23	7.31	1.51	1.68
37.40	310.55	6.94	1.42	1.61

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: For use between 293.15 and 310.55 K.

 $\ln x_1 = -7.4372 + 7.6609/(T/100K)$ 

The standard error about the regression line is  $5.37 \times 10^{-6}$ .

Mol Fraction 103x1
8.03 7.69 7.37 7.07

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The liquid is saturated with the gas at a partial pressure of one atm.

The apparatus is that described by Dymond and Hildebrand (1). It uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressures.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Western Gas, Inc. Dried.
- (2) Cyclohexane. Matheson, Coleman and Bell chromatoquality reagent. Dried and fractionally frozen. m.p. 6.45°C.

### ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

### REFERENCES:

 Dymond, J.; Hildebrand, J. H. *Ind. Eng. Chem. Fundam.* 1967, 6, 130.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]

### ORIGINAL MEASUREMENTS:

Wilhelm, E.; Battino, R.

J. Chem. Thermodyn. 1973, 5, 117-120.

### **VARIABLES:**

*T*/K: 283.82 - 313.34 p/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Т/К	Mol Fraction $10^3 x_1$	Bunsen Coefficient a	Ostwald Coefficient L
283.82	8.56	1.81	1.88
297.63	7.55	1.57	1.71
313.34	6.85	1.39	1.60

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa (1 atm) by Henry's law. The Bunsen coefficients were calculated by the compiler.

Smoothed Data: For use between 283.82 and 313.34 K

 $\ln x_1 = -7.1298 + 6.7089/(T/100K)$ 

The standard error about the regression line is  $9.86 \times 10^{-5}$ .

T/K	Mol Fraction 10 3 x 1
288.15	8.22
298.15	7.60
308.15	7.06

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm of solve is placed in a flask of such size Up to 500 cm3 of solvent that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N2 trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Matheson Co., Inc. Research grade. Minimum volume percent purity is 99.995.
- (2) Cyclohexane. Phillips Petroleum Co. Pure Grade. Distilled.

# ESTIMATED ERROR:

$$\delta T/K = 0.03$$
  
 $\delta P/mmHg = 0.5$   
 $\delta x_1/x_1 = 0.005$ 

- REFERENCES:
  1. Morrison, T. J.; Billett, F.
  J. Chem. Soc. 1948, 2033.
  2. Battino, R.; Evans, F. D.;
  Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Krauss, W.; Gestrich, W.
2. Cyclohexane; C <sub>6</sub> H <sub>12</sub> ; [110-82-7]	ChemTech. (Heidelberg), 1977, 6,
2.000	513-6.
VARIABLES:	PREPARED BY:
T/K = 283.15-313.15	C.L. Young
EXPERIMENTAL VALUES:	
T/K Solubility, $S/mol$	Mole fraction of dm-3 bar-1 carbon dioxide in liquid, $x_{\rm CO_2}$
283.15 0.08130 293.15 0.07150	
303.15 0.06341 313.15 0.05667	0.00698
313.13	0.00032
+ at a partial pressure	of 101.325 kPa.
AUXILIAR	Y INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric apparatus in which gas was dissolved in liquid in glass cell. Pressure measured. Amount of gas dissolved estimated from pressure measurements when gas was repeatedly expanded into known volume. Details in source. Values of solubility calculated from equations and graphs in	No details given.
original.	
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1; \ \delta x_{CO_2} = \pm 1-2$ %.
	REFERENCES:

	6
COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]</li> </ol>	Patyi, L.; Furmer, I. E.; Makranczy, J.; Sadilenko, A. S.; Stepanova, Z. G.; Berengarten, M. G.
	Zh. Prikl. Khim. <u>1978</u> , 51, 1296- 1300.
VARIABLES:	PREPARED BY:
T/K = 298.15	C. L. Young
EXPERIMENTAL VALUES:	
T/K a <sup>†</sup>	Mole fraction of carbon dioxide at a partial pressure of 101.325 kPa $^x\mathrm{CO}_2$
298.15 1.57	0.00747
<sup>†</sup> volume of gas (measured a dissolved by one volume o	t 101.325 kPa and 273.15 K)  of cyclohexane.

# 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 Corrections of known dimensions. 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:

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

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Cyclohexane, C<sub>6</sub>H<sub>12</sub>; [110-82-7] VARIABLES: T/K = 273.15-303.15 P/MPa = 0.767-5.805 CRIGINAL MEASUREMENTS: Kaminishi, G-I.; Yokoyama, C.; Takahashi, S. Fluid Phase Equilibria, 1987, 34, 83-99. PREPARED BY: P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Henry's la H/MPa	aw constant H/kPa	Mole fraction $x_{CO_2}$ at $p_{CO_2} = 101.3 \text{ k}$	Pa*
283.15	11.48	11480	0.00882	
298.15	13.30	13300	0.00762	
303.15	13.89	13890	0.00729	

$$H = \begin{bmatrix} \frac{f}{x_1} \end{bmatrix}$$

$$x_1 = x_{CO_2}$$
;  $f_1 = \text{fugacity of } CO_2$ 

### AUXILIARY INFORMATION

### METHOD APPARATUS / PROCEDURE:

Apparatus able to withstand pressures to 20 MPa was used to determine phase equilibria by the bubble point method. Henry's constants at zero pressure were obtained from the experimental data by using the method described by Prausnitz and Chueh (1)

## SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Showa Tansan Industry Co., Ltd; purity better than 99.9%
- Supplied by Wako Pure Chem. Co., Ltd.; purity better than 99.8%

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$  $\delta P/kPa = \pm 0.1$  (authors)

### REFERENCES:

 Prausnitz, J.M.; Chueh, P.L. Computer Calculations for High Pressure Vapor-Liquid Equilibria, Prentice-Hall, Englewood Cliffs, USA, 1968.

 $<sup>^*</sup>$  taken by the compiler to be given approximately by  $P_{\mathrm{CO}_2}/H$ 

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO<sub>2</sub>; [124-38-9] Alicyclics or 1-Tetradecene Luhring, P.; Schumpe, A. J. Chem. Eng. Data, 1989, 34, 250-252. VARIABLES: IREPARED BY: T/K = 293.2C.L. Young **EXPERIMENTAL VALUES:** T/KHenry's Constant\* Mole fraction of $CO_2$ at 1 atm $/(Pa^m^3/mol^{-1})$ partial pressure Cyclohexane; $C_6H_{12}$ ; [110-82-7] 293.2 1414 0.007746 Tetrahydronaphthalene, (tetralin); C<sub>10</sub>H<sub>12</sub>; [119-64-2] 293.2 1610 0.008576 Decahydronaphthalene, (decalin); C10H18; [91-17-8] 293.2 2001 1-Tetradecene; C14H28; [1120-36-1] 293.2 1551 0.001654 \*referred to as Henry's constant in source but appears to be usual Henry's constant multiplied by molar volume. tcalculated by compiler using density data taken from ref.(1).

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE

Little infomation given in source. Method consisted of equilibrating known amounts of degassed liquid and gas and measuring the change in pressure. Equilibration was reached in 3 to 6 minutes. Some details given in ref.(2).

### SOURCE AND PURITY OF MATERIALS:

Obtained from Merck at the highest available purity. No other details given.

ESTIMATED ERROR:  $\delta T/K = \pm 0.1$  (authors)  $\delta x/x = \pm 0.01$  to 0.15 (compiler)

- Riddick, J.A.; Bunger, W.B.;1970 Organic Solvents, Wiley-Interscience, New York.
- Schumpe, A.; Quiker, G.;
   Decker, W.D.
   Adv. Biochem. Eng., 1982, 24, 1.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cyclohexane; C<sub>6</sub>H<sub>12</sub>; [110-82-7]
   Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>;
   [108-87-2]

# ORIGINAL MEASUREMENTS:

Horsman-van den Dool, L. E. W.;
Warman, J. W.

Interuniversity Reactor Institute
(IRI)-Report 134-81-01

### VARIABLES:

$$T/K = 293.2, 294.3$$
  
 $p_1/kPa = not given$ 

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	rature	Ostwald Coefficient	Number of Runs
t/°C	T/K	$L/cm^3 cm^{-3}$	OI Ruiis
Cycloh	exane		
20.0	293.2	1.64	2
Methylcyclohexane			
21.1	294.3	1.78	2

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A cylindrical glass container of approximately 15 cm³ volume is partly filled with solvent and closed with a half-hole septum. An amount of the gaseous solute is added to the container. The closed container is shaken for 30 minutes. Samples of both the vapor and liquid phases are taken in a calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.

The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 200 cm Porapak column is used for the separation.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Baker Chemical Co. Instrument grade, 99.99 percent. Used as received.
- (2) Cyclohexane. Merck and Co.
  Uvasol spektroskopie grade.
  Methylcyclohexane. Fluka.
  UV-Spektroskopie grade.
  Impurities which gave same
  retension times as the gas were
  removed by absorption or distillation. Otherwise used as rcvd.

### ESTIMATED ERROR:

 $\delta L/L = \pm 0.05$ 

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Methylcyclohexane; C<sub>7</sub>H<sub>14</sub>; [108-87-2]

### ORIGINAL MEASUREMENTS:

Field, L. R.; Wilhelm, E.; Battino, R.

J. Chem. Thermodyn. 1974, 6, 237 - 243.

### VARIABLES:

T/K: 283.89 - 313.28 P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^3 x_1$	Bunsen Coefficient a/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-1
283.89	11.53	2.07	2.151
298.13	9.28	1.63	1.784
313.28	7.67	1.33	1.521

The gas solubility values were adjusted to a  $CO_2$  partial pressure of 101.325 kPa (1 atm) by Henry's law.

The Bunsen coefficients were calculated by the compiler.

Smoothed Data: For use between 283.15 and 313.28 K.

$$\ln x_7 = -8.8123 + 12.3390/(T/100 K)$$

The standard error about the regression line is  $7.36 \times 10^{-4}$ .

Т/К	Mol Fraction 10 3 x 1
283.15	11.63
293.15	10.02
298.15	9.34
303.15	8.72
313.15	7.66

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to  $500~\rm{cm}^3$  of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid  $N_2$  trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Either Matheson Co., Inc. or Air Products and Chemicals, Inc. Purest grade available, minimum purity greater than 99 mole per cent.
- (2) Methylcyclohexane. Phillips Petroleum Co. Pure Grade. Distilled.

### ESTIMATED ERROR:

 $\delta T/K = 0.03$   $\delta P/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.005$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cyclooctane; C<sub>8</sub>H<sub>16</sub>; [292-64-8]

# ORIGINAL MEASUREMENTS:

Wilcock, R. J.; Battino, R.; Wilhelm, E.

J. Chem. Thermodyn. 1977, 9, 111 - 115.

## VARIABLES:

T/K: 289.09 - 313.52 P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
·	3.03	Coefficient	Coefficient
	$10^3x_1$	α	${f L}$
289.09	7.548	1.268	1.342
298.27	6.860	1.142	1.247
313.52	6.036	0.9897	1.136

The Bunsen coefficients were calculated by the compiler.

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa by Henry's law.

Smoothed Data: For 288.15 to 313.15 K.

 $\ln x_1 = -7.7453 + 8.2561/(T/100K)$ 

The standard error about the regression line is 4.11  $\times$  10<sup>-5</sup>.

T/K	Mol Fraction
	$10^3 x_{1}$
288.15	7.60
298.15	6.90
308.15	6.31

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum mole per cent purity is 99.8.
- (2) Cyclooctane. Chemical Samples Co. 99 mole per cent, distilled, refractive index (NaD, 298.15 K) 1.4562.

### ESTIMATED ERROR:

 $\delta T/K = 0.03$   $\delta P/mmHg = 0.5$  $\delta x_1/x_1 = 0.005$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) trans-1,2-Dimethylcyclohexane; C<sub>8</sub>H<sub>16</sub>; [6876-23-9]

# ORIGINAL MEASUREMENTS:

Geller, E. B.; Battino, R. Wilhelm, E.

J. Chem. Thermodyn. 1976, 8, 197-202.

### VARIABLES:

298.19, 312.88 101.325 (1 atm) T/K: p/kPa:

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.19	10.197	1.598	1.734
312.88	8.778	1.345	1.541

The Bunsen coefficients were calculated by the compiler assuming ideal gas behavior.

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa by Henry's law.

### Smoothed Data:

The equation is based on only two pair of experimental points and should be used with caution.

For use between 298.19 and 312.88 K  $\ln x_1 = -7.7777 + 9.5187/(T/100K)$ 

т/к	Mol Fraction 103x1
298.15	1.020
308.15	0.920

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to  $500~{\rm cm}^3$  of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by differences between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals Co. Stated to be 99.8 mole percent minimum.
- (2) trans-1,2-Dimethylcyclohexane. Chemicals Samples Co. Fractionally distilled and stored in dark. Refractive index (Na-D, 298.15 K) 1.4248.

### ESTIMATED ERROR:

$$\delta T/K = 0.03$$
  
 $\delta p/mmHg = 0.5$   
 $\delta x_1/x_1 = 0.005$ 

- REFERENCES:
  1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.;
   Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) cis-1,2-Dimethylcyclohexane; C<sub>8</sub>H<sub>16</sub>; [2207-01-4]

# ORIGINAL MEASUREMENTS:

Geller, E. B.; Battino, R. Wilhelm, E.

J. Chem. Thermodyn. 1976, 8, 197-202.

### VARIABLES:

*T*/K: 297.88, 312.99 101.325 (1 atm) p/kPa:

### PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction 10 <sup>3</sup> x <sub>1</sub>	Bunsen Coefficient a/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient _L/cm³ cm <sup>-3</sup>
297.88	9.408	1.504	1.640
312.99	7.972	1.252	1.435

The Bunsen coefficients were calculated by the compiler assuming ideal

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa by Henry's law.

Smoothed Data:

The equation is based on only two pair of experimental points and should be used with caution.

For use between 297.88 and 312.99 K

 $\ln x_1 = -8.1034 + 10.2396/(T/100K)$ 

T/K	Mol Fraction 10 3 x 1
298.15 308.15	9.38 8.39
308.13	8.39

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Up to 500 cm3 of solvent Degassing. is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by differences between the initial and final volumes in the buret The solvent is collected in system. a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals Co. Stated to be 99.8 mole percent minimum.
- (2) cis-1,2-Dimethylcyclohexane. Chemical Samples Co. Fractionally distilled and stored in dark. Refractive index (Na-D, 298.15 K) 1.4337.

### ESTIMATED ERROR:

 $\delta T/K = 0.03$  $\delta_P/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.005$ 

- REFERENCES:
  1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
  - 2. Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) trans-1,4-Dimethylcyclohexane, 30 mol %; C<sub>8</sub>H<sub>16</sub>; [2207-04-7]
- (3) cis-1,4-Dimethylcyclohexane, 70 mol %;  $C_8H_{16}$ ; [624-29-3]

# ORIGINAL MEASUREMENTS:

Geller, E. B.; Battino, R. Wilhelm, E.

J. Chem. Thermodyn. 1976, 8, 197-202.

# VARIABLES:

298.32, 313.01 101.325 (1 atm) T/K: p/kPa:

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.32	10.300	1.605	1.753
313.01	8.783	1.347	1.544

The Bunsen coefficients were calculated by the compiler.

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa (1 atm) by Henry's law.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N2 trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by differences between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals Co. Stated to be 99.8 mole percent minimum.
- (2) trans-1,4-Dimethylcyclohexane.
- (3) cis-1,4-Dimethylcyclohexane. Chemical Samples Co. Binary mixture used as received. Authors analyzed mixture by refractive index.

### ESTIMATED ERROR:

 $\delta T/K = 0.03$  $\delta p/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.005$ 

- REFERENCES:
  1. Morrison, T. J.; Billett, F.
  J. Chem. Soc. 1948, 2033.
- 2. Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) trans-1,3-Dimethylcyclohexane, 41 mole %; C<sub>8</sub>H<sub>16</sub>; [2207-03-6]
- (3) cis-1,3-Dimethylcyclohexane, 59 mole %;  $C_8H_{16}$ ; [638-04-0]

### ORIGINAL MEASUREMENTS:

Geller, E. B.; Battino, R. Wilhelm, E.

J. Chem. Thermodyn. 1976, 8, 197-202.

### **VARIABLES:**

*T*/K: 298.03, 313.01 101.325 (1 atm) p/kPa:

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^3 x_4$	Bunsen Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
298.03	10.184	1.582	1.726
313.01	8.592	1.312	1.503

The Bunsen coefficients were calculated by the compiler.

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa (1 atm) by Henry's law.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm³ of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid No trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by differences between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

## SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals Co. Stated to be 99.8 mole per cent minimum.
- (2) trans-1,3-Dimethylcyclohexane.
- (3) cis-1,3-Dimethylcyclohexane. Chemical Samples Co. Binary mixture used as received. Authors analyzed mixture by refractive index.

# ESTIMATED ERROR:

$$\delta T/K = 0.03$$
  
 $\delta_p/\text{mmHg} = 0.5$   
 $\delta x_1/x_1 = 0.005$ 

- REFERENCES:
  1. Morrison, T. J.; Billett, F.

  J. Chem. Soc. 1948, 2033.
  2. Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

OMPONENTS:		ORIGINAL MEASUREMENTS:
. Carbon diox	ide; CO <sub>2</sub> ; [124-38-9]	Tremper, K.K.; Prausnitz, J.M.
. 1, 1'-Bicyc [92-51-3]	lohexyl; C <sub>12</sub> H <sub>22</sub> ;	J. Chem.Engng.Data, <u>1976</u> ,21,295-9
ARIABLES:		PREPARED BY:
T/K = 300-	475	C.L. Young
XPERIMENTAL VALI	JES:	
T/K	Henry's Con /atm	stant <sup>a</sup> Mole fraction <sup>b</sup> of carbon dioxide at latm partial pressure,
300	128.0	0.00781
325	155.0	0.00645
350	188.0	0.00532
375	222.0	0.00450
400	251.0	0.00398
425	270.0	0.00370
450		*******
475	258.0	0.00388
a.		ents were made at several . solubility used were all region.
b.	Calculated by compiler between mole fraction a	assuming linear relationship nd pressure.
	AUXILIARY	INFORMATION
lescribed by I 1). Pressure	S/PROCEDURE paratus similar to that pymond and Hildebrand measured with a null precision gauge. Details	SOURCE AND PURITY OF MATERIALS:  Solvent degassed, no other details given.
		ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta x_{CO_2} = \pm 1\%.$

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,1'-Bicyclohexyl; C<sub>12</sub>H<sub>22</sub>; [92-51-3]

# ORIGINAL MEASUREMENTS:

Horsman-van den Dool, L. E. W.; Warman, J. W.

Interuniversity Reactor Institute
(IRI)-Report 134-81-01

### VARIABLES:

T/K = 295.2 $p_1/kPa = not given$  PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	erature	Ostwald Coefficient	Number of Runs
t/°C	T/K	L/cm <sup>3</sup> cm <sup>-3</sup>	OI Runs
22.0	295.2	1.09	(2)

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A cylindrical glass container of approximately 15 cm³ volume is partly filled with solvent and closed with a half-hole septum. An amount of the gaseous solute is added to the container. The closed container is shaken for 30 minutes. Samples of both the vapor and liquid phases are taken in a calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.

The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 200 cm Porapak column is used for the separation.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Baker Chemical Co. Instrument grade, 99.99 percent. Used as received.
- (2) 1,1'-Bicyclohexyl. Fluka. purum grade. Impurities which give the same retention time as the gas are removed before the experiment by adsorption or distillation.

ESTIMATED ERROR:

 $\delta L/L = \pm 0.05$ 

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Decahydronaphthalene, (decalin);  $C_{10}H_{18}$ ; [91-17-8]

# ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1971, 16, 340-2.

### VARIABLES:

T/K = 298.2; 323.2

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

<i>T</i> /K	Henry's constan /atm /	kPa *CO2	at P <sub>CO2</sub> =	101.3	kPa*
298.2 323.2		146 3780	0.00909 0.00735		

\* calculated by the compiler assuming that  $x_{\rm CO_2} = P_{\rm CO_2}/H$ 

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

A conventional gas-liquid chromatographic unit was used with helium as carrier gas. Values of Henry's constant were calculated from retention times extrapolated to zero sample size. Values correspond to very low partial pressure of carbon dioxide. Surface adsorption can cause appreciable errors in this method of measuring Henry's law constants.

# SOURCE AND PURITY OF MATERIALS:

- 1. Sample from L'Air Liquide; minimum purity 99.9 mol%
- 2. Sample from Touzart and Matignon or from Serlabo of purity 99 mol%

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  (estimated by compiler)

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) cis-Decahydronaphthalene or cisdecalin; C<sub>10</sub>H<sub>18</sub>; [493-01-6]

trans-Decahydronaphthalene or trans-decalin;  $C_{10}H_{18}$ ; [493-02-7]

ORIGINAL MEASUREMENTS:

Horsman-van den Dool, L. E. W.; Warman, J. W.

Interuniversity Reactor Institute
(IRI)-Report 134-81-01

VARIABLES:

$$T/K = 296.3, 296.6$$
  
 $p_1/kPa = not given$ 

PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Temperature	Ostwald Coefficient	Number of Runs
t/°C T/K	$L/cm^3$ cm <sup>-3</sup>	or kuns
cis-Decalin		
23.4 296.6	1.10	3
trans-Decalin		
23.1 296.3	1.25	3

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A cylindrical glass container of approximately 15 cm³ volume is partly filled with solvent and closed with a half-hole septum. An amount of the gaseous solute is added to the container. The closed container is shaken for 30 minutes. Samples of both the vapor and liquid phases are taken in a calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.

The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 200 cm Porapak column is used for the separation.

- SOURCE AND PURITY OF MATERIALS:
- (1) Carbon dioxide.Baker Chemical Co. Instrument grade, 99.99 percent. Used as received.
- (2) cis-Decalin and trans-Decalin. Merck. Zur Synthese grade. Impurities which give the same retention time as the gas are removed before the experiment by adsorption or distillation.

ESTIMATED ERROR:

 $\delta L/L = \pm 0.05$ 

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Ethene;  $C_2H_4$ ; [74-85-1] Propene;  $C_3H_6$ ; [115-07-1] 1-Butene;  $C_4H_8$ ; [106-98-9]

### VARIABLES:

T/K = 231.55-273.15 $P_{CO_2} = 81-219 \text{ kPa}$ 

# P<sub>CO<sub>2</sub></sub> = 81-219 kPa EXPERIMENTAL VALUES:

### ORIGINAL MEASUREMENTS:

Nagahama, K.; Konishi, H. Hoshino, D.; Hirata, M.

J. Chem. Eng. Japan 1974, 7(5), 323-328.

### PREPARED BY:

P.G.T. Fogg

Solvent	T/K	Ptotal /atm	<sup>x</sup> CO₂	<sup>y</sup> CO₂	P <sub>CO2</sub> /atm	P <sub>CO₂</sub> /kPa
ethene	231.55	13.85	0.079	0.084	1.16	118
	252.95	25.15	0.071	0.072	1.81	183
propene	252.95	4.5	0.076	0.404	1.82	184
	273.15	6.7	0.014	0.119	0.80	81
	273.15	7.9	0.050	0.274	2.16	219
1-butene	273.15	3.1	0.059	0.616	1.91	193

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The data given above were obtained during studies of the systems to higher pressures over the whole of each composition range. The apparatus has been described previously (1). The components were charged into a glass-windowed equilibrium cell. A magnetic piston pump recirculated vapor, removed it from the top of the liquid and reintroduced it into the bottom of the liquid. After equilibrium was reached (c. 0.5 h) samples of the gas phase and of the liquid phase were analysed by gas chromatography.

## SOURCE AND PURITY OF MATERIALS:

- 1. Purity at least 99.8%
- 2. Ethene; purity at least 99.95%
  Propene; purity at least 99.32%
  1-Butene; purity at least 99.4%

### EXPERIMENTAL ERROR:

 $\delta T/K = \pm 0.05$  (authors)

### REFERENCES:

 Hakuta, T.; Nagahama, K.; Hirata, M. Bull. Japan Petrol. Inst. 1969, 11, 10.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Propene; C<sub>6</sub>H<sub>6</sub>; [115-07-1]

ORIGINAL MEASUREMENTS: Haselden, G.G.; Snowden, P.

Trans. Faraday Soc. 1962, 58, 1515-1528.

VARIABLES:

T/K = 166.4-229.1 $P_{total}/kPa = 9-218$  PREPARED BY:

P.G.T. Fogg

## EXPERIMENTAL VALUES:

Measurement	of	dew	points

<sup>y</sup> CO₂	Total P/atm	Total P/kPa*	T/K	<sup>y</sup> CO₂	Total P/atm	Total P/kPa*	T/K
0.2116	0.2486 0.4484 0.9925 1.4433 1.9438 0.2467 0.4866 1.0131 1.5607 2.0052	25.19 45.43 100.57 146.24 196.96 25.00 49.30 102.65 158.14 203.18	192.7 202.9 218.9 226.8 234.4 188.9 200.3 213.9 223.3 229.1	0.6001	0.2291 0.5103 1.0192 1.5363 1.9530 0.2553 0.5054 1.0167 1.5249 1.9245	23.21 51.71 103.27 155.67 197.89 25.87 51.21 103.02 154.51 195.00	182.4 194.7 206.4 214.6 220.1 173.2 183.4 195.3 203.2 207.4
<sup>x</sup> co₂	M Total P/atm	easurement Total P/kPa*	of bubbl	e points  *CO2	Total P/atm	Total P/kPa*	T/K
0.089	1.9979 1.5340 1.0019 0.6946 0.4926 0.3053 0.2096 0.1361 0.0919 2.0796	202.44 155.43 101.52 70.38 49.91 30.93 21.24 13.79 9.31 210.72	225.1 218.3 208.4 200.6 193.8 185.3 179.1 172.5 166.4 212.3	0.331	1.3145 1.0788 0.9215 0.7473 2.1490 1.8701 1.7397 1.4702 1.3412 2.1222	133.19 109.31 93.37 75.72 217.75 189.49 176.28 148.97 135.90 215.03	200.3 195.6 191.7 186.8 205.7 202.0 200.4 196.0 194.1 202.5
0.197	1.833	185.73 152.49	208.9 203.4	V.453	1.9788 1.8034	200.50 182.73	200.8 198.7

 $x_{\rm CO_2}$  = mole fraction of carbon dioxide in the liquid phase  $y_{\rm CO_2}$  = mole fraction of carbon dioxide in the gas phase calculated by the compiler

# AUXILIARY INFORMATION

200.8

### METHOD/APPARATUS/PROCEDURE:

Dew points and bubble points and bubble points of various mixtures of carbon dioxide and propene were measured. The dew and bubble points cells were immersed in a cryostat. Full details of the apparatus are described in the paper.

1.3629 138.10

# SOURCE AND PURITY OF MATERIALS:

No information

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$  (authors)

# ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Ethane; C<sub>2</sub>H<sub>6</sub>; [74-84-0] 3. Ethene; C<sub>2</sub>H<sub>4</sub>; [74-85-1] VARIABLES: T/K = 130-180 P<sub>CO<sub>2</sub></sub>/kPa = 0.033-27.6

### EXPERIMENTAL VALUES:

Mole percent solubility of solid carbon dioxide in various liquid mixtures of ethane and ethene

T/K	D *	Mole % com	position of	liquid be	fore CO₂ add	ded
1710	PCO2* /kPa	100% C2H4	70% C <sub>2</sub> H <sub>4</sub> 30% C <sub>2</sub> H <sub>6</sub>	50% C <sub>2</sub> H <sub>4</sub> 50% C <sub>2</sub> H <sub>6</sub>	25% C <sub>2</sub> H <sub>4</sub> 75% C <sub>2</sub> H <sub>6</sub>	100% C <sub>2</sub> H <sub>6</sub>
130	0.033	1.4	1.0	0.7	0.4	0.2
135	0.082	1.9	1.4	0.9	0.5	0.3
140	0.190	2.5	1.9	1.3	0.7	0.4
145	0.417	3.3	2.5	1.8	1.1	0.6
150	0.856	4.3	3.3	2.4	1.5	0.9
155	1.68	5.6	4.3	3.3	2.1	1.2
160	3.15	7.2	5.5	4.3	2.8	1.6
165	5.70	9.2	7.1	5.6	3.8	2.2
170	9.94	13.0	9.4	7.4	5.0	3.1
175	16.8			10.0	6.7	4.5
180	27.6					6.7

<sup>\*</sup> calculated by the compiler from vapor pressure equations for solid CO<sub>2</sub> given in the literature; 130-145 K ref.(1); 150-180 K ref.(2).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The experimental method is described in ref. (3). Vapor pressures of saturated solutions of carbon dioxide with excess solid in Various mixtures of ethane and ethene were measured over temperature ranges with a five junction copper constantin thermocouple. The vapor pressures of solutions of carbon dioxide of known composition were then measured at the point of appearance and of disappearance of the solid carbon dioxide. The corresponding temperatures were then found from the relationship between temperature and vapor pressure which had been established in the first series of measurements.

### SOURCE AND PURITY OF MATERIALS:

Components were obtained from commercial sources and purified as described in ref. (3).

# ESTIMATED ERROR:

- 1. Meyers, C.H.; van Dusen, M.S. Bur. Stand. J. Res. 1933, 10, 301.
- 2. Giauque, W.F.; Egan, C.J. J. Chem. Phys. 1937, 5, 45.
- Clark, A.M.; Din, F.
   Trans. Faraday Soc. 1950, 46, 901.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbon dioxide; CO <sub>2</sub> ; [123-38-9]	Bratzler, K. D.; Doerges, A.; Herbert, W.
(2) Various solvents. See table below.	German Patent No. 1,769,197 to Metallgesellschaft AG 6000 Frankfurt, FRG 1971, Oct 21
VARIABLES:	PREPARED BY:
T/K = 293 $p_1/kPa = 101.3$	H. L. Clever
EXPERIMENTAL VALUES:	
Coefficient Co	Ostwald Mol Fraction Defficient L/m <sup>3</sup> m <sup>-3</sup> × <sub>1</sub>
Water; H <sub>2</sub> O; [7732-18-5] 20 0.88	0.94 0.00071
Methanol; CH <sub>4</sub> O; [67-56-1] 20 3.5	3.7 <sub>5</sub> 0.0063
1,2,3,4-Tetrahydronaphthale 20 1.3	ne or tetralin; C <sub>10</sub> H <sub>12</sub> ; [119-64-2] 1.4 0.0079
Dimethylbenzene or xylene; 20 2.0	C <sub>8</sub> H <sub>10</sub> ; [1330-20-7] 2.1 <sub>5</sub> 0.011
4-Methyl-1,3-dioxolane-2-on C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> ; [108-32-7] 20 3.8	ne or propylene carbonate; 4.1 0.014
1-Methylpyrrolidinone; C <sub>5</sub> H <sub>9</sub> 20 4.0	NO; [872-50-4] 4.3 0.017
Hexamethylphosphoric triami 20 4.9	de; [(CH <sub>3</sub> ) <sub>2</sub> N] <sub>3</sub> PO; [680-31-9] 5.2 <sub>5</sub> 0.037
The Ostwald coefficient and were calculated by the compi	
AUXILIARY I	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing specified.	Nothing specified.
	ESTIMATED ERROR:
	Nothing specified.
	REFERENCES:

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Krauss, W.; Gestrich, W. Chem. - Tech (Heidelberg) 1977, 6, 2. 1,2,3,4- Tetrahydronaphthalene (Tetralin); C<sub>10</sub>H<sub>12</sub>; [119-64-2] 513-6. VARIABLES: PREPARED BY: C.L. Young T/K = 283.15-313.15EXPERIMENTAL VALUES: Mole fraction of Solubility, S<sup>+</sup>/mol dm<sup>-3</sup> bar<sup>-1</sup> carbon dioxide in T/Kliquid, x<sub>CO</sub>, 0.00895 283.15 0.06589 293.15 0.05795 0.00794 0.05140 0.00710 303.15 313.15 0.04595 0.00640 + at a partial pressure of 101.325 kPa. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus in which gas was dissolved in liquid in glass cell. Pressure measured. No details given. Amount of gas dissolved estimated from pressure measurements when gas was repeatedly expanded into known volume. Details in source. Values of solubility calculated from equations and graphs in original. ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta x_{\text{CO}_2} = \pm 1-2$ % REFERENCES:

# COMPONENTS: ORIGINAL MEASUREMENTS: [124-38-9] 1. Carbon dioxide; CO2; Horvath, M. J.; Sebastian, H. M.; Chao, K.-C. 2. 1,2,3,4-Tetrahydronaphthálene Ind. Eng. Chem. Fundam. (tetralin); C10H12; 1981, 20, 394-396. [119-64-2] VARIABLES: PREPARED BY: T/K = 300C. L. Young $P/kPa \simeq 101.3$ EXPERIMENTAL VALUES: Mole fraction of Henry's constant carbon dioxide in liquid, T/K/atm xco, 300 0.00691 144 † at a partial pressure of carbon dioxide of 1 atmosphere calculated by compiler assuming $\phi = 0.995$ . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Gas chromatographic analysis of a 1. No details given. saturated solution at barometric 2. Purity 99.06 mole per cent. pressure. Henry's constants determined from formula $H = (p - p_o)\phi(m + 1)/m$ where p is the total pressure, $p_{\bullet}$ the vapor pressure of the solvent and $\phi$ is the fugacity coefficient of ESTIMATED ERROR: $\delta T/K = \pm 0.25$ ; $\delta H/atm = \pm 3$ % The mole ratio, m, is the gas. (estimated by compiler). defined by Moles of carbon dioxide REFERENCES: in gas phase m = Moles of carbon dioxide in liquid phase

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Methyl-4-(1-Methylethenyl)cyclohexene or d-limonene or carvene; C<sub>10</sub>H<sub>16</sub>; [138-86-3]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

Mol Fraction	Bunsen	Ostwald
10 <sup>2</sup> x <sub>1</sub>	Coefficient α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm³cm-3
1.37	1.93	2.034
1.27	1.79	1.921
1.18	1.65	1.802
	$\frac{10^2 x_1}{1.37}$ 1.27	$ \begin{array}{ccc} 10^2 x_1 & & \text{Coefficient} \\ \hline 1.37 & & \text{1.93} \\ 1.27 & & \text{1.79} \\ \end{array} $

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1-Methyl-4-(1-Methylethenyl)cyclohexene. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic Hydrocarbons

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

Solubility of carbon dioxide in aromatic hydrocarbons

Solubility in benzene at pressures below 200 kPa has been studied by at least ten groups (1-10). Limiting values of Henry's constant from high pressure data published by Kaminishi et al.(11) can also be used to estimate the mole fraction solubility at lower pressures. Values of mole fraction solubility at a partial pressure of 101.3 kPa from the available data are not very consistent. Values for 283.2 K range from 0.0107 to 0.01208 and values for 293.2 K range from 0.0091 to 0.0099 with a value of 0.0105 at 293.6 K. There is better agreement at other temperatures. Over the whole temperature range the values of mole fraction solubility at a partial pressure of 101.3 kPa, based on (1-10), fit the equation given below.

$$\ln x_{CO_2} = -18.437 + 1296.5/(T/K) + 1.6511ln(T/K)$$

temperature range = 283.2-313.2 Kstandard deviation in  $x_{CO_2} = 0.00037$ 

At least ten groups (1,2,4,6,8,12-16) have measured solubility of carbon dioxide in methylbenzene at pressures below 200 kPa. There is, in general, good agreement between values for mole fraction solubility in this solvent at a partial pressure of 101.3 kPa. However the solubility at 193.2 K reported by Williams seems to be too low. Values of the mole fraction solubility at a partial pressure of 101.3 kPa from other measurements by Williams and by other workers fit the equation below.

$$\ln x_{CO_2} = -13.921 + 1547.7/(T/K) + 0.72764ln(T/K)$$

temperature range = 203.2-316.2 Kstandard deviation in  $x_{CO_2} = 0.00128$ 

Three groups (1,9,17) measured solubility in 1,2-dimethylbenzene. Values of mole fraction solubility at a partial pressure of 101.3 kPa are consistent with each other and fit the equation below.

$$\ln x_{CO_2} = -52.371 + 3066.3/(T/K) + 6.57571n(T/K)$$

temperature range = 253.2-313.2standard deviation in  $x_{CO_2}$  = 0.00016

Six groups (1,4,6,8,9,17) measured solubility in 1,3-dimethylbenzene. Again there is good consistency between different sets of data. Values of mole fraction solubility fit the following equation

$$\ln x_{CO_2} = -49.384 + 2960.3/(T/K) + 6.1263ln(T/K)$$

temperature range = 233.2-313.1 K standard deviation in  $x_{CO_2}$  = 0.00015

Solubility in 1,4-dimethylbenzene was measured at 293.15 K by Rosenthal (9) and by Piskovsky and Lakomy (1). Byrne et al.(17) measured the solubility at 313.13 K, 298.12 K and three temperatures between 288 K and 289 K. Values of mole fraction solubility at a partial pressure of 101.3 kPa are consistent with each other but the temperature range is small in comparison with measurements of the solubility in the other two isomers of dimethylbenzene. These values fit the following equation

$$\ln x_{CO_2} = -247.112 + 11816.1/(T/K) + 35.617ln(T/K)$$

temperature range = 288.2-313.1standard deviation in  $x_{CO_2} = 0.00021$ 

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic Hydrocarbons

### EVALUATOR:

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

Mole fraction solubilities at a partial pressure of 101.3 kPa at 293.15 K from smoothing equations for the three isomers are as follows:

1,2-dimethylbenzene 0.0105 1,3-dimethylbenzene 0.0113 1,4-dimethylbenzene 0.0114

Bratzler et al.(18) have published the Bunsen coefficient for a mixture of isomers of dimethylbenzene at 293 K. The corresponding mole fraction solubility at a partial pressure of 101.3 kPa is 0.011. The mole fraction solubility in a mixture of isomers at 293.15 K and 101.3 kPa from measurements by Vitovec (19) is 0.0109. These values are consistent with the values for the individual isomers.

Solubility in ethylbenzene has been measured by Piskovsky and Lakomy (1) from 198.2 K to 293.2 K and by Luhring and Schumpe (8) at 293.2 K. Piskovsky's measurements are self consistent. The mole fraction solubility at 293.2 K and a partial pressure of 101.3 kPa from Piskovsky's measurements is 0.0108 compared with Luhring's value of 0.01022. Values from the two sources fit the equation

$$\ln x_{CO_2} = -52.108 + 3033.9/(T/K) + 6.5525ln(T/K)$$

temperature range = 198.2-293.2 Kstandard deviation in  $x_{CO_2} = 0.00049$ 

Just (6) reported the solubility of carbon dioxide in (1-methylethyl)- . benzene at temperatures from 288.15 K to 298.15 K. Values of mole fraction solubility are close to those for ethylbenzene but no other data on this solvent are available for comparison.

Luhring and Schumpe (8) reported a Henry's constant for solubility in 1,2,4-trimethylbenzene at 293.2 K. This corresponds to a mole fraction solubility of 0.01125 at a partial pressure of 101.3 kPa which is close to values for solubility in the dimethylbenzenes under these conditions. No other measurements of the solubility in this solvent are available for comparison.

Tremper and Prausnitz (20) have published Henry's constants for 1,1'-methylenebisbenzene for 300 K to 475 K. Horvath et a1.(4) published a Henry's constant for 300 K of 124 atm. This is very close to Tremper's value of 123 atm. Mole fraction solubilities for a partial pressure of 101.3 kPa calculated from Henry's constants in the two papers fit the equation below.

$$\ln x_{CO_2} = -37.246 + 2368.7/(T/K) + 4.3008 \ln(T/K)$$

temperature range = 300-475 Kstandard deviation in  $x_{\text{CO}_2}$  =  $6.2 \times 10^{-5}$ 

Measurements by Glazunova (21) show that the mole fraction solubility in 1,1'-methylenebis(methylbenzene) in the temperature range 293 K to 393 K is greater than that in 1,1'-methylenebisbenzene under the same conditions. Mole fraction solubility in methylbenzene is greater than that in benzene under similar conditions. No other measurements of the solubility in 1,1'-methylenebis(methylbenzene) are available for comparison. Glazunova's measurements fit the equation given below. This equation can only be accepted on a tentative basis.

$$\ln x_{CO_2} = -8.3777 + 1156.2/(T/K)$$

temperature range = 293-393 K standard deviation in  $x_{CO_2} = 0.00019$ 

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic Hydrocarbons

### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

The solubility of carbon dioxide in (1-methylethyl)-1,1'-biphenyl has been measured to high pressures at 293.2 K, 373.2 K and 473.2 K by Bogdanov (22). The mole fraction solubility at 293.2 K and a partial pressure of 101.3 kPa is approximately 0.0113. No measurements by other authors are available for comparison.

Horvath et al.(4) have found a Henry's constant of 151 atm for dissolution in 1-methylnaphthalene at 300 K. Chai and Paulaitis (23) reported Henry's constants at temperatures from 298.6 K to 330.2 K. The interpolated value at 300 K is 151.4, close to the value reported by Horvath. Mole fraction solubilities calculated from Henry's constants published by the two groups fit the equation

$$\ln x_{CO_2} = -1.8516 + 759.73/(T/K) - 0.99967 \ln(T/K)$$

temperature range = 298.6-311.0standard deviation in  $x_{CO_2} = 3.4 \times 10^{-5}$ 

A selection of mole fraction solubilities in aromatic hydrocarbons is shown in Table 1 and Fig 1.

- 1. Piskovsky, L.; Lakomy, J. Chem. Prumys1. 1965, 15, 745-746.
- 2. Krauss, W.; Gestrich, W. Chem.-Tech. (Heidelberg) 1977, 6, 513-516.
- Patyi, L.; Furmer, I.E.; Makranczy, J.; Sadilenko, A.S.; Stepanova, Z.G.; Berengarten, M.G. Zh. Prikl. Khim. 1978, 51, 1296-1300.
- Horvath, M.J.; Sebastian, H.M.; Chao, K.-C. Ind. Eng. Chem. Fundam. 1981, 20, 394-396.
- 5. Gjaldbaek, J.H. Acta Chem. Scand. 1953, 7, 537-544.
- 6. Just, G. Z. Phys. Chem. 1901, 37, 342-367.
- Byrne, J.E.; Battino, R.; Danforth, W.F. J. Chem. Thermodyn. <u>1974</u>, 6, 245-250.
- 8. Luhring, P.; Schumpe, A. J. Chem. Eng. Data 1989, 34, 250-252.
- 9. Rosenthal, W. Thes. Fac. Sci. Univ. Strasbourg (France) 1954.
- 10. Koudelka, L. Chem. Zvesti 1964, 18, 178-185.
- 11. Kaminishi, G-I.; Yokoyama, C.; Takahashi, S. Fluid Phase Equilibria 1987, 34, 83-99.
- 12. Williams, D.L. U.S. Atomic Energy Commission Report LA-1484, 1952.
- 13. Gjaldbaek, J.C.; Andersen, E.K. Acta Chem. Scand. 1954, 8, 1398-1413.
- Field, L.R.; Wilhelm, E.; Battino, R. J. Chem. Thermodyn. 1974, 6, 237-243.
- 15. Chen, H.; Liu, M.; Zheng, L. Zhejiang Daxue Xuebao 1985, 19(1), 140-148.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic Hydrocarbons

### EVALUATOR: .

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

- Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P. Khim. Prom. 1960, (5), 18-22.
- 17. Byrne, J.E.; Battino, R.; Wilhelm, E. J. Chem. Thermodyn. <u>1975</u>, 7, 515-522.
- Bratzer, K.D.; Doerges, A.; Herbert, W. German Patent No. 1 769 197 to Metallgesellschaft AG, 1971.
- 19. Vitovec, J. Collect. Czech. Chem. Comm. 1968, 33, 1203-1310.
- 20. Tremper, K.K.; Prausnitz, J.M. J. Chem. Eng. Data 1976, 21, 295-299.
- 21. Glazunova, T.V.; Ryabov, M.I.; Lipshtein, R.A. Sov. At. Energ. <u>1987</u>, 62, 449-451.
- 22. Bogdanov, F.F. Issled. Teploprovodnosk. Inst. Telo. Mesoobmena Akad. Nauk. Beloruss. S.S.R. 1967, 230-236.
- 23. Chai, C-P.; Paulaitis, M.E. J. Chem. Eng. Data 1981, 26, 277-279.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic Hydrocarbons

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

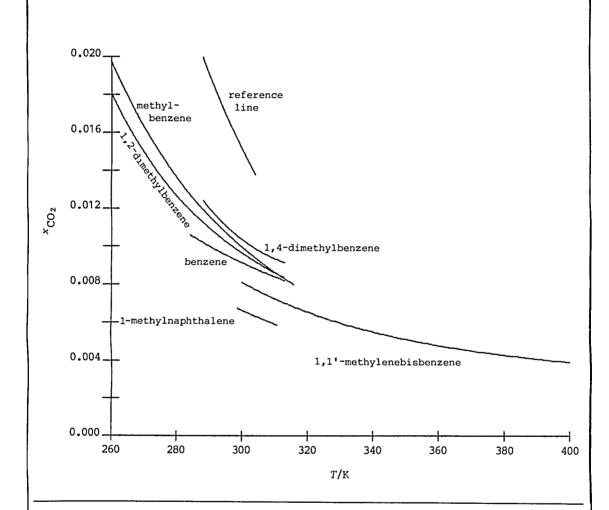


Fig. 1 Mole fraction solubility of carbon dioxide in various aromatic hydrocarbons at a partial pressure of gas of 101.3 kPa.

The curves showing the variation of solubility with temperature correspond to equations derived by the evaluator.

A reference line corresponding to values from the Raoult's law equation is also shown.

COMPONENTS:	EVALUATOR:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London,
2. Aromatic Hydrocarbons	Holloway Road, London, N7 8DB, U.K.
	July 1991

CRITICAL EVALUATION:

Table 1. Mole fraction solubilities of carbon dioxide at a partial pressure of 101.3 kPa in aromatic hydrocarbons.

Solvent	T/K	<sup>x</sup> co₂	Reference
Benzene	293.15 298.15	0.00969 ±0.00038 0.00926 ±0.00038	*
Methylbenzene	293.15 298.15	0.01102 ±0.00128 0.01021 ±0.00128	*
1,2-Dimethylbenzene	293.15 298.15	0.01050 ±0.00016 0.00984 ±0.00016	* *
1,3-Dimethylbenzene	293.15 298.15	0.01129 ±0.00015 0.01057 ±0.00015	* *
1,4-Dimethylbenzene	293.15 298.15	0.01138 ±0.00021 0.01057 ±0.00021	* *
1,2,4-Trimethylbenzer	ne 293.15	0.01125	8
Ethylbenzene	293.15 298.15	0.01072 ±0.00049 0.01006 ±0.00049	* *
(1-Methylethyl)benzer	ne 298.15	0.0101	6
1,1'-Methylenebisben	zene 298.15	0.00825 ±0.00006	*
1,1'-Methylenebis(me	thylbenze 293.15 298.15	ne) 0.01165 0.01111	21 21 †
1-Methylnaphthalene	298.15	0.00674 ±0.00003	*

 $<sup>\</sup>ensuremath{^{*}}$  from the equation given by the evaluator on a previous page  $\ensuremath{^{\dagger}}$  interpolated

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm $^{-1}$	Coefficient L/cm3cm-3
288.15	10.03	2.57	2.710
293.15	9.30	2.37	2.540
298.15	8.79	2.22	2.425

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Benzene. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. H.

Acta Chem. Scand. 1953, 7, 537 - 544.

# VARIABLES:

$$T/K = 293.55 - 307.35$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

J. Chr. Gjaldbaek

### EXPERIMENTAL VALUES:

Carbon Dioxide Pressure p <sub>1</sub> /mmHg	Mol Fraction <sup>1</sup> 10 <sup>3</sup> x <sub>1</sub>	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
714.2	10.6	2.65	2.85
556.6	10.5	2.62	2.82
656.1	9.76	2.43	2.65
663.5	9.42	2.33	2.58
609.4	8.82	2.17	2.44
	Dioxide Pressure p <sub>1</sub> /mmHg 714.2 556.6 656.1 663.5	Dioxide Pressure $p_1/\text{mmHg}$ $10^3 x_1$ $p_1/\text{mmHg}$ $10.6$ $10.5$	Dioxide Pressure $p_1/\text{mmHg}$

Mole fraction solubility values adjusted to a gas partial pressure of 101.325 kPa (1 atm) by the compiler.

Smoothed Data: For use between 293.55 and 307.35 K.

 $\ln x_1 = -8.4548 + 11.4497/(T/100 K)$ 

The standard error about the regression line is  $1.09 \times 10^{-4}$ .

T/K	Mol Fraction 103x1
293.15	10.58
298.15	9.91
303.15	9.30
308.15	8.75

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as confining liquid. The solvent was degassed in the apparatus.

The absorbed volume of gas is calculated from the initial and final amounts, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury.

The mole fraction solubility values are at 1 atm assuming Henry's law is obeyed.

Details of the apparatus and procedure are given in ref. 1 and 2.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate (analytical reagent) and concentrated sulfuric acid. 99.9 per cent CO<sub>2</sub>.
- (2) Benzene. Merck and Co.
  Analytical reagent. M.p./°C =
  5.43, b.p. (760 mmHg)/°C = 80.28.

## ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic hydrocarbons

### ORIGINAL MEASUREMENTS:

Piskovsky, L.; Lakomy, J.

Chem. Prumys1. 1965, 15, 745-746.

### VARIABLES:

T/K = 198-293P/kPa = 101.3

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	T/K	Kuenen coefficient <sup>†</sup>	x <sub>CO<sub>2</sub></sub> at P <sub>CO<sub>2</sub></sub> = 101.3 kPa*
Benzene	283.15	3.15	0.0109
C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	293.15	2.61	0.0091
Methylbenzene C <sub>7</sub> H <sub>8</sub> ; [108-88-3]	198.15 213.15 233.15 253.15 273.15 283.15 293.15	36.32 17.73 9.07 5.49 3.67 3.10 2.64	0.1307 0.0684 0.0362 0.0222 0.0150 0.0127 0.0108
1,2-Dimethylbenzene C <sub>8</sub> H <sub>10</sub> ; [95-47-6]	253.15	4.47	0.0209
	263.15	3.63	0.0170
	273.15	3.00	0.0141
	283.15	2.53	0.0119
	293.15	2.17	0.0102

<sup>†</sup> The Kuenen coefficient is defined as the volume of gas, reduced to 273.15 K and 101.325 kPa, dissolved by one gram of solvent when the partial pressure of the gas is 101.325 kPa.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The volume of gas dissolved in a weighed quantity of solvent in an absorption vessel was measured by use of a gas buret. The temperature of the absorption vessel was controlled by an alcohol bath to which solid carbon dioxide could be added as required. The vessel was shaken until equilibrium was reached.

# SOURCE AND PURITY OF MATERIALS:

 Obtained from solid carbon dioxide.

# ESTIMATED ERROR:

 $\delta$ (Kuenen coeff.) = ±0.67% (authors)

<sup>\*</sup> calculated by the compiler

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Aromatic hydrocarbons

### ORIGINAL MEASUREMENTS:

Piskovsky, L.; Lakomy, J.

Chem. Prumys1. 1965, 15, 745-746.

# EXPERIMENTAL VALUES:

Solvent	т/к	Kuenen coefficient <sup>†</sup>	x <sub>CO<sub>2</sub></sub> at P <sub>CO<sub>2</sub></sub> = 101.3 kPa*
1,3-Dimethylbenzene C <sub>8</sub> H <sub>10</sub> ; [108-38-3]	233.15 243.15 253.15 263.15 273.15 283.15 293.15	8.09 6.20 4.88 3.94 3.26 2.75 2.35	0.0372 0.0287 0.0228 0.0185 0.0153 0.0130
1,4-Dimethylbenzene; C <sub>8</sub> H <sub>10</sub> ; [106-42-3]	293.15	2.38	0.0112
Ethylbenzene C <sub>8</sub> H <sub>10</sub> ; [100-41-4]	198.15 213.15 233.15 253.15 273.15 283.15 293.15	27.92 14.22 7.48 4.58 3.11 2.65 2.29	0.1176 0.0635 0.0345 0.0214 0.0146 0.0125 0.0108

 $<sup>^\</sup>dagger$  The Kuenen coefficient is defined as the volume of gas, reduced to 273.15 K and 101.325 kPa, dissolved by one gram of solvent when the partial pressure of the gas is 101.325 kPa.

<sup>\*</sup> calculated by the compiler

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

# ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Danforth, W. F.

J. Chem. Thermodyn. 1974, 6, 245-250.

### VARIABLES:

T/K: 310.65

P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction 10 <sup>3</sup> x 1	Bunsen Coefficient α/cm³(STP)cm-3 atm-1	Ostwald Coefficient L/cm³cm-3
310.64	8.07	2.008	2.284 2.283
310.69	8.07	2.007	

The mole fraction and Bunsen coefficient values were calculated by the compiler assuming ideal gas behavior.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm³ of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid nitrogen trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum purity is 99.8 mole per cent.
- (2) Benzene. J. T. Baker Analyzed Reagent Grade. 99.9 mole per cent, thiophene free.

ESTIMATED ERROR:  $\delta T/K = 0.01$ 

 $\delta P/\text{mmHg} = 0.5$ 

 $\delta L_{0}/L_{0} = 0.01$ 

 $\delta L_{w}/L_{w} = 0.02$ 

- 1. Morrison, T. J.; Billett, F.
- J. Chem. Soc. 1948, 2033.
   Battino, R.; Evans, F. D.; Danforth, W.F.
   J.Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

# COMPONENTS: ORIGINAL MEASUREMENTS: Krauss, W.; Gestrich, W. 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2] Chem.-Tech. (Heidelberg), 1977, 6, 513-6. VARIABLES: PREPARED BY: T/K = 283.15-313.15C.L. Young EXPERIMENTAL VALUES: Mole fraction of carbon dioxide in Solubility, S/mol dm<sup>-3</sup> bar<sup>-1</sup> T/Kliquid, $x_{\text{CO}_2}$ 0.1220 0.0107 283.15 293.15 0.1088 0.00970 303.15 0.09779 0.00883 0.08848 0.00810 313.15 + at a partial pressure of 101.325 kPa. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus in which gas was dissolved in liquid in glass cell. Pressure measured. Amount of gas dissolved estimated No details given. from pressure measurements when gas was repeatedly expanded into known volume. Details in source. Values of solubility calculated from equations and graphs in original. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta x_{CO_2} = \pm 1-2$ % REFERENCES:

102		
COMPONENTS:		ORIGINAL MEASUREMENTS:
	cide; CO <sub>2</sub> ; [124-38-9]	Patyi, L.; Furmer, I. E.; Makranczy, J.; Sadilenko, A. S.; Stepanova, Z. G.; Berengarten, M. G.
,		Zh. Prikl. Khim. <u>1978</u> , 51, 1296- 1300.
VARIABLES:		PREPARED BY:
T/K = 29	8.15	C. L. Young
EXPERIMENTAL VALU	JES:	
T/K	α†	Mole fraction of carbon dioxide at a partial pressure of 101.325 km $^x$ CO <sub>2</sub>
298.15	2.23	0.00888
	AUXILIAR	INFORMATION
METHOD/APPARATUS	/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
were added, in known amount of known dimester were made for	thod. Pressure known amounts of gas n increments, to a of liquid in a vessel nsions. Corrections the partial pressure Details in ref. (1).	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:

1. Bodor, E.; Bor, G. J.; Mohai, B.; Sipos. G. Veszpremi. Vegyip. Egy. Kozl. <u>1957</u>, *1*, 55.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]</li> </ol>	Horvath, M. J.; Sebastian, H. M.; Chao, KC.  Ind. Eng. Chem. Fundam.  1981, 20, 394-396.
VARIABLES: T/K = 300 P/kPa ≃ 101.3	PREPARED BY:  C. L. Young

EXPERIMENTAL VALUES:

Mole fraction of carbon dioxide in liquid,
/atm \*\*CO2 †\*

300 109 0.0091

 $^{\dagger}$  at a partial pressure of carbon dioxide of 1 atmosphere calculated by compiler assuming  $\phi$  = 0.995.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula

$$H = (p - p_o)\phi(m + 1)/m$$

where p is the total pressure,  $p_o$  the vapor pressure of the solvent and  $\phi$  is the fugacity coefficient of the gas. The mole ratio, m, is defined by

 $m = \begin{array}{c} \text{Moles of carbon dioxide} \\ \underline{\text{in gas phase}} \\ \underline{\text{Moles of carbon dioxide}} \\ \text{in liquid phase} \end{array}$ 

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Purity stated as "∿ 100%".

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.25$ ;  $\delta P/\text{atm} = \pm 3\%$  (estimated by compiler).

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Benzene, C<sub>6</sub>H<sub>6</sub>; [71-43-2] VARIABLES: T/K = 273.15-303.15 P/MPa = 0.826-5.688 ORIGINAL MEASUREMENTS: Kaminishi, G-I.; Yokoyama, C.; Takahashi, S. Fluid Phase Equilibria, 1987, 34, 83-99. PREPARED BY: PREPARED BY:

### EXPERIMENTAL VALUES:

T/K	Henry's la H/MPa	aw constant H/kPa	Mole fraction ${}^{x}_{CO_{2}}$ at ${}^{p}_{CO_{2}}$ = 101.3kPa $^{*}$
283.15	8.39	8390	0.01208
298.15	10.37	10370	0.00977
303.15	11.06	11060	0.00916

$$H = \begin{bmatrix} f_1 \\ x_1 \to 0 \end{bmatrix}$$

$$x_1 = x_{CO_2}$$
;  $f_1 = \text{fugacity of } CO_2$ 

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Apparatus able to withstand pressures to 20 MPa was used to determine phase equilibria by the bubble point method. Henry's constants at zero pressure were obtained from the experimental data by using the method described by Prausnitz and Chueh (1)

### SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Showa Tansan Industry Co., Ltd; purity better than 99.9%
- Supplied by Merck Co. Ltd; purity better than 99.7%

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$  (authors)  $\delta P/kPa = \pm 0.1$ 

# REFERENCES:

 Prausnitz, J.M.; Chueh, P.L. Computer Calculations for High Pressure Vapor-Liquid Equilibria, Prentice-Hall, Englewood Cliffs, USA, 1968.

 $<sup>^*</sup>$  taken by the compiler to be given approximately by  $^P{}_{\mathrm{CO}_2}/H{}$ 

	105		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9] 2. Benzene and methylbenzenes	Luhring, P.; Schumpe, A. <i>J. Chem. Eng. Data</i> , 1989, 34, 250-252.		
VARIABLES:	PREPARED BY:		
T/K = 293.2	C.L. Young		
EXPERIMENTAL VALUES:			
T/K Henry's Constant /(Pa m³/mol <sup>-1</sup> )	* Mole fraction of CO <sub>2</sub> at 1 atm partial pressure		
Benzene; C <sub>6</sub>	H <sub>6</sub> ; [71-43-2]		
293.2 946	0.009518		
Methylbenzene, (toluene); $C_7H_8$ ; [108-88-3]			
293.2 965	0.009080		
1,3-Dimethylbenzene, (m-xylene); C <sub>8</sub> H <sub>10</sub> ; [108-38-3]			
293.2 1067	0.01167		
1,2,4-Trimethylben	nzene; C <sub>9</sub> H <sub>12</sub> ; [95-63-6]		
293.2 1251	0.01125		
Ethylbenzene; C <sub>8</sub> H <sub>10</sub>	; [100-41-4]		
293.2 1124	0.01022		
*referred to as Henry's constant in Henry's constant multiplied by 'calculated by compiler using dens	molar volume.		
AUXILIARY IN	FORMATION		
METHOD/APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:		
Little infomation given in source. Method consisted of equilibrating known amounts of degassed liquid angas and measuring the change in pressure. Equilibration was reached in 3 to 6 minutes. Some details given in ref			

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  (authors)  $\delta x/x = \pm 0.01$  to 0.15 (compiler)

- Riddick, J.A.; Bunger, W.B.;1970 Organic Solvents, Wiley-Interscience, New York.
   Schumpe, A.; Quiker, G.; Decker, W.D. Adv. Biochem. Eng., 1982, 24, 1.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Methyl benzene or toluene;  $C_7H_8$ ; [108-88-3]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. <u>1901</u>, 37, 342 - 367.

### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^3 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	11.30	2.42	2.557
293.15	10.61	2.26	2.426
298.15	9.97	2.11	2.305

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Methyl benzene. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]

2. Methylbenzene (Toluene); C7H8; [108-88-3]

Williams, D. L.

U.S. Atomic Energy Commission Report LA-1484, 1952.

VARIABLES:

$$T/K = 193.2-273.2$$
  
 $P/kPa = 78.1-78.5$ 

PREPARED BY:

C. L. Young

EXPERIMENTA	L V	AT.	UES:
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DVI DKITIDKILI	. VALUES.			
t/°C	T/K	Total pressure /mmHg	Observed Solubility cm³ (NTP)/ g solvent	Solubility at 760 mmHg total pressure cm <sup>3</sup> (NTP)/ g solvent
) o	273.2	588.6	2.95	3.81
-10	263.2	586.1	3.57	4.62
-20	253.2	588.8	4.34	5.60
-30	243.2	588.2	5.34	6.90
-40	233.2	589.1	6.82	8.80
-50	223.2	587.4	8.53	11.04
-60	213.2	587.8	12.34	15.96
-70	203.2	587.2	15.81	20.46
-80	193.2	588.2	17.25	22.27

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Toluene admitted to absorption flask. Amount determined by Carbon dioxide disweighing. solved in toluene, amount added being measured volumetrically. Contents of absorption flask stirred with magnet enclosed in Pressure measured with glass. mercury manometer.

### SOURCE AND PURITY OF MATERIALS:

- 1. Dried with anhydrous calcium chloride.
- 2. Merck research grade, dried and redistilled. Degassed.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/\text{mmHg} = \pm 0.2$ ;  $\delta x_{\mathrm{CO}_2}$  = ±2% (estimated by compiler).

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Methylbenzene or toluene; C<sub>7</sub>H<sub>8</sub>; [108-88-3]

### ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

J. Chr. Gjaldbaek

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2 x_{1}$	Bunsen Coefficient α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	1.05 1.05	2.22 2.20	2.42 2.40

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1,2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO<sub>2</sub>.
- (2) Methylbenzene. Riedel-de-Haën.
  Analytical reagent. Fractionated
  by distillation. B.p.
  (760 mmHg)/°C = 110.75 110.80,
  refractive index n<sub>D</sub>(25.1°C) =
  1.4936 1.4938.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. 1930, 52, 68.
- 2. Gjaldbaek, J. C.

  Acta Chem. Scand. 1952, 6, 623.

- Carbon dioxide; CO2; [124-38-9]
- 2. Methanol; CH<sub>4</sub>O; [67-56-1] 2-Butanone; C<sub>4</sub>H<sub>8</sub>O; [78-93-3] Acetic acid, ethyl ester, (ethyl acetate); C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>; [141-78-6] Methylbenzene, (toluene); C7H8; [108-88-3]

### ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Khim. Prom. 1960, (5), 18-22.

### VARIABLES:

T/K = 228-248P/kPa = 101-1621 PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	T/K	H*/atm	Henry's H*/kPa§	constant, H**/atm	H H**/kPa§	<sup>x</sup> CO <sub>2</sub> at <sup>P</sup> CO <sub>2</sub> = 101.3 kPa†
Methanol¶	248.0	42.2	4276	41.5	4205	0.0241
	238.2	29.5	2989	27.5	2786	0.0364
	228.1	20.9	2118	19.8	2006	0.0505
2-Butanone	248.0	15.7	1591	15.3	1550	0.0654
	238.2	11.5	1165	11.6	1175	0.0862
	228.1	8.0	811	7.7	780	0.1299
Ethyl acetate	248.0	12.2	1236	12.3	1246	0.0813
	238.2	9.1	922	9.0	912	0.1111
	228.1	6.3	638	6.2	628	0.1613
Methylbenzene	248.0	41.4	4195	40.5	4104	0.0247
	238.2	33.2	3364	32.3	3273	0.0310
	228.1	24.8	2513	23.7	2401	0.0422

Values of Henry's constant based upon measurements made in the pressure range 101-1621 kPa and calculated by a graphical method from the relationship

 $RT\ln(f_2/x_2) = RT\ln H + \int \overline{V}_2 dP - Ax_2$ 

where  $f_2$  is the fugacity of the carbon dioxide at pressure P

 $\overline{V}_2$  is the partial molar volume of carbon dioxide at infinite dilution H is equal to the limiting value of  $P_2/x_2$  at  $P_2=0$ ; A is a constant.

- \*\* Values of Henry's constant based upon measurements of the solubility of carbon dioxide at a partial pressure of 101.3 kPa. † calculated by the compiler and equal to the reciprocal of  $H^{**}/atm$

§ calculated by the compiler

¶ the authors used data for methanol which they had published earlier (1).

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A static method was used. A compressure) section of the A glass apparatus was connected to a high pressure section made of metal. Carbon dioxide in the low pressure section was allowed to condense in a cooled metal bulb in the high pressure section. The quantity of gas collected was found from pressure changes in the glass section. The valve connecting the two section was then closed and the condensed gas allowed to evaporate

SOURCE AND PURITY OF MATERIALS: No information

# ESTIMATED ERROR

 $\delta x_{\text{CO}_2} = \pm 5\% \text{ (compiler)}$ 

### REFERENCES:

1. Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P. Khim. Prom. 1959, (4), 328.

to generate the required pressure and to come in contact with the solvent under test which was held in an absorption cell in a thermostat bath. cell was stirred magnetically. The quantity of unabsorbed gas when equilibrium was reached was calculated from the final pressure and volume of the gas in the high pressure section.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Methylbenzene or toluene;  $C_7H_8$ ; [108-88-3]

# ORIGINAL MEASUREMENTS:

Field, L. R.; Wilhelm, E.; Battino, R.

J. Chem. Thermodyn. 1974, 6, 237 - 243.

### VARIABLES:

*T*/K: 283.67 - 313.24 P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2 x_7$	Bunsen Coefficient a/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm3cm-3
283.67	1.257	2.71	2.816
298.43 313.24	1.013 0.861	2.15 1.79	2.343 2.054

The gas solubility values were adjusted to a  $\rm CO_2$  partial pressure of 101.325 kPa (1 atm) by Henry's law.

The Bunsen coefficients were calculated by the compiler.

Smoothed Data: For use between 283.15 and 313.24 K.

$$\ln x_1 = -8.3963 + 11.3873/(T/100 K)$$

The standard error about the regression line is 1.48 x 10-4.

T/K	Mol Fraction 10 <sup>2</sup> x <sub>1</sub>
283.15	1.259
293.15	1.098
298.15	1.029
303.15	0.966
313.15	0.857

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Up to 500 cm3 of solvent Degassing. is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is applied intermittently through a liquid N2 trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Either Matheson Co., Inc. or Air Products and Chemicals, Inc. Purest grade available, minimum purity greater than 99 mole per cent.
- (2) Methylbenzene. Phillips Petroleum. Pure Grade. Distilled.

### ESTIMATED ERROR:

 $\delta T/K = 0.03$  $\delta P/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.005$ 

- REFERENCES: 1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO<sub>2</sub>; [124-38-9] Krauss, W.; Gestrich, W. Chem.-Tech. (Heidelberg), 1977, 6, Methylbenzene, (Toluene), C7H8; [108-88-3] 513-6. VARIABLES: PREPARED BY: C.L. Young T/K = 283.15-313.15EXPERIMENTAL VALUES: Mole fraction of Solubility<sup>+</sup>, S/mol dm<sup>-3</sup> bar<sup>-1</sup> carbon dioxide in T/Kliquid, x 283.15 0.1262 0.0133 0.1087 0.0113 293.15 0.09461 0.0102 303.15 313.15 0.08305 0.00906 at a partial pressure of 101.325 kPa. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus in which gas was dissolved in liquid in glass cell. Pressure measured No details given. Amount of gas dissolved estimated from pressure measurements when gas was repeatedly expanded into known volume. Details in source. Values of solubility calculated from equations and graphs in original. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta x_{CO_2} = \pm 1-2%.$ REFERENCES:

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Horvath, M. J.; Sebastian, H. M.; Chao, K.-C. 2. Methylbenzene, (toluene); C7H8; Ind. Eng. Chem. Fundam. [108-88-3] 1981, 20, 394-396. VARIABLES: PREPARED BY: T/K = 298 or 300C. L. Young P/kPa = 101.3EXPERIMENTAL VALUES:

Т/К	Henry's constant /atm	Mole fraction of carbon dioxide in liquid, ${}^x{\text{CO}}_2$
298	102	0.0098
300	106	0.0094

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Gas chromatographic analysis of a saturated solution at barometric Henry's constants deterpressure. mined from formula

$$H = (p - p_0)\phi(m + 1)/m$$

where p is the total pressure,  $p_o$ the vapor pressure of the solvent and  $\phi$  is the fugacity coefficient of ESTIMATED ERROR: the gas. The mole ratio, m, is defined by

Moles of carbon dioxide  $m = \frac{\text{in gas phase}}{\text{Moles of carbon dioxide}}$ in liquid phase

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Purity stated as "∿ 100%".

 $\delta T/K = \pm 0.25$ ;  $\delta P/\text{atm} = \pm 3\%$ (estimated by compiler).

<sup>†</sup> at a partial pressure of carbon dioxide of 1 atmosphere calculated by compiler assuming  $\phi = 0.995$ .

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Chen, H.; Liu, M.; Zheng, L.; Zhu, Z.		
2. Methylbenzene; C <sub>7</sub> H <sub>8</sub> ; [108-88-3]	Zhejiang Daxue Xuebao <u>1985</u> , 19(1), 140-148.		
VARIABLES:	PREPARED BY:		
T/K = 298.15-316.15 P/kPa ≃ 101.3	P.G.T. Fogg		

# EXPERIMENTAL VALUES:

T/K	Henry's c	onstant <sup>†</sup>	x <sub>CO₂</sub> at	
	H/atm	H/kPa*	$P_{\text{CO}_2} = 101.3 \text{ kPa}^*$	
298.15	95.78	9705	0.01044	
303.15	101.25	10259	0.00988	
316.15	118.83	12040	0.00842	

† Henry's constant, H, is based upon the relationship

$$H = P_{CO_2}/x_{CO_2}$$

where  $P_{\text{CO}_2}$  is equal to barometric pressure.

\* calculated by the compiler

# AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Solubilities were measured with a modified Novak and Conway apparatus. Details of the apparatus are given by the authors. The pressure was measured with a mercury manometer. The solvent in the absorption vessel was stirred with a magnetic stirrer. Gas was circulated through the apparatus by means of a gas pump until no further gas was absorbed (see ref. 1).

### SOURCE AND PURITY OF MATERIALS:

- 1. purity 97.3%
- analytical grade supplied by Hongzhou Chlorophyll Plant.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  (absorption vessel)  $\delta T/K = \pm 1.0$  (entire system) (authors)

# REFERENCES:

1. Novak-Adamic, D.M.; Conway, B.F. Chem. Instrum. 1973, 5, 79.

(1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]

1,4-Dimethylbenzene;  $C_8^{H}_{10}$ ; [106-42-3]

(2) Benzene; C<sub>6</sub>H<sub>6</sub>; 1,2-Dimethylbenzene;  $C_8^H_{10}$ ; [95-47-6] 1,3-Dimethylbenzene;  $C_8H_{10}$ ; [108-38-3]

# ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thes. fac. sci. Univ. Strasbourg (France) 1954.

### VARIABLES:

T/K = 293.15p/kPa = 101.325

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K <sup>b</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>	Bunsen b Coefficient a/cm³(STP)cm-³atm-1	Mole Fraction <sup>b</sup>
Benzene	:		
293.15	2,66	2.47	0.00988
1,2-Dim	ethylbenzene		
293.15	2.085	1.940	0.01051
1,3-Dim	ethylbenzene		
293.15	2.19	2.04	0.0112
1,4-Dim	ethylbenzene		
293.15	2.20	2.05	0.0113

a Original data.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and ESTIMATED ERROR: below atmospheric.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Aromatic hydrocarbons.

 $\delta T/K = \pm 0.2$  $\delta p/kPa = \pm 0.1$  $\delta L/L = \pm 0.02$  (compiler)

### REFERENCES:

Some data in the thesis have been published. See:

1. Maillard, A.; Rosenthal, W. Compt. rend. 1952, 234, 2546-8.

b Calculated by compiler using real gas molar volumes.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2-Dimethylbenzene or o-xylene;  $C_8H_{10}$ ; [95-47-6]

### ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Wilhelm, E.

J. Chem. Thermodyn. 1975, 7, 515-522.

# VARIABLES:

T/K: 283.08 - 313.17  $p_1/kPa$ : 101.325 (1 atm)

### PREPARED BY:

H. L. Clever A. L. Cramer

# EXPERIMENTAL VALUES:

AL.	AWTOED!			
****	<i>T</i> /K	Mol Fraction $10^3 x_{1}$	Bunsen Coefficient α/cm³ (STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
	283.08 283.21	12.30 12.34	2.335 2.344	2.420 2.430
	298.19	9.94	1.855	2.026
	313.06 313.17	8.34 8.30	1.533 1.526	1.757 1.750

The Bunsen coefficients were calculated by the compiler. The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa (1 atm) by Henry's law.

Smoothed Data: For use between 283.08 and 313.17 K.

 $\ln x_1 = -8.5010 + 11.6175/(T/100 K)$ 

The standard error about the regression line is  $4.91 \times 10^{-5}$ .

T/K	Mol Fraction 103x1
283.15	12.30
293.15	10.69
298.15	10.01
303.15	9.38
313.15	8.30

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Either Air Products & Chemicals, Inc., or Matheson Co., Inc. 99 mol per cent or better.
- (2) 1,2-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

### ESTIMATED ERROR:

$$\delta T/K = 0.03$$
  
 $\delta P/\text{mmHg} = 0.5$   
 $\delta x_1/x_1 = 0.005$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.;
   Danforth, W. F. J. Am. Oil
   Chem. Soc. 1968, 45, 830.
   Battino, R.; Banzhof, M.;
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

ITAL	AUTORO.			
	T/K	Mol Fraction	Bunsen	Ostwald
_		10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
:	288.15	1.20	2.22	2.346
2	293.15	1.12	2.06	2.216
2	298.15	1.04	1.91	2.090

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1,3-Dimethylbenzene. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) <u>1894</u>, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,3-Dimethylbenzene or m-xylene;  $C_8H_{10}$ ; [108-38-3]

### ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Wilhelm, E.

J. Chem. Thermodyn. 1975, 7, 515-522.

### VARIABLES:

T/K: 283.01 - 313.14  $p_1/k$ Pa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever A. L. Cramer

# EXPERIMENTAL VALUES:

T AUTORS.			
T/K	Mol Fraction 103x 1	Bunsen Coefficient a/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
283.01 283.13	12.99 13.21	2.425	2.513
283.13	13.21	2.466 2.471	2.556 2.561
298.17	10.63	1.949	2.127
313.14	8.89	1.603	1.838

The Bunsen coefficients were calculated by the compiler. The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa (1 atm) by Henry's law.

Smoothed Data: For use between 283.01 and 313.15 K.

 $\ln x_{\tau} = -8.4234 + 11.5806/(T/100 K)$ 

The standard error about the regression line is  $1.24 \times 10^{-4}$ .

<i>T</i> /K	Mol Fraction 10 <sup>3</sup> x <sub>1</sub>
283.15	13.12
293.15	11.41
298.15	10.68
303.15	10.02
313.15	8.87

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm³ of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is applied intermittently through a liquid N2 trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Either Air Products & Chemicals, Inc., or Matheson Co., Inc. 99 mol per cent or better.
- (2) 1,3-Dimethylbenzene. Phillips Petroleum Co. Pure grade.

### ESTIMATED ERROR:

 $\delta T/K = 0.03$   $\delta P/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.005$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.
   Battino, R.; Evans, F. D.;
- 2. Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil
- Chem. Soc. 1968, 45, 830.

  Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>1,3-Dimethylbenzene (m-xylene);</li> <li>C<sub>8</sub>H<sub>10</sub>; [108-38-3]</li> </ol>	Horvath, M. J.; Sebastian, H. M.; Chao, KC.  Ind. Eng. Chem. Fundam.  1981, 20, 394-396.
VARIABLES:	PREPARED BY:
T/K = 298  or  300 $P/\text{kPa} \simeq 101.3$	C. L. Young

### EXPERIMENTAL VALUES:

T/K	Henry's constant /atm	Mole fraction of carbon dioxide in liquid, $^{x}\mathrm{CO}_{2}$ †
298	94	0.0106
300	95	0.0105

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Gas chromatographic analysis of a saturated solution at barometric pressure. Henry's constants determined from formula

$$H = (p - p_o) \phi (m + 1) / m$$

where p is the total pressure,  $p_o$  the vapor pressure of the solvent and  $\phi$  is the fugacity coefficient of the gas. The mole ratio, m, is defined by

 $m = \frac{ \mbox{Moles of carbon dioxide}}{ \mbox{Moles of carbon dioxide} } \\ \mbox{in liquid phase}$ 

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Purity 99.93 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.25$ ;  $\delta P/\text{atm} = \pm 3\%$  (estimated by compiler).

 $<sup>^{\</sup>dagger}$  at a partial pressure of carbon dioxide of 1 atmosphere calculated by compiler assuming  $\phi$  = 0.995.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,4-Dimethylbenzene or p-xylene;  $C_8H_{10}$ ; [106-42-3]

# ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Wilhelm, E.

J. Chem. Thermodyn. 1975, 7, 515-522.

VARIABLES:

T/K: 288.17 - 313.13  $p_1/kPa$ : 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

m valiono.			
т/к	Mol Fraction 10 <sup>3</sup> x <sub>1</sub>	Bunsen Coefficient α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
288.17	12.54	2.319	2.447
288.23	12.33	2.280	2.406
288.55	12.53	2.317	2.448
298.12	10.87	1.987	2.169
313.13	9.10	1.636	1.876

The Bunsen coefficients were calculated by the compiler.

The solubility values were adjusted to a carbon dioxide partial pressure of 101.325 kPa (1 atm) by Henry's law.

Smoothed Data: For use between 288.17 and 313.15 K.

 $\ln x_1 = -8.3698 + 11.4868/(T/100 K)$ 

The standard error about the regression line is  $1.15 \times 10^{-4}$ .

<i>T</i> /K	Mol Fraction 103x1
293.15	11.66
298.15	10.92
303.15 313.15	10.25 9.08

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Either Air Products & Chemicals, Inc., or Matheson Co., Inc. 99 mol per cent or better.
- (2) 1,4-Dimethylbenzene. Phillips Petroleum Co. Pure grade. Used as received.

ESTIMATED ERROR:

$$\begin{array}{lll} \delta \ T/K &=& 0.01 \\ \delta \ P/\text{mmHg} &=& 0.5 \\ \delta \ x_{1}/x_{1} &=& 0.001 \end{array}$$

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- 2. Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.;
   Bogan, M.; Wilhelm, E.
   Anal. Chem. 1971, 43, 806.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; Vitovec, J. [124-38-9] 2. Dimethylbenzene; C<sub>8</sub>H<sub>10</sub>; 33, 1203-1310. VARIABLES: P/kPa = 101.3 T/K = 293.15 PRIGINAL MEASUREMENTS: Vitovec, J. Collect. Czech. Chem. Comm. 1968, 33, 1203-1310. PREPARED BY: P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Absorption /kg m <sup>-3</sup>	$x_{\text{CO}_2}$ at $P_{\text{CO}_2} = 101.3 \text{ kPa}$	* 1
293.15	3.96	0.0109	_

 $<sup>^</sup>st$ calculated by the compiler.

The compiler has assumed that a mixture of dimethylbenzene isomers was used for the experiment and has taken the density of the solvent to be the average of the values for the three isomers.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility of carbon dioxide was measured by a saturation method as described in ref. (1). Carbon dioxide was passed through the solvent and the final concentration in the solution was measured by a titration method as described in ref. (2).

# SOURCE AND PURITY OF MATERIALS:

- Obtained from a pressure vessel. Purity at least 99%.
- 2. Technical grade material.

ESTIMATED ERROR:

- Vitovec, J.; Fried, V. Collect. Czech. Chem. Comm. 1960, 25, 1522.
- Emmert, R.E.; Pigford, R.L. Chem. Eng. Progr. 1955, 50, 86.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) (1-Methylethyl)-benzene or isopropyl benzene or cumene; C<sub>9</sub>H<sub>12</sub>; [98-82-8]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

1d
ient m-3
8
9
2
,

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) (1-Methylethyl)-benzene. No information.

ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	
<ol> <li>Carbon dloxide; Co<sub>2</sub>; [124-38-9]</li> <li>1,1'-Methylenebisbenzene; (Diphenyl methane); C<sub>13</sub>H<sub>12</sub>; [101-81-5]</li> </ol>	Tremper, K.K.; Prausnitz, J.M.  J. Chem.Engng.Data 1976,21,295-9
VARIABLES:	PREPARED BY:
T/K = 300-475	C.L. Young
EXPERIMENTAL VALUES:	
T/K Henry's Con /atm	stant <sup>a</sup> Mole fraction <sup>b</sup> of carbon dioxide at 1 atm partial pressure, <sup>x</sup> CO <sub>2</sub>
300 123.0	0.00813
325 161.0	
350 196.0	
375 228.0	***************************************
400 259.0	
425 287.0	0.00348
450 309.0	0.00324
475 306.0	0.00327
within the Henry's-Law	assuming linear relationship
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE Volumetric apparatus similar to that described by Dymond and Hildebrand (1) Pressure measured with a null detector and precision gauge. Details in ref. (2).	
	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta x_{\text{CO}_2} = \pm 1 \%.$ REFERENCES:  1. Dymond, J.; Hildebrand J.H.  Ind. Eng. Chem. Fundam. 1967, 6, 130.  2. Cukor, P.M.; Prausnitz, J.M.  Ind. Eng. Chem. Fundam. 1971, 10, 638.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Horvath, M. J.; Sebastian, H. M.; Chao, K.-C. 2. Diphenylmethane (1,1'-methylene-Ind. Eng. Chem. Fundam. bisbenzene); C13H12; 1981, 20, 394-396. [101-81-5] VARIABLES: PREPARED BY: T/K = 300 $P/kPa \simeq 101.3$ C. L. Young EXPERIMENTAL VALUES: Mole fraction of Henry's constant carbon dioxide in liquid, T/K /atm <sup>x</sup>CO₂ †

124 0.0080 300

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Gas chromatographic analysis of a saturated solution at barometric Henry's constants deterpressure. mined from formula

$$H = (p - p_o)\phi(m + 1)/m$$

where p is the total pressure, p. the vapor pressure of the solvent and  $\phi$  is the fugacity coefficient of the gas. The mole ratio, m, is defined by

Moles of carbon dioxide in gas phase m = Moles of carbon dioxide in liquid phase

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Purity 99.06 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.25$ ;  $\delta P/\text{atm} = \pm 3\%$ (estimated by compiler).

<sup>†</sup> at a partial pressure of carbon dioxide of 1 atmosphere calculated by compiler assuming  $\phi = 0.995$ .

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1,1'-Methylenebis (methylbenzene),
   (ditolyl methane); C<sub>15</sub>H<sub>16</sub>;
   [1335-47-3]

# ORIGINAL MEASUREMENTS:

Glazunova, T.V.; Ryabov, M.I.; Lipshtein, R.A. Sov. At. Energ., 1987, 62, 449-451.

### VARIABLES:

T/K = 293-393P/kPa = 101.3 PREPARED BY:

C.L. Young

# EXPERIMENTAL VALUES:

t/°C	T/K	Bunsen coefficient	Mole fraction at partial pressure of 1 atm.
20	293	131.63	0.01165
50	323	93.63	0.008314
70	343	77.40	0.006883
120	393	47.83	0.004265

 $^{\rm a}$  Calculated by compiler assuming the ideal gas law and the molar volume of component 2 is 200.7  ${\rm cm}^{\rm 3}~{\rm mol}^{\rm -1}$ 

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE

Single pass flow system. In which sample of solvent was saturated with gas at or near atmospheric pressure. Sample of solvent withdrawn and analysed using gas chromatography fitted with thermal conductivity detector.

# SOURCE AND PURITY OF MATERIALS:

- Purity at least 99.8 per cent by volume.
- 2. Technical grade to TU 3810298-76 standard.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5; \quad \delta x/x = \pm 0.10$ 

### COMPONENTS: ORIGINAL MEASUREMENTS: Bogdanov, F.F. 1. Carbon dioxide; CO2; [124 - 38 - 9]Issled. Teploprovodnosk. Inst. Telo. (1-Methylethyl)-1,1'-biphenyl, Mesoobmena Akad. Nauk. Beloruss. S.S.R. 1967, 230-236. (monoisopropylbiphenyl); $C_{15}H_{17}$ ; [25640-78-2] VARIABLES: PREPARED BY: T/K = 293-473P.G.T. Fogg P/kPa = 500-6000

# EXPERIMENTAL VALUES:

The author has plotted graphs of absorption of gas (vol.of gas\*/vol. solvent) against pressure at temperatures of 20, 100 and 200°C. The points for 20°C fall on a straight line passing through the origin. Points for the other temperatures are scattered. The compiler has estimated absorption at a pressure of 101.3 kPa and 20°C from the graph.

P/kPa	T/K	vol.gas /vol.solvent	<sup>x</sup> CO₂ <sup>†</sup>	
101.3	293.2	1.35	0.0113	

<sup>\*</sup> the compiler considers that volumes of gas have been corrected to 1.013 kPa and 273.15 K.

### AUXILIARY INFORMATION

The author has given details of absorption apparatus for use at high pressures. Gas under test was introduced from a gas cylinder into the absorption cell containing the liquid under test. A sample of solution could be withdrawn and the volume of absorbed gas measured when the system had reached equilibrium.

METHOD /APPARATUS / PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No information

### ESTIMATED ERROR:

Experimental points on graph accurate to ±10% (author)

 $<sup>^\</sup>dagger$  calculated by the compiler. The density of the solvent was assumed to be 1.048 g cm $^{-3}$ . This is the value for 3-ethylbiphenyl at 273.2 K.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. l-Methylnaphthalene;  $C_{11}^{H}_{10}$ ; [90-12-0]

### ORIGINAL MEASUREMENTS:

Chai, C-P.; Paulaitis, M. E.;

J. Chem. Eng. Data, 1981, 26,
277-279.

### VARIABLES:

T/K = 298.6-330.2

### PREPARED BY:

C. L. Young

### **EXPERIMENTAL VALUES:**

T/K	Henry´s constant /atm	Mole fraction a of carbon dioxide	T/K	Henry's constant /atm	Mole fraction <sup>5</sup> of carbon dioxide
298.6	147.75	0.0067682	316.2	180.78	0.0055316
298.6	149.80	0.0066756	316.2	183.29	0.0054558
298.6	149.24	0.0067006	316.2	181.10	0.0055218
302.7	157.04	0.0063678	320.2	191.32	0.0052268
304.3	159.32	0.0062767	323.6	194.79	0.0051337
307.1	163.75	0.0061069	323.6	198.42	0.0050398
307.1	165.48	0.0060430	323.6	195.13	0.0051248
307.1	164.18	0.0060909	330.2	210.85	0.0047427
311.0	172.37	0.0058015			

a Calculated by compiler for a partial pressure of 1 atm.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus similar to that described in ref.(1). Known amount of carbon dioxide brought into contact with known amount of solvent. Reduction in pressure measured.

# SOURCE AND PURITY OF MATERIALS:

- 1. Linde "bone dry" grade.
- 2. Fisher certified grade.

# ESTIMATED ERROR:

### REFERENCES:

 Dymond, J. H.; Hildebrand, J. H.; Ind. Eng. Chem. Fundam., 1967, 6, 130.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 1-Methylnaphthalene; C<sub>11</sub>H<sub>10</sub>; [90-12-0]

# ORIGINAL MEASUREMENTS:

Horvath, M. J.; Sebastian, H. M.; Chao, K.-C. Ind. Eng. Chem. Fundam. 1981, 20, 394-396.

VARIABLES:

T/K = 300 $P/kPa \simeq 101.3$  PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

T/K

Henry's constant /atm

Mole fraction of carbon dioxide in liquid, <sup>x</sup>co₂ †

300

151

0.00659

at a partial pressure of carbon dioxide of 1 atmosphere calculated by compiler assuming  $\phi$  = 0.995.

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

Gas chromatographic analysis of a saturated solution at barometric Henry's constants deterpressure. mined from formula

$$H = (p - p_0)\phi(m + 1)/m$$

where p is the total pressure,  $p_{o}$ the vapor pressure of the solvent and  $\phi$  is the fugacity coefficient of | ESTIMATED ERROR: The mole ratio, m, is the gas. defined by

Moles of carbon dioxide in gas phase m = Moles of carbon dioxide in liquid phase

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Purity 99.51 mole per cent.

 $\delta T/K = \pm 0.25$ ;  $\delta P/\text{atm} = \pm 3\%$ (estimated by compiler).

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alcohols

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

Solubility of carbon dioxide in alcohols.

Measurements by Makranczy et al.(1) indicate that mole fraction solubilities in straight chain primary alkanols at 298.2 K and a partial pressure of carbon dioxide of 101.3 kPa increase linearly with carbon number from methanol to dodecanol. This trend has not been confirmed by other workers. In cases where comparison is possible, the higher the carbon number the greater the divergence of Makranczy's data from other data which are available (Fig. 1).

Shenderei et al.(2) published values of the solubility in methanol from 13.33 kPa to 101.3 kPa at 194.5 K to 273.2 K. These measurements show linear variation of mole fraction solubility with pressure at every temperature even to a value of 0.25 at 194.5 K and 93.33 kPa. Linear variation to such a high value appears to be inconsistent with the measurements at high pressures and higher temperatures by Krichevskii and Lebedeva (3). These authors found that mole fraction solubility curves at constant temperature were convex towards the pressure axis.

Values of the mole fraction solubility at a partial pressure of 101.3 kPa may be found from published data for 202.6 K to 307.2 K (1-14). Values for 293.2 range from 0.00602 (6) to 0.00719 (7) and for 298.2 from 0.00568 (6) to 0.00635 (10). The evaluator recommends the smoothing equation for mole fraction solubilities at a partial pressure of 101.3 kPa which is given below. This is based upon ten of the papers (2-4,7-10,13,14).

$$\ln x_{CO_2} = -49.919 + 3484.7/(T/K) + 5.8265\ln(T/K)$$

temperature range = 202.6-323.0 Kstandard deviation in  $x_{CO_2} = 0.00139$ 

Solubility in ethanol at a partial pressure of 101.3 kPa in the temperature range 212.7 K to 333.4 K has been published in at least nine papers (1,2,4,6,10-12,15,16). Shenderei et a1.(2) measured the solubility in ethanol from 13.33 kPa to 101.3 kPa at 212.7 K to 248.0 K. Data are self consistent and there is no reason to doubt the reliability. The value of the mole fraction solubility at 298.15 ranges from 0.00624 (Takahashi et a1.(16)) to 0.00728 (Won et a1.(11)). Takahashi calculated solubility from the rate of absorption of gas. The method is an interesting one but is likely to be less reliable than conventional methods. Kunerth's measurements (6) from 291.2 K to 307.2 K may again be too low. The evaluator considers that measurements by Cargill and MacPhee (15) to be the most reliable in the temperature range 277.9 K to 333.4 K. These measurements agree with the solubility at 298.15 K measured by Won et a1. (11) and are close to measurements by Kosakewitsch (12), Makranczy et a1.(1) and by Luhring and Schumpe (4). The only measurements below 277 K are by Shenderei et a1.(2). These appear to be consistent with measurements at higher temperatures and can be tentatively recommended.

The following equation for mole fraction solubility at a partial pressure of 101.3 kPa is based upon measurements by Cargill and MacPhee and by Won  $et\ al$ .

$$\ln x_{CO_2} = -22.278 + 2027.1/(T/K) + 1.8521\ln(T/K)$$

temperature range = 277.9-333.4 K standard deviation in  $x_{CO_2}$  = 1.56 × 10<sup>-5</sup>

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alcohols

# **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

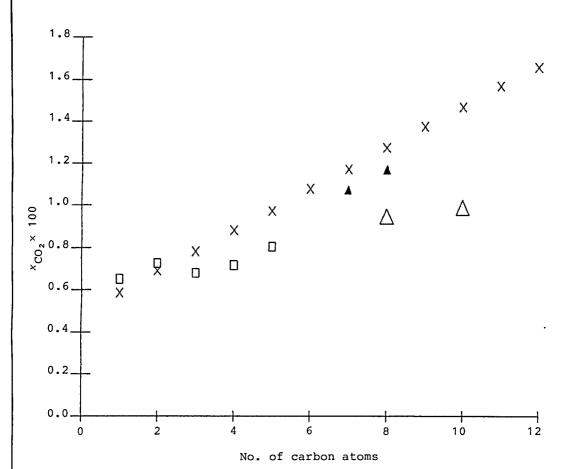


Fig. 1 Values from various sources of the mole fraction solubility of carbon dioxide in straight chain primary alkanols at 298.15 K and a partial pressure of gas of 101.3 kPa.

- from the smoothing equations given by the evaluator
- X Makranczy et al. (1)
- ▲ Dim et al. (21)
- $\triangle$  Wilcock et a1. (20)

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. Alcohols

### **EVALUATOR:**

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July 1991

### CRITICAL EVALUATION:

The equation given below for mole fraction solubility at a partial pressure of 101.3 kPa is based upon measurements by Cargill and MacPhee, by Won  $et\ al.$ , and by Shenderei  $et\ al.$ 

$$\ln x_{CO_2} = -56.735 + 3560.0/(T/K) + 6.9952ln(T/K)$$

temperature range = 212.7-333.4 Kstandard deviation in  $x_{CO_2} = 0.00038$ 

Solubility in 1-propanol was measured by Shenderei et al.(2) from 13.3 kPa to 101.3 kPa at 212.7 K to 248.0 K. There is no reason to doubt the reliability but no similar measurements in this temperature and pressure range are available for comparison. Tokunaga (17) reported Ostwald coefficients and Henry's constants measured at or close to 101.3 kPa from 283.2 K to 313.2 K. Mole fraction solubility at 298.2 K is available from work by Macranczy et al.(1), Takahashi et al.(16) and Just (10). These values range from 0.00470 (Takahashi) to 0.00782 (Makranczy). The interpolated value from Tokunaga's work is 0.00679. Takahashi used a method which depended upon measuring absorption rates and the value is much too low. Measurements by Makranczy et al. for primary alkanols show a trend which differs from that shown by other measurements. The equation for mole fraction solubility given below and based upon measurements by Shenderel et al. and by Tokunaga et al. is recommended on a provisional basis. i.e.

$$\ln x_{\text{CO}_2} = -52.708 + 3312.9/(T/K) + 6.4248\ln(T/K)$$

temperature range = 212.7-313.2 Kstandard deviation in  $x_{CO2} = 0.00028$ 

Solubility in 2-propanol was also measured by Shenderei et al.(2) from 13.3 kPa to 101.3 kPa at 212.7 K to 248.0 K. Again there is no reason to doubt the reliability of these measurements but no other measurements in this temperature and pressure range are available for comparison. Tokunaga (17) measured the solubility in this solvent at about 101.3 kPa in the temperature range 283.2 K to 313.2 K. A measurement at 293.2 K by Luhring and Schumpe (4) corresponds to a mole fraction solubility of 0.00720. The value from Tokunaga's work is 0.00685.

An equation for mole fraction solubility at a partial pressure of 101.3 kPa which is based upon measurements by Shenderei  $et\ al.$  and by Tokunaga is recommended on a provisional basis. i.e.

$$\ln x_{CO_2} = -83.277 + 4450.3/(T/K) + 11.112ln(T/K)$$

temperature range = 212.7-313.2 Kstandard deviation in  $x_{CO_2} = 0.00032$ 

Shenderei et al.(2) measured solubility in 1-butanol from 13.3 kPa to 101.3 kPa at 212.7 K to 248.0 K. The data is self consistent but no other measurements under these conditions are available for comparison. The solubility reported by Makranczy et al.(1) corresponds to a mole fraction of 0.008832 at 298.15 K and a partial pressure of 101.3 kPa. Luhring and Schumpe's data (4) correspond to a mole fraction solubility of 0.00781 at 293.15 K and a partial pressure of 101.3 kPa. This latter value is not compatible with Makranczy's data. The evaluator considers that Luhring's value is more likely to be reliable. The following smoothing equation based upon measurements by Shenderei et al. and by Luhring and Schumpe is

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alcohols

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

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### CRITICAL EVALUATION:

recommended on a tentative basis until further measurements on the system are available.

$$\ln x_{CO_2} = -52.475 + 3272.5/(T/K) + 6.4171ln(T/K)$$

temperature range = 212.7-293.2 K standard deviation in  $x_{CO_2}$  = 0.00038

Shenderei et al.(2) measured the solubility in 2-methyl-1-propanol from 13.3 kPa to 101.3 kPa at 212.7 K to 248.0 K. The data is self consistent but no other measurements at these temperatures and pressures are available for comparison. Battino et al.(18) measured solubility at 101.3 kPa from 274.0 K to 328.0 K. Battino's measurements are in satisfactory agreement with earlier measurements by Just (10) from 288.2 K to 298.2 K. Takahashi et al.(16) estimated the solubility from absorption studies. Their data correspond to a mole fraction solubility of 0.00628 at 298.2 compared with a value of 0.00697 from Battino and 0.0698 from Just.

The following equation based upon data from Battino  $et\ al.$  and from Just is recommended as likely to be reliable.

$$\ln x_{CO_2} = -7.5561 + 1195.7/(T/K) -0.24941ln(T/K)$$

temperature range = 274.0-328.0 K standard deviation in  $x_{\rm CO_2}$  = 9.7 × 10<sup>-5</sup>

The following equation based upon data from Shenderei  $et\ al.$ , Battino  $et\ al.$  and from Just can be accepted on a tentative basis

$$\ln x_{CO_2} = -75.542 + 4061.4/(T/K) + 9.9928ln(T/K)$$

temperature range = 212.7-328.0standard deviation in  $x_{CO_2}$  = 0.00055

Shenderei et al.(2) measured solubility in 2-butanol from 13.3 kPa to 101.3 kPa at 211.7 K to 248.0 K. The data is self consistent. No other measurements of solubility of carbon dioxide in this solvent are available for comparison.

Solubility in 1-pentanol has been measured by Just (10) in the range 288.2 K to 298.2 K and by Pedrosa et al.(19) in the range 288.2 K to 318.2 K. There is good agreement between the two sets of measurements. A smoothing equation for mole fraction solubility at a partial pressure of 101.3 kPa based on these two sets of measurements is given below. Solubility reported by Makranczy et al.(1) for 298.15 K seems to be too high.

$$\ln x_{CO_2} = -119.31 + 6103.7/(T/K) + 16.501\ln(T/K)$$

temperature range = 288.3-318.2 K standard deviation in  $x_{CO_2}$  = 5.9 × 10<sup>-5</sup>

Kunerth (6) published values of the solubility in 3-methyl-1-butanol at 101.3 kPa for 293.2 K to 307.2 K. These are close to values for 1-pentanol discussed above. A smoothing equation for mole fraction solubility at a partial pressure of 101.3 kPa is given below. It should be noted that values of solubility in methanol and in ethanol published in

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alcohols

### **EVALUATOR:**

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July 1991

### CRITICAL EVALUATION:

the same paper are slightly low in comparison with values measured more recently.

 $\ln x_{CO_2} = 9.5281 + 390.83/(T/K) - 2.7484ln(T/K)$ 

temperature range = 293.2-307.2 K standard deviation in  $x_{\rm CO_2}$  = 3.6 × 10<sup>-5</sup>

Solubilities in 1-hexanol and 1-heptanol have been published by Makranczy et al.(1). Solubility in 1-heptanol has also been measured by Dim et al.(21). Values from both sources are high compared with solubilities in other alkanols (Fig 1).

The solubility in 1-octanol at a partial pressure of 101.3 kPa was measured by Wilcock et al.(20) from 282.7 K to 313.6 K. Solubilities at 298.2 K reported by Makranczy et al.(1) and by Dim et al.(21) are high in comparison with Wilcock's measurements. Takahashi et al.(16) published a value at 298 K from a study of the rate of absorption of gas. This value is unlikely to be reliable and is low relative to Wilcock's values. Measurements by Wilcock et al. are recommended on a provisional basis.

The solubility in 1-nonanol has been published by Macranczy  $et \ al.(1)$ . (Fig 1)

Wilcock et al.(20) published values of solubility in 1-decanol at 284.0 K to 313.5 K. and a partial pressure of 101.3 kPa. The data can be recommended on a provisional basis. Macranczy et al.(1) published a value for 298.2 K which is very high in comparison with Wilcock's value (Fig 1).

Makranczy et al.(1) measured solubility in 1-undecanol and 1-dodecanol at 298.2 K (Fig 1).

Solubility in an equimolar mixture of 1-decanol and 1-dodecanol was measured by Luther and Hiemenz (22) from 293.2 K to 355.2 K. The mole fraction solubility at 293.2 K and a partial pressure of 101.3 kPa is given as 0.0107 compared with a value for the solubility in pure 1-decanol of 0.0106 from measurements by Wilcock  $et\ al.(20)$ .

The solubility in cyclohexanol was measured by Begley et al.(23) at a partial pressure of 101.3 kPa from 298.3 K to 321.0 K. The value of the mole fraction solubility at 298.3 K is 0.00442 which may be compared with a value of 0.00286 from much earlier measurements by Cauquil (24). Begley's measurements are likely to be the more reliable. It is clear that mole fraction solubility in cyclohexanol is much lower than solubility in 1-hexanol or in cyclohexane under similar conditions.

The solubility in benzenemethanol to high pressures was measured by Emel'yanova et al.(25) over the temperature range 323.2 K to 398.2 K. Solubility at a partial pressure of 101.3 kPa can be estimated from the data. Extrapolation to 298.2 K and a partial pressure of 101.3 kPa gives a value of the mole fraction solubility of about 0.0044. This is in contrast to the value of 0.00781 estimated from measurements of the limiting value of Henry's constant measured by gas-liquid chromatography and reported by Lenoir et al.(26). Surface adsorption can give erroneous values of Henry's constants measured by chromatography. Mole fraction solubility at a partial pressure of 101.3 kPa from Emel'yanova's measurements can be provisionally recommended in the absence of measurements conducted at barometric pressure.

Mole fraction solubilities in dihydric alkanols are lower than in monohydric alkanols. The mole fraction solubility at a partial pressure of 101.3 kPa in 1,2-ethanediol from work by Byeseda *et al.*(27) is 0.0031 at 297.1 K and from work by Hayduk and Malik (29) is 0.0022 at 298.2 K.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alcohols

### **EVALUATOR:**

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### CRITICAL EVALUATION:

The value at 298.2 K from chromatographic measurements by Lenoir  $et\ al.(26)$  is 0.00382. The corresponding value for ethanol is 0.00725. Further work on the system is required before a solubility value can be recommended

Semenova et al.(28) measured the solubility in butane-1,4-diol to high pressures at 323.2 K to 398.2 K. Data can be extrapolated to 101.3 kPa. Further extrapolation to 298.2 K and 101.3 kPa indicates a mole fraction solubility of about 0.00395 compared with a value of 0.00717 for 1-butanol. Semenova's data may be accepted on a provisional basis until there is confirmation by other workers.

Just (10) measured solubility in 1,2,3-propanetriol at 298.2 K. Measurements indicate a mole fraction solubility of 0.0000903 at 101.3 kPa. Such a low value must be treated with suspicion until it has been confirmed by other workers.

A selection of mole fraction solubilities in alcohols is given in Table 1.

- Makranczy, J.; Rusz, L.; Balog-Megyery, K. Hung. J. Ind. Chem. <u>1979</u>, 7, 41-6.
- Shenderei, E.R.; Zel'venskii, Ya. D.; Ivanovskii, F.P. Gaz. Prom. 1958, 12, 36-42.
- Krichevskii, I.R.; Lebedeva, E.S. Zhur. Fiz. Khim. <u>1947</u>, 21(6), 715-718.
- 4. Luhring, P.; Schumpe, A.; J. Chem. Eng. Data 1989, 34, 250-252.
- Bratzler, K.D.; Doerges, A.; Herbert, W. German Patent No. 1 769 197 to Metallgesellschaft AG 1971.
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- 7. Vitovec, J. Collect. Czech. Chem. Comm. 1968, 33, 1203-1310.
- 8. Koudelka, L. Chem. Zvesti 1964, 18, 178-185.
- 9. Yorizane, M.; Sadamoto, S.; Masuoka, H.; Eto, Y. Kogyo Kagaku Zasshi 1969, 72, 2174-2177.
- 10. Just, G. Z. Phys. Chem. 1901, 37, 342-367.
- Won, Y.S.; Chung, D.K.; Mills, A.F. J. Chem. Eng. Data <u>1981</u>, 26, 140-141.
- 12. Kosakewitsch, P.P. Zeit. Phys. Chem. (A) 1929, 143, 216-224.
- 13. Usyukin, I.P.; Shleynikov, V.M. Neftepererab. Neftekhim. 1963, No.1, 39-43.
- Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P. Khim. Prom. 1960, (5), 18-22.
- Cargill, R.W.; MacPhee, D.E. J. Chem Research (S) 1981, 232; J. Chem. Research (M) 1981, 2743-2755.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alcohols

### **EVALUATOR:**

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July 1991

### CRITICAL EVALUATION:

- Takahashi, M.; Kobayashi, Y.; Takeuchi, H. J. Chem. Eng. Data 1982, 27, 328-331.
- 17. Tokunaga, J. J. Chem. Eng. Data 1975, 20, 41-46.
- Battino, R.; Evans, F.D.; Danforth, W.F.; Wilhelm, E. J. Chem. Thermodyn. <u>1971</u>, 3, 743-751.
- Pedrosa, G.C.; Salas, J.A.; Katz, M. Anal. Asoc. Quim. Argent. 1988, 76(3), 199-206.
- Wilcock, R.J.; Battino, R.; Danforth, W.F.; Wilhelm, E. J. Chem. Thermodyn. 1978, 10, 817-822.
- 21. Dim, A.; Gardner, G.R.; Ponter, A.B.; Wood, T. J. Chem. Eng. Japan 1971, 4, 92-95.
- 22. Luther, H.; Hiemenz, W. Chem. Ing. Tech. 1957, 29, 530-535.
- Begley, J.W.; Maget, J.R.; Williams, B. J. Chem. Eng. Data 1965, 10, 4-8.
- 24. Cauquil, G. J. Chim. Phys. 1927, 24, 53-55.
- Emel'yanova, E.A.; Tsimmerman, S.S.; Semenova, A.I.; Tsiklis, D.S. Zhur. Fiz. Khim. 1980, 54, 382-384; Russian J. Phys. Chem. 1980, 54(2), 219-220.
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- 27. Byeseda, J.J.; Deetz, J.A.; Manning, W.P. Proc. Laurance Reid Gas Cond. Conf. 1985
- 28. Semenova, A.I.; Tsimmerman, S.S.; Emel'yanova, E.A. Zhur. Fiz, Khim. 1981, 55, 1941-1943; Russian J. Phys. Chem. 1981, 55(8), 1105-1107.
- 29. Hayduk, W.; Malik, V.K. J. Chem. Eng. Data 1971, 16, 143-146.

COMPONENTS:		EVALUATOR:	
1.	Carbon dioxide; CO <sub>2</sub> ; [124-38-9] Alcohols	Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.	
		July 1991	

CRITICAL EVALUATION:

Table 1. Solubility of carbon dioxide at a partial pressure of 101.3 kPa in alcohols.

Solvent	T/K	<sup>x</sup> CO₂	Reference
Methanol	298.15	0.006511 ±0.00139	*
Ethanol	298.15	0.007251 ±0.000016	*
1-Propanol	298.15	0.00680 ±0.00038	*
2-Propanol	298.15	0.00654	17
1-Butanol	298.15	0.00718 ±0.00038	* †
2-Methyl-1-propanol	298.15	0.006966 ±0.000097	*
1-Pentanol	298.15	0.008050 ±0.000059	*
3-Methyl-1-butanol	298.15	0.008064 ±0.000036	6
1-Octanol	298.15	0.00938	20
1-Decanol	298.15	0.00973	20
Cyclohexanol	298.25	0.00442	23
1,2-Ethanediol	298.15 297.1 298.15	0.00382 0.00306 0.00220	26 27 29

<sup>\*</sup> from the  $\rm \acute{e}quation$  given by the evaluator on a previous page  $\rm \dagger$  extrapolated.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Methanol; CH<sub>4</sub>O; [67-56-1]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick

H. L. Clever

EXPERIMENTAL VALUES:

IVE	AWPORD:			
	T/K	Mol Fraction	Bunsen	Ostwald
_		10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
:	288.15	7.78	4.37	4.606
2	293.15	7.03	3.92	4.205
2	298.15	6.35	3.52	3.837

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Methanol. No information.

ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alkanols

### VARIABLES:

T/K = 291.15-307.15  $P/kPa \simeq 101.3$ 

### ORIGINAL MEASUREMENTS:

Kunerth, W.

Phys. Rev. 1922, 19, 512-524.

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	T/K	Ostwald coefficient L	$x_{\text{CO}_2}$ at $P_{\text{CO}_2} = 101.3 \text{ kPa}^*$
Methanol; CH <sub>4</sub> O; [67-56-1]	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15	3.63 3.57 3.51 3.44 3.37 3.28 3.19 3.09 2.97	0.00614 0.00602 0.00589 0.00575 0.00561 0.00544 0.00527 0.00508
Ethanol; C <sub>2</sub> H <sub>6</sub> O; [64-17-5]	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15	2.95 2.87 2.80 2.73 2.66 2.58 2.48 2.41 2.31	0.00719 0.00697 0.00677 0.00657 0.00637 0.00615 0.00589 0.00570
3-Methyl-1-butanol, (isoamyl alcohol); C <sub>5</sub> H <sub>12</sub> O; [123-51-3]	293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15	1.91 1.88 1.85 1.81 1.76 1.72 1.69	0.00861 0.00842 0.00823 0.00800 0.00773 0.00750 0.00733

<sup>\*</sup> calculated by the compiler

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The method is based upon that described by McDaniel (1). The apparatus consisted of a gas buret attached to a levelling tube containing mercury and to the absorption cell containing the solvent under test. The volume of gas absorbed by a measured volume of liquid was measured at a total pressure equal to barometric pressure. The mercury in the gas buret was covered with a layer of solvent so that the gas in the buret was saturated with solvent vapor. Buret and absorption cell were surrounded by heating wire and water jackets fitted with thermometers.

### SOURCE AND PURITY OF MATERIALS:

- produced by heating NaHCO<sub>3</sub>; dried with CaCl<sub>2</sub>; frozen in liquid air and volatile impurities pumped away; passed over P<sub>2</sub>O<sub>5</sub>.
- commercial sample; purity attested by boiling point and density.

## ESTIMATED ERROR:

 $\delta x_{CO_2} = \pm 5\%$ 

(compiler)

- 1. McDaniel, A.S.;
  - J. Phys. Chem. 1911, 15, 587.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Methanol; CH<sub>4</sub>O; [67-56-1] Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5] VARIABLES: T/K = 288.15-296.15 P/kPa = 101.3 PRIGINAL MEASUREMENTS: Kosakewitsch, P.P. Zeit. Phys. Chem. (A) 1929, 143, 216-224. PREPARED BY: P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	T/K	P/kPa	Solubility† 100n(CO <sub>2</sub> ) /n(alkanol)	Mole fraction solubility* <sup>*</sup> CO <sub>2</sub>
Methanol	288.15	101.3	0.825	0.00818
Ethanol	289.90 290.40 291.65 294.40 295.40 296.15	101.3	0.813 0.802 0.788 0.750 0.739 0.736	0.00762 0.00796 0.00782 0.00744 0.00734 0.00731

 $\dagger$  100 × (number of moles of  $CO_2$ )/(number of moles of alkanol)

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Carbon dioxide was bubbled through the solvent for two to four days. A portion of the saturated solution was then added to CO<sub>2</sub>-free water containing a measured quantity of sodium hydroxide. The mixture of sodium hydroxide and carbonate was then titrated against hydrochloric acid using phenolphthalein as indicator.

Solubilities were corrected to a partial pressure of carbon dioxide of 101.3 kPa.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide was prepaed by the action of hydrochloric acid on calcium carbonate. The gas was purified and dried by the usual methods.
- Alcohols were said to be free of water.

ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9] 2. Methanol; CH <sub>4</sub> O; [67-56-1]	Krichevskii, I.R.; Lebedeva, E.S.  Zhur. Fiz. Khim. 1947, 21(6), 715-718.
VARIABLES: T/K = 273.2-323.0 P/kPa = 101.3	PREPARED BY: P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	P <sub>CO2</sub> /kPa	Solubility of CO <sub>2</sub> cm <sup>3</sup> g <sup>-1</sup> *	Mole fraction solubility  *CO2 +
273.15	101.3	8.13	0.01157
298.15	101.3	4.33	0.00620
322.95	101.3	3.11	0.00446

<sup>\*</sup> volume of gas corrected to 101.3 kPa, 273.15 K dissolved by one gram of methanol  $\,$ 

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Apparatus described in an earlier paper (1). The measurements at 101.3 kPa were part of a study which extended to 6970 kPa.

### SOURCE AND PURITY OF MATERIALS:

- 1. From a commercial source; purity
  99.9%
- 2. Synthetic purified sample; density indicated that the water content did not exceed several tenths of a percent.

### ESTIMATED ERROR:

 $\delta$ (solubility) =  $\pm 1\%$ 

### REFERENCES:

 Krichevskii, I.R.; Zhavoronkov, N.M.; Tsiklis, D.S.
 Zhur. Fiz. Khim. 1937, 9, 317.

<sup>&</sup>lt;sup>†</sup> calculated by the compiler

- Carbon dioxide; CO<sub>2</sub>
  [124-38-9]
- 2. Methanol; CH<sub>4</sub>O; [67-56-1]

### ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Gaz. Prom. 1958, 12, 36-42.

### VARIABLES:

P/kPa = 13.3-101.3T/K = 212.7-298.2

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

т/к	P/mmHg	P/kPa*	Solubility*	* *CO2
194.5	100 300	13.33 40.00	25.745 83.343	0.0358 0.1073
	500 700	66.66 93.33	138.647 231.130	0.1785 0.2500
202.6	100 300 500	13.33 40.00 66.66	15.743 49.475 90.282	0.0222 0.0666 0.1138
	760	101.32	142.523	0.1705
212.7	100 300 500	13.33 40.00 66.66	9.132 24.383 48.129	0.0130 0.0388 0.0649
227.9	760 100 300	101.32 13.33 40.00	74.909 4.607 13.790	0.0975 0.0066 0.0195
	500 760	66.66 101.32	24.034 36.879	0.0335 0.0505
240.7	100 300 500	13.33 40.00 66.66	2.715 8.209 14.064	0.0039 0.0117 0.0199
248.0	760 100 300	101.32 13.33 40.00	28.870 1.212 6.672	0.0306 0.00318 0.00953
	500 760	66.66 101.32	11.196 17.123	0.01589 0.02410
273.2	100 300 500 760	13.33 40.00 66.66 101.32	1.090 3.274 5.371 8.351	0.00157 0.00470 0.00783 0.01190

<sup>\*</sup> calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A static method was used. A weighed quantity of solvent was placed in the absorption pipet which was subsequently cooled in a cryostat with automatic temperature control. The solvent was then degassed under vacuum. Liquid lost during this process was collected in an absorption column and weighed so appropriated correction could be made to the weight of solvent. Carbon dioxide was then supplied from a calibrated gas buret. The liquid was stirred by an electromagnetic stirrer until equilibrium was reached.

### SOURCE AND PURITY OF MATERIALS:

- from commercial solid carbon dioxide; purified twice by evaporation, freezing and pumping with a vacuum pump.
- 2. No information

### ESTIMATED ERROR:

<sup>\*\*</sup> defined as the volume of gas, corrected to 273.15 K and 101.325 kPa, dissolved by one gram of solvent at the stated temperature and pressure.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Methanol; CH<sub>4</sub>O; [67-56-1]</li> </ol>	Usyukin, I.P.; Shleynikov, V.M.  Neftepererab. Neftekhim. 1963, (1), 39-43.	
VARIABLES: T/K = 203.2-293.2	PREPARED BY: P.G.T. Fogg	
P/kPa = 101.3		

### EXPERIMENTAL VALUES:

	f solubility
	_
.3 3.56	0.00644
4.86	0.00867
6.67	0.01172
9.25	0.01598
12.30	0.02089
17.76	0.02952
26.30	0.04259
40.00	0.06261
65.50	0.09741
124.00	0.1677
	/vol. o solven  .3 3.56 4.86 6.67 9.25 12.30 17.76 26.30 40.00 65.50

 $<sup>^{*}</sup>$  volume of gas corrected to 273.15 K and 101.3 kPa

# METHOD APPARATUS/PROCEDURE: No information Source and purity of materials: No information ESTIMATED ERROR: REFERENCES:

<sup>\*\*</sup> calculated by the compiler

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO2; Vitovec, J. [124-38-9] Collect. Czech. Chem. Comm. 1968, 2. Methanol; CH<sub>4</sub>O; [67-56-1] 33, 1203-1310. **VARIABLES:** PREPARED BY: P/kPa = 101.3P.G.T. Fogg T/K = 293.15EXPERIMENTAL VALUES: $x_{CO_2}$ at $P_{CO_2} = 101.3 \text{ kPa}^*$ Absorption /kg m<sup>-3</sup> T/K7.87 0.00719 293.15 \*calculated by the compiler. AUXILIARY INFORMATION METHOD APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: The solubility of carbon dioxide was measured by a saturation method as 1. Obtained from a pressure vessel. Purity at least 99%. described in ref.(1). Carbon dioxide was passed through the solvent and the final concentration 2. Chemically pure reagent. in the solution was measured by a titration method as described in ref.(2). ESTIMATED ERROR: $\delta x_{\rm CO_2} = \pm 0.5\%$ REFERENCES: 1. Vitovec, J.; Fried, V. Collect. Czech. Chem. Comm. <u>1960</u>, 25, 1552. 2. Emmert, R.E.; Pigford, R.L. Chem. Eng. Progr. 1955, 50, 86.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9] 2. Methanol; CH <sub>4</sub> O; [67-56-1]	Yorizane, M.; Sadamoto, S.; Masuoka, H.; Eto, Y. Kogyo Kagaku Zasshi 1969, 72, 2174-7	
VARIABLES: T/K = 243.15-273.15 P/kPa = 202.7-3333.6	PREPARED BY: P.G.T. Fogg	

### EXPERIMENTAL VALUES:

Solubility measurements were made over pressure ranges to a maximum of 3333.6 kPa. Limiting values of Henry's law constants, H, were given by the authors. The compiler has estimated the mole fraction solubility at a partial pressure of 101.3 kPa by extrapolation of the solubility data by use of a simplified Krichevsky-Il'inskaya equation of the form

$$\log_{10}(P_2/x_2) = \log_{10}H - \beta(1-x_1^2)$$

where  $P_2$  is the partial pressure of carbon dioxide,  $x_2$  the mole fraction of carbon dioxide in the liquid phase,  $\beta$  a constant and  $x_1$  the mole fraction of solvent in the liquid phase.

T/K	H/atm*	H/kPa	$x_2$ at $P_2 = 101.3 \text{ kPa**}$
243.15 258.15	38 59	3850 5978	0.0233 0.0179
273.15	92	9322	0.0118

- \* defined by the authors as  $H = \lim_{x_2 \to 0} \frac{f_2}{x_2}$  where  $f_2$  is the fugacity of CO<sub>2</sub>.
- \*\* calculated by the compiler as indicated above.

# METHOD/APPARATUS/PROCEDURE: Vapor-liquid equilibrium cell. Diagram given in source. (Original in Japanese) ESTIMATED ERROR: REFERENCES:

	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Makranczy, J.; Rusz, L.;
_	Balog-Megyery, K.
2. Methanol; CH <sub>4</sub> O; [67-56-1]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6
VARIABLES:	PREPARED BY:
T/K = 298.15	C.L. Young
P/kPa = 101.3	
EXPERIMENTAL VALUES:	
	vald Mole fraction of carbon dioxide*,
	<sup>x</sup> CO₂
	A PROGRAM AND THE PROGRAM AND
298.15 101.3 3.5	0.005871
* calculated by co	ompiler
+ partial pressure	e of carbon dioxide.
AUXILIARY	INFORMATION
	INFORMATION SOURCE AND PURITY OF MATERIALS:
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:	
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:  No details given.
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:  No details given.
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS: No details given. ESTIMATED ERROR: $\delta x_{\rm CO_2} = \pm 3\%$
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS: No details given. $\delta x_{\rm CO_2} = \pm 3\%$ REFERENCES:
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR: $\delta x_{\rm CO_2} = \pm 3 \%$ REFERENCES:  1. Bodor, E.; Bor, Gy.; Mohai, B.;
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR: $\delta x_{\text{CO}_2} = \pm 3\%$ REFERENCES:  1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos. G. Veszpremi Vegyip. Egy. Kozl.
METHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR: $\delta x_{\text{CO}_2} = \pm 3\%$ REFERENCES:  1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos. G.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Methanol; CH<sub>4</sub>O; [64-56-1]

### ORIGINAL MEASUREMENTS:

Won, Y. S.; Chung, D. K.; Mills, A. F

J. Chem. Eng. Data 1981, 26, 140 - 141.

### VARIABLES:

T/K = 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	rature	Solubility	Mol Fraction	Ostwald
t/ºC	T/K	$c_1/\text{kmol m}^{-3}\text{atm}^{-1}$	$10^3 x_{1}$	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
25	298.15	0.159	6.43	3.89

The mole fraction and Ostwald coefficient were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The carbon dioxide solubility was determined by saturating the liquid phase in a gas bubbler immersed in an isothermal bath. The liquid phase carbon dioxide concentration was determined by using a standard wet chemistry technique (1). The partial pressure of the carbon dioxide over the liquid was calculated by subtracting the vapor pressure of the liquid from the measured total pressure.

The diffusivity of carbon dioxide was measured.  $10^9 D/m^2 s^{-1} = 8.37$ 

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information.
- (2) Methanol. Source not given. The density, kinematic viscosity, and surface tension were measured and reported in the paper. Values are  $\rho/kg \text{ m}^{-3} = 786.6$ ,  $10^6 \text{ v/m}^2 \text{ s}^{-1} = 0.695$ , and  $10^3 \text{ σ/N m}^{-1} = 22.2$ .

### ESTIMATED ERROR:

$$\delta c_1/c_1 = \pm 0.02$$

### REFERENCES:

1. Chung, D. K.
 Ph. D. Dissertation, 1974
 University of California,
 Los Angeles

COMPONENTS:		ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dio [124-38-9]</li> <li>Alcohols</li> </ol>		Luhring, P.; Schumpe, A.  J. Chem. Eng. Data 1989, 34, 250-252
VARIABLES:		PREPARED BY:
T/K = 293.	2	C.L. Young; P.G.T. Fogg
EXPERIMENTAL VALUE	S:	
T/K	Henry's Constant* /(Pa m³/mol <sup>-1</sup> )	Mole fraction of CO₂ at 1 atm <sup>†</sup> partial pressure
	Methanol; CH	40; [67-56-1]
293.2	601	0.00683
	Ethanol; C <sub>2</sub> H	60; [64-17-5]
293.2	802	0.00737
	2-Propanol;	C <sub>3</sub> H <sub>8</sub> O; [67-63-0]
293.2	1070	0.00720
	1-Butanol; C	4H <sub>10</sub> ; [71-36-3]
293.2	1179	0.00781
Henry's cons	tant multiplied by the	source but appears to be the usual molar volume density data taken from ref. (1).
	AUXILIARY	'INFORMATION
METHOD /ADDADATHS /D	DOGERNING	COURSE AND DUDING OF MARCHIALC

### METHOD APPARATUS / PROCEDURE:

Little information is given in source. Method consisted of equilibrating known amounts of degassed liquid and gas and measuring the change in pressure. Equilibration was reached in 3 to 6 minutes. Some details given in ref. 2.

### SOURCE AND PURITY OF MATERIALS:

2. Obtained from Merck at the highest available purity. No other details given.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  (authors)  $\delta x/x = \pm 0.01$  to 0.15 (compilers)

- 1. International Critical Tables McGraw Hill, New York 1929.
- Schumpe, A.; Quiker, G.;
   Decker, W.D. Adv. Biochem. Eng. 1982, 24, 1.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### **EXPERIMENTAL VALUES:**

<i>T/</i> K	Mol Fraction	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	7.38	2.97	3.130
293.15 298.15	7.04 6.45	2.72 2.48	2.973 2.706

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Ethanol. Source not given. Stated to be 97 per cent.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- Carbon dioxide; CO<sub>2</sub>
  [124-38-9]
- 2. Alkanols

### ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Gaz. Prom. 1958, 12, 36-42.

### VARIABLES:

P/kPa = 13.3-101.3T/K = 212.7-298.2

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

EXPERIMENTAL	VALUES:				
Solvent	T/K	P/mmHg	P/kPa*	Solubility** cm³g-1	X <sub>CO2</sub>
Ethanol; C <sub>2</sub> H <sub>6</sub> O; [64~17-5]	248.0	100 300 500 760 100	13.33 40.00 66.66 101.32 13.33	1.37 1.10 6.89 10.52 2.78	0.00282 0.00842 0.01400 0.02130 0.00572
	212.7	300 500 760 100	40.00 66.66 101.32	8.43 14.23 21.97	0.01715 0.02860 0.04350
	212.7	300 500 760	13.33 40.00 66.66 101.32	5.30 16.28 27.80 43.50	0.01085 0.03260 0.05440 0.08260
1-Propanol; C <sub>3</sub> H <sub>8</sub> O; [71-23-8]	248.0	100 300 500 760	13.33 40.00 66.66 101.32	0.836 2.852 4.785 7.315	0.00255 0.00764 0.01275 0.01936
	227.9	100 300 500 760	13.33 40.00 66.66 101.32	1.851 5.604 9.445 14.538	0.00497 0.01490 0.02486 0.03776
	212.7	100 300 500 760	13.33 40.00 66.66 101.32	3.345 10.065 17.011 26.774	0.00895 0.02645 0.04390 0.06740

<sup>\*</sup> calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A static method was used. A weighed quantity of solvent was placed in the absorption pipet which was subsequently cooled in a cryostat with automatic temperature control. The solvent was then degassed under vacuum. Liquid lost during this process was collected in an absorption column and weighed so appropriate correction could be made to the weight of solvent. Carbon dioxide was then supplied from a calibrated gas buret. The liquid was stirred by an electromagnetic stirrer until equilibrium was reached.

### SOURCE AND PURITY OF MATERIALS:

- from commercial solid carbon dioxide; purified twice by evaporation, freezing and pumping with a vacuum pump.
- 2. No information

### ESTIMATED ERROR:

<sup>\*\*</sup> defined as the volume of gas, corrected to 273.15 K and 101.325 kPa, dissolved by one gram of solvent at the stated temperature and pressure.

Carbon dioxide; CO<sub>2</sub>
[124-38-9]

2. Alkanols

ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Gaz. Prom. 1958, 12, 36-42.

EXPERIMENTAL VA	LUES:
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Solvent	T/K	P/mmHg	P/kPa*	Solubility** cm³g-1	*CO <sub>2</sub>
2-Propanol; C <sub>3</sub> H <sub>8</sub> O; [67-63-0]	248.0	100 300 500	13.33 40.00 66.66	0.817 2.461 4.121	0.00220 0.00660 0.01100
	227.9	760 100 300 500 760	101.32 13.33 40.00 66.66	6.280 1.626 4.922 8.276 12.719	0.01667 0.00437 0.01311 0.02185
	212.7	100 300 500 760	101.32 13.33 40.00 66.66 101.32	3.013 9.188 15.540 24.090	0.03319 0.00806 0.02420 0.04025 0.06101
1-Butanol; C <sub>4</sub> H <sub>10</sub> O; [71-36-3]	248.0	100 300 500	13.33 40.00 66.66	0.786 2.374 3.373	0.00261 0.00781 0.01305
	227.9	760 100 300 500 760	101.32 13.33 40.00 66.66 101.32	6.076 1.586 4.591 7.736 11.931	0.01982 0.00525 0.01505 0.02510 0.03819
	212.7	100 300 500 760	13.33 40.00 66.66 101.32	2.715 8.175 13.820 21.740	0.00895 0.02650 0.04400 0.06750
2-Methyl-1- propanol; C <sub>4</sub> H <sub>10</sub> O;	248.0	100 300 500	13.33 40.00 66.66	0.618 1.843 3.125	0.00205 0.00610 0.01030
[78-83-1]	227.9	760 100 300 500 760	101.32 13.33 40.00 66.66 101.32	4.728 1.236 3.679 6.190 9.480	0.01550 0.00401 0.01210 0.02020 0.03060
	212.7	100 300 500 760	13.33 40.00 66.66 101.32	2.178 6.786 11.571 18.010	0.00720 0.02210 0.03710 0.05660
2-Butanol; C <sub>4</sub> H <sub>10</sub> O; [78-92-2]	248.0	100 300 500 760	13.33 40.00 66.66 101.32	0.568 1.71 2.87	0.00189 0.00566 0.00943
	227.9	100 300 500 760	13.33 40.00 66.66 101.32	4.38 1.01 3.05 5.08 7.82	0.01435 0.00334 0.01000 0.01665 0.02535
	212.7	100 300 500 760	13.33 40.00 66.66 101.32	1.70 5.17 7.75 13.40	0.00562 0.01685 0.02810 0.04270

 $<sup>^{\</sup>star}$  calculated by the compiler.

<sup>\*\*</sup> defined as the volume of gas, corrected to 273.15 K and 101.325 kPa, dissolved by one gram of solvent at the stated temperature and pressure.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5]</li> </ol>	Makranczy, J.; Rusz, L.; Balog-Megyery, K.	
	Hung. J. Ind. Chem. 1979, 7, 41-6.	
VARIABLES:	PREPARED BY:	
T/K = 298.15 P/kPa = 101.3	C.L. Young	
EXPERIMENTAL VALUES:		
	wald Mole fraction of carbon dioxide*, ${}^{x}_{\text{CO}_2}$	
298.15 101.3 2.	892 0.006889	
* calculated by c	ompiler	
+ partial pressur	e of carbon dioxide	
	INFORMATION	
WETHOD/APPARATUS/PROCEDURE:  Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1) was used.	SOURCE AND PURITY OF MATERIALS:  No details given	
	ESTIMATED ERROR:	
	δx <sub>CO2</sub> = ±3%	
	REFERENCES:	
	1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G.  Veszpremi Vegyip. Egy. Kozl.  1957, 1, 55.  Chem. Abstr. 1961, 55, 3175h.	

- Carbon dioxide; CO2; [124-38-9]
- 2. Ethanol;  $C_2H_6O$ ; [64-17-5]

### ORIGINAL MEASUREMENTS:

Cargill, R.W.; MacPhee, D.E.

J. Chem. Research (S) 1981, 232; J. Chem. Research (M) 1981, 2743-2755.

### VARIABLES:

T/K = 277.9 - 334.6 $P_{\rm CO_2}/{\rm kPa} = 101.3$ 

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

P <sub>CO2</sub> /kPa	T/K	$S_0/\text{cm}^3\text{kg}^{-1}$	<sup>*</sup> CO₂
101.3	277.9	4820	0.010451
	284.8	4300	
	285.8		0.008977
	294.2		0.007729
	294.3	3720	
	303.2		0.006670
	305.9	3010	
	312.6		0.005770
	312.7	2700	
	322.7		0.005002
	323.7	2380	
	333.4		0.004346
	334.6	2140	

 $S_{\rm o}$  is the volume of gas, reduced to 1.013 bar and 273.15 K, which is dissolved by 1 kg of solvent.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The authors measured solubilities by the flowing film method as described by Morrison (1) and modified by Cargill (2). Solubilities were corrected to a partial pressure of carbon dioxide of 1.013 bar (3).

### SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by British Oxygen Company; purity 99.9%.
- 2. Purity 99.9%

### ESTIMATED ERROR:

- 1. Morrison, T.J.; Billett, F. J. Chem. Soc. 1948, 2033; J. Chem. Soc. 1952, 3819
- 2. Cargill, R.W.; Morrison, T.J. J. Chem. Soc., Faraday Trans. 1, 1975, 618.
- 3. Private communication.

<sup>\*</sup> smoothed data given by the authors.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5]

### ORIGINAL MEASUREMENTS:

Won, Y. S.; Chung, D. K.; Mills, A. F.

J. Chem. Eng. Data 1981, 26, 140-141.

VARIABLES:

T/K = 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Temp	erature	Solubility	Mol Fraction	Ostwald
t/°C	<i>T</i> /K	$e_1/\text{kmol m}^{-3} \text{ atm}^{-1}$	10³x <sub>1</sub>	Coefficient _L/cm³cm-3
25	298.15	0.125	7.28	3.06

The mole fraction and Ostwald coefficients were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The carbon dioxide solubility was determined by saturating the liquid phase in a gas bubbler immersed in an (2) Ethanol. Source not given. isothermal bath. The liquid phase The density, kinematic visc carbon dioxide concentration was determined by using a standard wet chemistry technique (1). The partial pressure of the carbon dioxide over the liquid was cal-culated by subtracting the vapor pressure of the liquid from the measured total pressure.

The diffusivity of carbon dioxide was measured.  $10^9 \text{ C/m}^2 \text{ s}^{-1} = 3.88.$ 

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information.
- The density, kinematic viscosity, and surface tension were measured values are  $\rho/kg$  m<sup>-3</sup> = 785.0,  $10^6 v/m^2$  s<sup>-1</sup> = 1.400, and  $10^3 \sigma/N$  m<sup>-1</sup> = 22.7.

### ESTIMATED ERROR:

$$\delta c_1/c_1 = \pm 0.02$$

### REFERENCES:

1. Chung, D. K. Ph.D. Dissertation, 1974 University of California, Los Angeles

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Takahashi, M.; Kobayashi, Y.; Takeuchi, H.

J. Chem. Eng. Data 1982, 27, 328-31.

VARIABLES: T/K = 298 $p_1/kPa = 101.3$ 

Composition.

PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Ethanol Mol Fraction	Viscositya	Diffusion Coefficient	Solubility
	x_2	$10^3 \mu_{\rm m}/Pa$ s	$\frac{10^9 D_{\rm A}}{\rm m^2 s^{-1}}$	$c_1/\text{mol m}^{-3}$
298	0.00 0.20 0.40 0.60 0.80 1.00	1.97 1.71 1.55 1.39 1.24 1.08	3.06 3.26 3.33 3.50 3.72 3.86	62.9 71.8 76.5 76.6 88.8

a Literature values taken from Ishikawa, T. "Kongoeki Nendo no Riron" (Theories of Viscosity for Mixed Solvents); Maruzen, Tokyo, 1968.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An indirect method (1) was used in which the absorption rate of carbon dioxide into the mixed solvent was measured as a function of time.

It was assumed that the film-theory model of the gas absorption process applied. A plot of ln (absorption rate) vs. time is linear. The slope is a function of the diffusion coefficient and the intercept is a function of both the diffusion coefficient and the solubility.

A diaphram cell with interfacial area 5.81 cm² and lower compartment volume for the liquid was 53.5 cm³. The diaphram was Millipore Teflon of mean pore size 10.0  $\mu$ m, thickness 125  $\pm$  15  $\mu$ m, and porosity 0.68. The liquid was stirred at a constant rate of 1.33 rotations s<sup>-1</sup>.

The solutions were prepared and then degassed by refluxing for five hours. Their compositions were determined by density or refractive index. The CO<sub>2</sub> was presat. with solvent vap.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not identified. From cylinder.
- (2, 3) Ethanol and 1-Propanol. It was stated that the chemicals were of special grade.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.1$$
  
 $\delta c_{1}/c_{1} = \pm 0.05 - 0.10$  (compiler).

### REFERENCES:

 Takeuchi, H.; Fujine, M.; Sato, T.; Onda, K.
 J. Chem. Eng. Jpn. 1975, 8, 25 and 252.

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]

(2) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 298.15 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^3 x_1$	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm³cm-3	_
298.15	7.62	2.29	2.498	

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1-Propanol. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]
   2-Propanol; C<sub>3</sub>H<sub>8</sub>O; [67-63-0]

### ORIGINAL MEASUREMENTS:

Tokunaga, J.

J. Chem. Eng. Data 1975, 20, 41-46.

### VARIABLES:

T/K = 283.15-313.15 $P_{CO_2} = 101.3 \text{ kPa}$ 

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	T/K	Ostwald coef. L	H/atm	H/kPa*	* at CO <sub>2</sub> = 101.3 kPa
1-Propanol	283.15 293.15 303.15 313.15	2.76 2.27 2.1 1.88	113 137 157 179	11450 13882 15908 18137	0.00877 0.00725 0.00633 0.00556
2-Propanol	283.15 293.15 303.15 313.15	2.53 2.18 1.95 1.86	122 145 166 178	12362 14692 16820 18036	0.00813 0.00685 0.00599 0.00559

Henry's constant, H, was taken to be given by

mole ratio solubility of  $CO_2$ 

partial pressure of CO<sub>2</sub>, P<sub>CO<sub>2</sub></sub>

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Solvents were refluxed for several hours to remove dissolved gases. a measured volume of the solvent was then transferred to an absorption chamber fitted with a magnetic stirrer and connected to a system of gas burets, vacuum line and mercury reservoir. A measured volume of the gas then came in contact with the liquid which was agitated until equilibrium was reached. The final volume of the gas was then measured.

### SOURCE AND PURITY OF MATERIALS:

- super pure grade from Nippon Tansan Co. Ltd.; 98.96% pure.
   from Wako Pure Chemicals Ind.;
- 2. from Wako Pure Chemicals Ind.; fractionated before use. 1-propanol:

 $\rho_{25} = 0.7990; \, \eta_{25} = 1.38345$  2-propanol:

 $\rho_{25} = 0.78087; \, \eta_{25} = 1.37500$ 

ESTIMATED ERROR:

<sup>\*</sup> calculated by the compiler

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Makranczy, J.; Rusz, L.; Balog-Megyery, K.		
2. 1-Propano1; C <sub>3</sub> H <sub>8</sub> O; [71-23-8]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6		
VARIABLES:	PREPARED BY:		
T/K = 298.15 P/kPa = 101.3	C.L. Young		
EXPERIMENTAL VALUES:			
	wald Mole fraction of icient carbon dioxide*,  **CO2		
298.15 101.3 2.	0.007817		
* calculated by c	ompiler		
+ partial pressur	e of carbon dioxide.		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1) was used.	No details given		
	ESTIMATED ERROR:		
	$\delta x_{\text{CO}_2} = \pm 3\%$		
	REFERENCES:  1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G.		

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9] 2. 1-Butanol; C <sub>4</sub> H <sub>10</sub> O; [71-36-3]	Makranczy, J.; Rusz, L.; Balog-Megyery, K.  Hung. J. Ind. Chem. 1979, 7, 41-6.		
VARIABLES:	PREPARED BY:		
T/K = 298.15 P/kPa = 101.3	C.L. Young		
EXPERIMENTAL VALUES:			
T/K P <sup>+</sup> /kPa Ost coeff	wald Mole fraction ficient of carbon dioxide,*  xCO2		
298.15 101.3 2.	369 0.008827		
* calculated by c	compiler		
	e of carbon dioxide		
AUVILLAD	/ INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS;		
Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1) was used.	No details given.		
	ESTIMATED ERROR:		
	ESTIMATED ERROR: $\delta x_{\text{CO}_2} = \pm 3\%$		

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Methyl-1-propanol; C<sub>4</sub>H<sub>10</sub>O; [78-83-1]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

	• •		
	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm³cm-3
288.15	5 8.06	1.98	2.088
293.15	7.49	1.83	1.964
298.15	6.98	1.69	1.849

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 2-Methyl-1-propanol.
  No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Methyl-1-propanol or isobutyl alcohol;  $C_AH_QOH$ ; [78-83-1]

### ORIGINAL MEASUREMENTS:

Battino, R.; Evans, F. D.; Danforth, W. F.; Wilhelm, E.

J. Chem. Thermodyn. 1971, 3, 743 - 751.

### VARIABLES:

T/K: 273.98 - 328.00 P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen Coefficient α/cm <sup>3</sup> (STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
	<u></u>		
273.98	10.24	2.55	2.56
283.01	8.50	2.09	2.17
297.71	6.96	1.69	1.84
297.77	7.01	1.71	1.86
298.17	7.11	1.73	1.89
298.22	7.04	1.72	1.87
312.75	5.71	1.36	1.56
312.77	5.72	1.37	1.57
328.00	4.68	1.09	1.32
		*** * * * *	

The Bunsen coefficients were calculated by the compiler with the assumption the gas was ideal.

Smoothed Data: For 273.15 to 328.15 K

 $\ln x_1 = -9.2306 + 12.7124/(T/100K)$ 

The standard error about the regression line is  $1.22 \times 10^{-4}$ .

T/K	Mol Fraction $10^3 x_1$	<i>T/</i> K	Mol Fraction $10^3 x_1$
278.15	9.46	308.15	6.065
288.15	8.08	318.15	5.33
298.15	6.965	328.15	4.72

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. The Matheson Co. Inc. Commercial grade stated to be better than 99 mol per cent.
- (2) 2-Methyl-1-propanol. Fisher Co. Certified grade (99 mol per cent)

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.03$   $\delta P/\text{mmHg} = \pm 0.5$  $\delta x_1/x_1 = \pm 0.005$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Pentanol or amyl alcohol;  $C_5H_{12}O$ ; [71-41-0]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^3 x_1$	Bunsen Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
288.15	9.29	1.95	2.058
293.15	8.65	1.81	1.941
298.15	8.07	1.68	1.831

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1-Pentanol. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52,
   275.

				101
COMPO	NENTS:			ORIGINAL MEASUREMENTS:
1. 2.				Makranczy, J.; Rusz, L.; Balog-Megyery, K.
		or C <sub>6</sub> H <sub>14</sub> O; [111-2	27-3]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6.
VARIA	BLES:			PREPARED BY:
	T/K = 298 P/kPa = 1			C.L. Young
EXPER	IMENTAL VALUES	:		
	T/K	p <sup>+</sup> /kPa		wald Mole fraction of cient carbon dioxide*, $^{x}$ CO $_{2}$
			l- Per	ntanol
	298.15	101.3	2.2	0.00974
			1- He	anol
	298.15	101.3	2.3	0.0108
		A	AUXILIARY	INFORMATION
METHO	D/APPARATUS/PR	OCEDURE:		SOURCE AND PURITY OF MATERIALS:
of		hod. The appar Mohai, and Sir		No details given.
				ESTIMATED ERROR:
				$\delta x_{\text{CO}_2} = \pm 3\%$
				REFERENCES:  1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G.     Veszpremi Vegyip. Egy. Kozl.     1957, 1, 55.     Chem. Abstr. 1961, 55, 3175h

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Pentanol; C<sub>5</sub>H<sub>12</sub>O; [71-41-0]

### ORIGINAL MEASUREMENTS:

Pedrosa, G.C.; Salas, J.A.; Katz, M.

Anal. Asoc. Quim. Argent. 1988, 76(3), 199-206.

### VARIABLES:

T/K = 288.15-318.15 $P/kPa \approx 101.3$ 

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	density of solvent /kg m <sup>-3</sup>	Bunsen coeff. $\alpha$	Ostwald coeff. $\stackrel{L}{\iota}$	Henry's constant† /Mpa	${}^{x}_{CO_{2}}^{at} {}^{P}_{CO_{2}}^{P}$ = 101.3 kPa*
288.15	818.4	1.957	2.065	10.87	0.00924
298.15	811.5	1.657	1.809	12.72	0.00790
308.15	804.8	1.472	1.660	14.19	0.00709
318.15	800.6	1.324	1.542	15.58	0.00646

 $P_{\text{CO}_2} \simeq 101.3 \text{ kPa}$ 

†Henry's constant, H, was assumed by the compiler to be given by:

$$H = P_{CO_2}/N$$

where N is the mole ratio solubility of carbon dioxide.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Densities of the pure solvent were measured using a digital densitometer AP, model DMA 45 with temperatures controlled to 0.01 K with a Haake thermostat and measured to 0.01 K by a Digtec thermometer. The densitometer was first calibrated with distilled water.

The method and details of apparatus for measuring the absorption of gas are given in ref. (1). An Erlenmeyer flask connected to a pressure transducer was used. The transducer was first calibrated against a manometer containing dibutyl phthalate.

### SOURCE AND PURITY OF MATERIALS:

- 1. from a cylinder; purity 99.5%
- Merck p.a. grade was used without further purification apart from degasification by boiling.

### **ESTIMATED ERROR:**

 $\delta \rho / \text{kg m}^{-3} = \pm 0.1$  $\delta L = \pm 1\%$  (authors)

### REFERENCES:

 Postigo, M.A.; Pedrosa, G.C.; Katz, M.

Anal. Asoc. Quim. Argent. 1978, 66, 25.

<sup>\*</sup>calculated by the compiler

COMPO				
1.			ORIGINAL MEASUREMENTS:	
2.		ride; $CO_2$ ; [124-38-9] $C_7H_{16}O$ ; [111-70-6]	Makranczy, J.; Rusz, L.; Balog-Megyery, K.	
	or		Hung. J. Ind. Chem. 1979, 7, 41-6.	
VARIA	BLES:		PREPARED BY:	
	T/K = 29 P/kPa =		C.L. Young	
EXPER	IMENTAL VALUES:	:		
	T/K		twald Mole fraction of . ficient carbon dioxide*, $^x\mathrm{CO}_2$	
		lF	eptanol	
	298.15	101.3	.052 0.01175	
		1-0	ctanol	
	298.15	101.3	.997 0.01277	
		* calculated by	compiler	
			re of carbon dioxide.	
	· · · · · · · · · · · · · · · · · · ·			
		AUXILIA	Y INFORMATION	
METHO	DD/APPARATUS/PR		SOURCE AND PURITY OF MATERIALS:	
Vol	lumetric metl			
Vol	lumetric meth Bodor, Bor,	OCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Vol	lumetric meth Bodor, Bor,	OCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Vol	lumetric meth Bodor, Bor,	OCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Vol	lumetric meth Bodor, Bor,	OCEDURE:	SOURCE AND PURITY OF MATERIALS:  - No details given.	
Vol	lumetric meth Bodor, Bor,	OCEDURE:	SOURCE AND PURITY OF MATERIALS:  No details given.  ESTIMATED ERROR: $\delta x_{\text{CO}_2} = \pm 3\%$	
Vol	lumetric meth Bodor, Bor,	OCEDURE:	SOURCE AND PURITY OF MATERIALS:  - No details given.  ESTIMATED ERROR:	

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. 1-Heptanol; C<sub>7</sub>H<sub>16</sub>O; [111-70-6] 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5] VARIABLES: T/K = 298.2 P/kPa ~ 101.3

### EXPERIMENTAL VALUES:

Solvent	P <sub>CO2</sub> /kPa†	T/K	Solubility /mol cm <sup>-3</sup>	*CO2*
1-heptanol	101.3	298.15	7.63 × 10 <sup>-5</sup>	0.01069
1-octanol	101.3	298.15	$7.42 \times 10^{-5}$	0.01166

- + the presure of gas is not stated in the paper. It has been assumed by the compiler that the pressure was equal to barometric.
- \* calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Barium carbonate precipitated from a saturated solution of carbon dioxide was subsequently back titrated with hydrochloric acid. Details of the method have been given in refs (1) and (2). Densities of solvents were measured with a calibrated pycnometer.

### SOURCE AND PURITY OF MATERIALS:

- 2. 1-Heptanol; density = 0.8209 g cm<sup>-3</sup>
  - 1-octanol; density =  $0.8190 \text{ g cm}^{-3}$

### ESTIMATED ERROR:

- 1. Dim. A. Eng. Sc. Thesis, University of Sydney, 1969.
- 2. Gardner, G.R. M.Sc. Thesis, University of Manchester, 1968.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Octanol; C<sub>8</sub>H<sub>17</sub>OH; [111-87-5]

### ORIGINAL MEASUREMENTS:

Wilcock, R. J.; Battino, R.; Danforth, W. F.; Wilhelm, E.

J. Chem. Thermodyn. 1978, 10, 817 - 822.

VARIABLES: T/K: 282.66 - 313.64 p/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^3 x_1$	Bunsen Coefficient \alpha/cm3 (STP) cm-3 atm-1	Ostwald Coefficient _L/cm³ cm-3
282.66	11.53	1.662	1.720
298.12	9.301	1.322	1.443
313.64	7.849	1.100	1.263

The Bunsen coefficients were calculated by the compiler.

It is assumed that the gas is ideal and that Henry's law is obeyed.

Smoothed Data: For use between 283.15 to 313.15 K

 $\ln x_7 = -8.3646 + 11.0172/(T/100K)$ 

The standard error about the regression line is  $9.97 \times 10^{-5}$ .

T/K	Mol Fraction $10^3 x_1$
283.15	11.41
293.15	9.99
298.15	9.38
303.15	8.82
313.15	7.86

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Up to 500 cm3 of solvent Degassing. is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and Vacuum is intermittently applied through a liquid N2 trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum mole per cent purity stated to be 99.8.
- (2) 1-Octanol. Eastman Organic Chemicals. Distilled, density at 298.15 K, /g cm - 0.8247.

ESTIMATED ERROR:

$$\delta T/K = 0.02$$
  
 $\delta p/mmHg = 0.5$   
 $\delta x_1/x_1 = 0.01$ 

- 1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- 2. Battino, R.; Evans, F. D.;
   Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>1-Nonanol; C<sub>9</sub>H<sub>20</sub>O; [143-08-8]</li> </ol>	Makranczy, J.; Rusz, L.; Balog-Megyery, K.
or 1-Decanol; C <sub>10</sub> H <sub>22</sub> O; [112-30-1]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6
VARIABLES:	PREPARED BY:
T/K = 298.15 P/kPa = 101.3	C.L. Young
EXPERIMENTAL VALUES:	
T/K P <sup>+</sup> /kPa Ostwal coeffici	
l-Nona	nol
298.15 101.3 1.954	0.01378
1-Deca	nol
298.15 101.3 1.910	0.01473
* calculated by co	ompiler
+ partial pressure	e of carbon dioxide
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method. The apparatus of Bodor, Bor, Mohai and Sipos (1) was used.	No details given
	ESTIMATED ERROR:
	$\delta x_{\text{CO}_2} = \pm 3\%$
	REFERENCES:  1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos. G.  Veszpremi Vegyip. Egy. Kozl.  1957, 1, 55.  Chem. Abstr. 1961, 55, 3175h

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Decanol; C<sub>10</sub>H<sub>21</sub>OH;

# ORIGINAL MEASUREMENTS:

Wilcock, R. J.; Battino, R.; Danforth, W. F.; Wilhelm, E.

J. Chem. Thermodyn. 1978, 10, 817 - 822.

# VARIABLES:

T/K: 284.01 - 313.49 p/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

 T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³ cm <sup>-3</sup>
284.01	12.32	1.468	1.526
298.15	9.733	1.144	1.249
313.49	7.914	0.917	1.053

The Bunsen coefficients were calculated by the compiler.

It is assumed that the gas is ideal and that Henry's law is obeyed. Smoothed Data: For use between 283.15 to 313.15 K

 $\ln x_7 = -9.1079 + 13.3691/(T/100K)$ 

The standard error about the regression line is 1.01 x  $10^{-4}$ .

Т/К	Mol Fraction 103x1
283.15	12.45
293.15	10.59
298.15	9.81
303.15	9.11
313.15	7.92

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to  $500~\rm{cm}^3$  of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid  $N_2$  trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum mole per cent purity stated to be 99.8.
- (2) 1-Decanol. Eastman Organic Chemicals. Distilled, density at 298.15 K, ρ/g cm<sup>-3</sup> 0.8206.

ESTIMATED ERROR:

 $\delta T/K = 0.02$   $\delta p/mmHg = 0.5$  $\delta x_1/x_1 = 0.01$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.
- Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO<sub>2</sub>; [124-38-9] Makranczy, J.; Rusz, L.; Balog-Megyery, K. 2. 1-Undecanol; C<sub>11</sub>H<sub>24</sub>O; [112-42-5] Hung. J. Ind. Chem. 1979, 7, 41-6. 1-Dodecanol; C<sub>12</sub>H<sub>26</sub>O; [112-53-8] VARIABLES: PREPARED BY: T/K = 298.15C.L. Young P/kPa = 101.3EXPERIMENTAL VALUES: P<sup>+</sup>/kPa T/KOstwald Mole fraction of coefficient carbon dioxide\*, $x_{CO_2}$ 1-Undecanol; $C_{11}H_{24}O$ ; [112-42-5] 101.3 0.01571 298.15 1.877 1-Dodecanol; $C_{12}H_{26}O$ ; [112-53-8] 101.3 298.15 1.845 0.01664 \* calculated by compiler + partial pressure of carbon dioxide. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric method. The apparatus No details given. of Bodor, Bor, Mohai, and Sipos (1) was used. ESTIMATED ERROR: $\delta x_{\text{CO}_2} = \pm 3\%$ REFERENCES: 1. Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55. Chem. Abstr. 1961, 55, 3175h.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. 1-Decanol; C<sub>10</sub>H<sub>22</sub>O; [112-30-1] 3. 1-Dodecanol; C<sub>12</sub>H<sub>26</sub>O; [112-53-8] VARIABLES: T/K = 293.15-355.15 P/kPa = 0-80 kPa ORIGINAL MEASUREMENTS: Luther, H.; Hiemenz, W. Chem. Ing. Tech. 1957, 29, 530-535. PREPARED BY: P.G.T. Fogg

### EXPERIMENTAL VALUES:

The solvent consisted of an equimolar mixture of 1-decanol and 1-dodecanol.

T/K	Concentr	_	Ostwald coeff. $L$	Henry's const		Mole fraction solubility at 101.3 kPa
	/mol m <sup>-</sup> liquid	gas	L	/atm	/kPa**	101+3 RF4
293.15 314.15 334.65 355.15	7.56 5.43 4.30 3.48	5.61 5.25 5.00 4.75	1.35 1.03 0.850 0.733	93.7±1.9	9490±190	0.0107

At 293.15 K the mole fraction solubility was shown to be proportional to the partial pressure of carbon dioxide to a pressure of at least 600 Torr (80  $\,\mathrm{kPa}$ ).

- \* concentrations correspond to partial pressures of carbon dioxide of about 13 kPa.
- \*\* calculated by the compiler.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A spectroscopic method was used. The gas and solution under test was circulated through cuvettes. The concentration of carbon dioxide in the gas and liquid phases were calculated from the integrated extinction coefficient due to the infra-red band at 2350 cm<sup>-1</sup>

SOURCE AND PURITY OF MATERIALS:

 from a cylinder; purified by the usual methods.

ESTIMATED ERROR:

 $\delta L \leq \pm 7.5\%$  (authors)

# ORIGINAL MEASUREMENTS: COMPONENTS: (1) Carbon dioxide; CO2; [124-38-9] Cauquil, G. (2) Cyclohexanol; C<sub>6</sub>H<sub>12</sub>O; J. Chim. Phys. 1927, 24, [108-93-0] 53-55. VARIABLES: PREPARED BY: T/K = 299 $p_1/kPa = 102$ H. L. Clever EXPERIMENTAL VALUES: The author states that one liter of cyclohexanol absorbs 677 $\rm cm^3$ carbon dioxide at 26 $^{\circ}C$ and 766 mmHg. The compiler calculates an Ostwald coefficient of $L/{\rm cm}^3$ cm<sup>-3</sup> = 0.677 and a mole fraction solubility of $x_1$ = 2.86 x $10^{-3}$ at 299 K and a gas partial pressure of 101.325 kPa (1 atm). AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) Carbon dioxide. The apparatus appears to be of the No information. Bunsen type. (2) Cyclohexanol. Distilled, boiling point 160.9 °C at 766 mmHg. The initial and final volumes of gas in contact with the liquid were measured. The vapor pressure Degassed and tested to be air of the liquid was ignored. free. ESTIMATED ERROR: $\delta L/L = \pm 0.05$ (compiler) REFERENCES:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Cyclohexanol; C<sub>6</sub>H<sub>12</sub>O; [108-93-0]

# ORIGINAL MEASUREMENTS:

Begley, J.W.; Maget, J.R.;
Williams, B.

J. Chem. Eng. Data 1965, 10, 4-8.

# VARIABLES:

P/kPa = 101.3T/K = 298.25-320.95

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

т/к	Ostwald coefficient L	Mole fraction solubility  x at PCO2 = 101.3 kPa*
298.25	1.017	0.00442
301.45	0.990	0.00427
303.75	0.980	0.00420
306.75	0.957	0.00408
309.45	0.925	0.00391
312.75	0.910	0.00382
314.95	0.887	0.00370
320.95	0.830	0.00342

<sup>\*</sup>calculated by the compiler using the expression for the density of the solvent given in The International Critical Tables.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solvent was boiled to remove any gases in solution and was then introduced into the absorption vessel without coming into contact with the air. The volume of carbon dioxide absorbed by the liquid from gas buret was then measured. The composition of the solution after equilibrium was attained was measured by chemical analysis. enabled a check to be made of solubility as calculated from the volume of gas absorbed. The absorption vessel and the gas buret were kept at constant temperature by circulation of water from a thermostat bath.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide 99.99% pure, from a cylinder supplied by Mathiesen Chemical Company.
- 2. Cyclohexanol technical grade from Dow Chemical Company. Impurities were phenol max.0.5 wt%; cyclohexanone max. 0.1wt%; water max. 0.5 wt%

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  Solubility measurements reproducible to about  $\pm 0.5\%$  (authors).

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Benzenemethanol (Benzyl alcohol);
   C<sub>7</sub>H<sub>8</sub>O; [100-51-6]

1,2-Ethanediol (Ethylene glycol); C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>; [107-21-1]

# ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data, 1971, 16, 340-2.

### VARIABLES:

T/K = 298.2

### PREPARED BY:

C. L. Young

# EXPERIMENTAL VALUES:

Solvent	T/K	Henry's constant  HCO2/atm	Mole fraction at $1atm^*$
Benzenemethanol	298.2	128	0.00781
1,2-Ethanediol	298.2	262	0.00382

\* Calculated by the compiler assuming a linear function of  $p_{\text{CO}_2}$  vs  $x_{\text{CO}_2}$ , i.e.  $x_{\text{CO}_2}$  (1 atm) =  $1/H_{\text{CO}_2}$ 

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

### SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Benzenemethanol, (benzyl
  alcohol); C<sub>7</sub>H<sub>8</sub>O; [100-51-6]

# ORIGINAL MEASUREMENTS:

Emel'yanova, E.A.; Tsimmerman, S.S.; Semenova, A.I.; Tsiklis, D.S.

Zhur. Fiz. Khim. 1980, 54, 382-384. Russian J. Phys. Chem. 1980, 54(2), 219-220.

### VARIABLES:

T/K = 323.15-398.25P/kPa = 500-14000 kPa

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Measurements were made over the pressure range 500-14000 kPa. Mole fraction solubilities were interpreted by the Krichevskii-Il'inskaya equation in the form

$$\log_{10} \frac{f_2}{x_2} - \frac{\overline{v_2}P}{2.303RT} = \log_{10}H - \frac{A}{2.303RT} (1 - x_1^2)$$

where  $f_2$  is the fugacity of carbon dioxide,  $x_2$  is the mole fraction of carbon dioxide in the liquid phase,  $x_1$  is the mole fraction of benzenemethanol in the liquid phase,  $v_2$  is the partial molar volume of carbon dioxide as  $x_2 \! + \! 0$ , H is the limiting value of Henry's constant at zero pressure and A is a constant. Henry's constant is defined as the ratio of pressure of carbon dioxide to mole fraction solubility.

T/K	$\bar{v}_2/\text{cm}^3\text{mol}^{-1}$	H/bar	A/cm³mol-1bar-1	H/kPa*	$x_2$ at $P_2 = 101.3 \text{ kPa}^*$
323.15	38.7	282	2708	28200	0.00360
348.15 373.15 398.15	51.1 63.5 75.9	336 392 443	30200 31800 34870	33600 39200 44300	0.00303 0.00260 0.00230

<sup>\*</sup> calculated by the compiler

# AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Carbon dioxide and benzenemethanol were allowed to reach equilibrium at various pressures to a maximum of 14000 kPa. Samples of the liquid phase were removed and analysed.

Partial molar volumes of carbon dioxide were found by measuring the volume of the liquid phase at different temperatures in sealed glass tubes.

# SOURCE AND PURITY OF MATERIALS:

- From a cylinder; dried and freed from gaseous impurities by repeated refreezing with liquid nitrogen.
- 2. Purified by vacuum distillation; m.pt. 15.2-15.4°C.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$   $\delta x_2 = \pm 5\%$ 

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2-Ethanediol or ethylene glycol; C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>; [107-21-1]
- (3) Water; H<sub>2</sub>O; [7732-18-5]

# ORIGINAL MEASUREMENTS:

Hayduk, W.; Malik, V.K.

J. Chem. Eng. Data 1971, 16,
143-146.

\_\_\_\_

VARIABLES:

T/K: 298.15 P/kPa: 101.325 x<sub>2</sub>: 0-1.00 PREPARED BY:

W. Hayduk

# EXPERIMENTAL VALUES:

	<del></del>		
Mole Fraction 1 glycol/ $x_2$	Ostwald Coefficient <sup>1</sup> L/cm <sup>3</sup> cm <sup>-3</sup>	Bunsen Coefficient <sup>2</sup> α/cm <sup>3</sup> (STP)cm <sup>-3</sup> atm <sup>-1</sup>	Mole Fraction <sup>2</sup> CO <sub>2</sub> /10 4x <sub>1</sub>
0.0	0.825	0.756	6.08
0.072	0.823	0.661	6.08
1			
0.165	0.660	0.605	6.48
0.222	0.638	0.585	6.81
0.291	0.630	0.577	6.55
0.420	0.660	0.605	9.03
0.453	0.643	0.589	9.13
0.651	0.751	0.688	13.0
0.685	0.760	0.696	13.5
0.748	0.793	0.727	14.9
0.874	0.871	0.798	18.1
0.932	0.903	0.827	19.6
0.983	0.945	0.866	21.2
0.997	0.962	0.881	21.8
1.00	0.966³	0.885	22.0 <sup>3</sup>
1			

- 1 Original data
- <sup>2</sup> Calculated by compiler using solvent density data given
- Extrapolated by authors allowing for water content of ethylene glycol used.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solubility was measured by saturating the solvent solution in a water-jacketed contactor at atmospheric pressure and using a fritted-glass bubbler to disperse the gas. Samples of saturated solution were allowed to drain by gravity into a 50-cm pipet for analysis. The analysis consisted of reacting the sample with an excess of standard sodium hydroxide and back-titrating with standard acid. The composition of solvent was determined from the mass of the components.

# SOURCE AND PURITY OF MATERIALS:

- Matheson Co. Specified as instrument grade of purity 99.5 per cent.
- Fisher Chemical. Certified reagent grade of maximum water content 0.2 per cent.
- 3. Distilled.

# ESTIMATED ERROR:

 $\delta T/K = 0.1$ 

 $\delta x_1/x_1 = 0.015$   $\delta x_2/x_2 = 0.005$ 

· · · · · · · · · · · · · · · · · · ·	ORIGINAL MEASUREMEN	TTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>;</li> <li>[124-38-9]</li> </ol>	Byeseda, J.J.; Manning, W.P.	Deetz, J.A.;
2. Ethylene glycols	j	Reid Gas Cond.Conf.
VARIABLES:	PREPARED BY:	
T/K = 297.1 P/kPa = 101.6	P.G.T. 1	gogg
EXPERIMENTAL VALUES:	L	
Solvent	Ostwald coeff. $\it L$	in liquid*
		<sup>X</sup> CO₂
1,2-Ethanediol, (ethylene glycol); C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> ; [107-21-1]	1.33	0.0031
2,2'-[1,2-Ethanediylbis(oxy)]bis- ethanol, (triethylene glycol); C <sub>6</sub> H <sub>1</sub> ,O <sub>4</sub> ; [112-27-6]	1.70	0.0093
$T/K = 297.1$ $P_{CO_2}/psia = 14$	$P_{\text{CO}_2}/\text{kP}$	a = 101.6
AUXILIARY	INFORMATION	
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY	OF MATERIALS:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Butane-1,4-diol; C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>;
  [25265-75-2]

# ORIGINAL MEASUREMENTS:

Semenova, A.I.; Tsimmerman, S.S.; E.A. Emel'yanova

Zhur. Fiz. Khim. 1981, 55, 1941-1943 Russian J. Phys. Chem. 1981, 55(8), 1105-1107.

### VARIABLES:

T/K = 323.2-398.2P/kPa to 8000 kPa

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/°C	T/K	Henry's law /Mpa	constant, H /kPa	$x_{\text{CO}_2}$ at $P_{\text{CO}_2} = 101.3 \text{ kPa}^*$
50	323.2	36	36000	0.00280
75	348.2	46	46000	0.00219
100	373.2	56	56000	0.00180
125	398.2	76	76000	0.00133

<sup>\*</sup> estimated by the compiler

The Henry's law constant, H is defined as

$$H = P \to 0 \left[ \frac{f}{x} \right]$$

where f is the fugacity of  $CO_2$  and x is the mole fraction of  $CO_2$  in solution.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Solubilities were measured at pressures to 8000 kPa by a method described in ref. (1). The liquid phase was sampled and analysed after the systems had reached equilibrium. Mole fraction solubilities of carbon dioxide fitted the Krichevskii-Il'inskaya equation (3) from which limiting values of Henry's law were found.

### SOURCE AND PURITY OF MATERIALS:

- Obtained from a cylinder; frozen solid evacuated to remove gaseous impurities.
- 2. Purified by repeated freezing; M.pt 16.0-16.2°C; vapor pressure in the range 50-75°C measured with an isoteniscope and found to be consistent with literature data for a higher temperature (2).

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$  $\delta H = \pm 5\%$  (authors)

- Tsiklis, D.S. The Technique of Physicochemical Studies at High and Ultrahigh Pressures, 1976, Izd. Khimiya, Moscow, p.431
   Handbook of Chemistry and
- Handbook of Chemistry and Physics, 37th ed., 1955-56, Chemical Rubber Publ. Co., Vol.1, p.812
- Krichevskii, I.R.
   Phase Equilibria in Solutions at High Pressures, 1952,
   Goskhimizdat, Moscow, p.67.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2,3-Propanetriol or glycerol; C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>; [56-81-5]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 298.15 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

	Mol Fraction	Bunsen	Ostwald
	10 <sup>5</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
298.15	9.03	0.0277	0.0302

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1,2,3-propanetriol. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. <u>1890</u>, 6, 141.
- 2. Steiner, P.

  Ann. Phys. (Leipzig) 1894, 52, 275.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

# CRITICAL EVALUATION:

Solubility of carbon dioxide in solvents, other than alcohols, containing carbon, hydrogen and oxygen.

Bodor et al.(1) measured solubility in 2-propanone from 198 K to 318.2 K at partial pressures of carbon dioxide of 7.7 kPa to 97.2 kPa with extrapolation to 101.3 kPa. This data is self consistent and there is no reason to doubt its reliability. Solubility at a partial pressure of 101.3 kPa is given in nine papers (1-9) which together cover the range 198 K to 307.2 K. The general pattern of data is consistent except at 293.2 K and 298.2 K. At 293.2 K values for the mole fraction solubility range from 0.02022 (Felsing(7)) to 0.02317 (Koudelka(4)) and at 298.15 K from 0.01870 (Just(8)) to 0.02108 (Gjaldbaek(9)). The only measurements above 298.2 K are those of Kunerth (5). These need to be confirmed by further work. The following equation for mole fraction solubility at a partial pressure of 101.3 kPa is based upon all the data mentioned above.

$$\ln x_{CO_2} = -10.599 + 1980.7/(T/K) - 0.00280\ln(T/K)$$
 (I)

temperature range = 198-318.2 K standard deviation in  $x_{\rm CO2}$  = 0.0143

The following equation is based on data for the temperature range 200.0-298.2 K from (1,6-9).

$$\ln x_{CO_2} = -10.313 + 1905.1/(T/K) + 0.0017\ln(T/K)$$
 (II)

temperature range = 200.1-298.2 K standard deviation in  $x_{\text{CO}_2}$  = 0.0055

Shenderei (10) measured the solubility of carbon dioxide in various solutions of ethyne in 2-propanone at 217.2 K. Extrapolation of the mole fraction solubility for a partial pressure of carbon dioxide to zero concentration of ethyne gives a value of 0.234 for dissolution in pure 2-propanone. The value from equation II is 0.216.

Balog-Megyery et al.(2) have published solubilities in sixteen alkanones at 298.15 K and a partial pressure of gas of 101.3 kPa. These range from 2-propanone to 2-undecanone. There is very little change in the mole fraction solubilities calculated from the data. The value for 2-undecanone is 0.0212 and that for 2-propanone is 0.0192. This last value may be compared with the value of 0.0199 from equation II above.

Shenderei et al.(11) measured solubility in 2-butanone to high pressures and reported Henry's constants. Estimated mole fraction solubilities at  $228.1~\mathrm{K}$  and  $248.0~\mathrm{K}$  are  $0.1299~\mathrm{and}$   $0.0654~\mathrm{compared}$  with smoothed values of  $0.142~\mathrm{and}$   $0.073~\mathrm{for}$  2-propanone. No other data for 2-butanone at these temperatures are available for comparison.

Mole fraction solubilities in cyclopentanone (12), cyclohexanone (13) and in 2,6-dimethylcyclohexanone (14) have been measured at a partial pressure of 101.3 kPa from 273.15 K to 303.15 K by Gallardo et al. Solubility curves lie below that for 2-propanone. There is very little difference in mole fraction solubilities under the same conditions in the three solvents. Mole fraction solubilities are also close to that for 2-methyl-5- (1-methylethenyl)-2-cyclohexen-1-one from Just's data (8) (see Table 1). These measurements on cyclic ketones can be tentatively accepted as reliable.

Bodor  $et\ al.(1)$  measured solubilities in acetaldehyde at 33.2 kPa to 101.3 kPa from 198 K to 248.2 K. The data are self-consistent but no other measurements are available for comparison. Mole fraction solubility

- Carbon dioxide; CO₂; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

### **EVALUATOR:**

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# CRITICAL EVALUATION:

values are lower than those for 2-propanone under the same conditions. At  $248.2~\rm K$  and a partial pressure of 1.013 kPa the value for acetaldehyde is 0.047 compared with a value of 0.072 for 2-propanone.

Just (8) measured solubility in benzaldehyde at about 101.3 kPa from 288.2 K to 298.2 K. These measurements are in close agreement with measurements by Kunerth (5) from 291.2 K to 309.2 K. An equation for mole fraction solubility at a partial pressure of 101.3 kPa given below is recommended. It is based on the two sets of data.

$$\ln x_{CO_2} = -90.097 + 5108.0/(T/K) + 12.023ln(T/K)$$

temperature range = 288.2-309.2 K standard deviation in  $x_{CO_2}$  = 8.9 × 10<sup>-5</sup>

Solubility in 4-methyl-1,3-dioxolan-2-one (propylene carbonate) has been measured to high pressures by Mantor et al.(15), Zubchenko et al.(16), Shakhova et al.(17), Isaacs et al.(18) and by Murrieta-Guevara et al.(19). These authors have used the data to obtain limiting values of Henry's constant from which the solubility at 101.3 kPa may be estimated. Makranczy et al.(20) have also made measurements to high pressures but values of solubility at 101.3 kPa from these measurements are inconsistent with measurements by other groups. Lenoir et al.(21) have measured limiting values of Henry's constant by a chromatographic method. These values are high compared with other values and may be subject to the limitations of the chromatographic method. Limiting values of Henry's constant from chromatographic measurements by Sweeney (22) are in better agreement with other data. Rivas and Prausnitz (23,24) have reported values of Henry's constant at 263.2 K to 373.2 K calculated from volumes of gas absorbed. The solubility at 293.2 K is also given by Bratzer (25). The evaluator recommends an equation for mole fraction solubility at a partial pressure of gas of 101.3 kPa which is based upon data given in references (15-19,22-25). i.e.

$$\ln x_{CO_2} = -36.218 + 2856.7/(T/K) + 3.9003\ln(T/K)$$

temperature range = 228.2-423.2 Kstandard deviation in  $x_{CO_2} = 0.00060$ 

Meder et al.(26) measured the solubility at partial pressures from 9.3 kPa to 93.0 kPa at 293.2 K. Extrapolation to 101.3 kPa gives a value of  $x_{\rm CO}$  of about 0.015 compared with a value of 0.0133 from the above equation. These measurements at lower pressures need confirmation by other workers.

Vilcu et al.(27) have reported the mole fraction solubility in 1,3-dioxolan-2-one (ethylene carbonate) to be 0.00703 at 101.3 kPa and 313.2 K. This compares with a value of 0.00926 for solubility in propylene carbonate under these conditions.

Just (8) measured solubilities in acetic, propanoic and butanoic acids at about 101.3 kPa from 288.2 K to 298.2 K. Kunerth (5) measured solubility in acetic acid at about the same pressure over the range 291.2 K to 309.2 K. These measurements are consistent with those of Just. A smoothing equation for solubility at a partial pressure of 101.3 kPa, based on the two sets of measurements, is given below.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

**EVALUATOR:** 

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CRITICAL EVALUATION:

$$\ln x_{CO_2} = 76.937 - 2231.8/(T/K) - 12.978\ln(T/K)$$

temperature range = 288.2-309.2 Kstandard deviation in  $x_{CO_2} = 0.00012$ 

No other measurements are available to confirm Just's data for propanoic and butanoic acids.

Ouellet and Dubois (28) measured solubility in 9-octadecanoic acid at 11 kPa to 59 kPa from 296.2 K to 335.2 K. This work is self consistent but no measurements on this or other long chain carboxylic acids are available for comparison. These data for acetic, propanoic, butanoic and 9-octadecanoic acids indicate that mole fraction solubility at a partial pressure of 101.3 kPa increases with carbon number. (Table 1)

Just (8) measured solubility in acetic acid anhydride from 288.2 K to 298.2 K. No other data are available.

Mole fraction solubilities in alkyl esters of carboxylic acids from the literature are higher than in carboxylic acids or ketones under the same conditions. There is a tendency for values of mole fraction solubilities at 298.2 K and 101.3 kPa to increase with chain length of the parent alkanol and of the parent carboxylic acid. (see Table 1)

Just (8) measured solubility in pentyl formate from 288.2 K to 298.2 K. No other data on this system are available for comparison. The mole fraction solubility in methyl acetate at 298.2 K and 101.3 kPa from Just (8) is 0.02260 and from Gjaldbaek and Andersen (9) is 0.00207. The latter measurements are probably the more reliable.

Bodor et al.(29) measured solubility in ethyl acetate at partial pressures from 9.6 kPa to 102.4 kPa at 198 K to 318.2 K. The data is self-consistent. Shenderei et al.(11) measured solubility to high pressures at 228.0 K to 248.0 K. Bodor's value of mole fraction solubility at 248.2 K and a partial pressure of 101.3 kPa is 0.0890. The value at 248.0 K and 101.3 kPa from Shenderei is 0.0813. The following smoothing equation for mole fraction solubility at a partial pressure of 101.3 kPa is based upon data from both sources. Differences between the two sets of data must be borne in mind when this equation is used.

$$\ln x_{CO_2} = 11.689 + 1063.1/(T/K) - 3.3435 \ln(T/K)$$

temperature range = 198-318.2 K standard deviation in  $x_{CO_2}$  = 0.0095

Solubility in propyl acetate at 298.2 K and a partial pressure of 101.3 kPa was measured by Gjaldbaek and Andersen (9). Solubility in 2-methylpropyl acetate at 293.2 K and 298.2 K was measured by Just (8). There is no reason to doubt the reliability of these measurements but confirmation by other workers is needed.

Solubility in pentyl acetate at or close to 101.3 kPa was measured by Just (8) from 288.2 K to 298.2 K and by Kunerth (5) from 291.2 K to 307.2 K. Values of mole fraction solubility at 293.2 K are 0.0266 (Just) and 0.0280 (Kunerth). The following smoothing equation is based on the two sets of data.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

**EVALUATOR:** 

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July 1991

CRITICAL EVALUATION:

 $\ln x_{CO_2} = -79.380 + 4337.8/(T/K) + 10.737\ln(T/K)$ 

temperature range = 288.2-307.2 K standard deviation in  $\times_{\text{CO}_2} = 0.00056$ 

Ouellet and Dubois (28) measured solubility in ethyl stearate at 8 kPa to 78 kPa from 307.2 K to 347.2 K. The data are self-consistent but no other measurements are available for comparison.

Arai et al.(30) measured solubility in methyl, ethyl and butyl oleate at 30kPa to 90 kPa from 273.2 K to 343.2 K. There is very little difference between mole fraction solubilities in the three solvents. The data are self-consistent. No other measurements on these systems are available. Comparison with Oullet's measurements indicate that mole fraction solubility in oleates is greater than in stearates under the same conditions.

There are significant differences between solubilities in 1,2,3-propanetriol triacetate measured by Shakhova et al.(17) from 273.2 K to 328.2 K and those measured by Makranczy et al.(20) from 273.2 K to 303.2 K. Values of mole fraction solubility at a partial pressure of 101.3 kPa at 273.2 K are 0.0466 (Shakhova) and 0.0414 (Makranczy). At 298.2 K the two values are 0.0284 (Shakhova) and 0.0222 (Makranczy). Further measurements on this system are required.

The solubility in 1,1'-oxybisethane was measured by Christoff (31) in 1912 at barometric pressure from 273.2 K to 288.2 K. This work indicates that mole fraction solubility, corrected to a partial pressure of 101.3 kPa is close to that in 2-propanone under the same conditions. There is no recent work on the system under these conditions.

Bodor (32) measured solubility in tetrahydrofuran at 10.5 kPa to 97.7 kPa from 198 K to 318.2 K. Measurements are self-consistent and there is no reason to doubt their reliability. Mole fraction solubility is high compared with other solvents. No other work on the system is available for comparison.

Gallardo et a1.(33) reported the mole fraction solubility in 1,4-dioxane at a partial pressure of 101.3 kPa from 285.2 K to 303.2 K. Kassim et a1.(34) reported values from 303.2 K to 333.2 K. Values for 303.2 K are 0.01974 (Gallardo) and 0.0192 (Kassim). However Gallardo's measurements show a steep fall in mole fraction solubility with increase in temperature whereas Kassim's measurements show negligible change through the temperature range. The two sets of measurements are therefore not compatible. Further work on this system is required

The limiting value of Henry's constant for dissolution in dipropylene glycol at 298.2-343.2 K was measured by Lenoir et al.(21) by gas-liquid chromatography. No other measurements are available for comparison. Jou et al.(35) measured solubility in triethylene glycol to high pressures at 298.15 K to 398.15 K. Mole fraction solubility at 101.3 kPa can be calculated from the data. Makranczy et al.(36) also investigated this system at 273.15-303.15 K to high pressures. Values of mole fraction solubility at 298.15 K; 101.3 kPa from the two sources are 0.00677 (Makranczy); 0.00846 (Jou). The data from Jou et al. shows greater consistency over the pressure range in which studies were carried out and are likely to be the more reliable. Byeseda et al.(37) measured the solubility in this solvent at 297.1 K and a pressure of 101.6 K. The corresponding value of the mole fraction solubility is 0.0093 compared with a value of 0.0086 by extrapolation of Jou's measurements.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

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### CRITICAL EVALUATION:

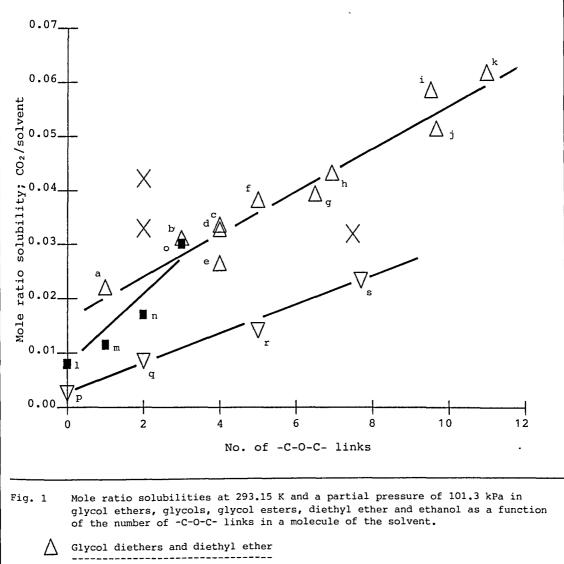
Makarov et al.(38) measured solubility to high pressures at 293.15 K in two samples of polyethylene glycol having average relative molecular masses of 280 and 400 respectively. In one case the average degree of polymerisation was 6 and in the other case 8.7. Comparison with Jou's data (35) shows that, at a partial pressure of gas of 101.3 K the mole fraction solubility of carbon dioxide increases with the average number of ether linkages in molecules of the solvent. A plot of mole ratio solubility of these compounds with two hydroxyl groups against the number of ether linkages is close to a straight line passing through the mole ratio solubility in ethylene glycol which has no ether linkages (Fig. 1). This indicates that Makarov's data is consistent with Jou's data. The solubility of hydrogen sulfide in polyethylene glycols shows a similar variation with the number of ether linkages (39).

Bodor et al.(40) measured solubility in 2-methoxyethanol (ethylene glycol monomethyl ether) at pressures to 99 kPa from 198 K to 318.2 K. Data can be extrapolated to give the solubility at 101.3 kPa. The measurements are self consistent and may be accepted on a tentative basis. Sciamanna and Lynn (41) measured solubility in diethylene glycol monomethyl ether and in triethylene glycol monobutyl ether at 3 to 100 kPa from 288.2 K to 373.2 K. Comparison of these measurements with Bodor's measurements on ethylene glycol monomethyl ether shows again that mole fraction solubility at a pressure of gas of 101.3 kPa increases with the number of ether linkages. When mole ratio solubilities in these compounds with one hydroxyl group are plotted against the number of ether linkages values lie close to a stright line. This line is close to the solubility in ethanol which has no ether linkages (Fig 1).

Solubilities in polyethylene glycol diethers have been published by various authors. Makarov (38) measured solubilities in triethyleneglycol diethyl ether, polyethylene glycol diethyl, dipropyl and methylpropyl ethers to high pressures at 293.2 K to 323.2 K. Sciamanna and Lynn (41) measured solubilities in di- and tri- and tetraethylene glycol dimethyl ethers at pressures to 100 kPa from 288.2 K to 373.2 K. Zubchenko and Shakhova (42) also measured the solubility in tetraethylene glycol dimethyl ether at 298.15 K. Sweeney (22) measured the limiting value of Henry's constant at 298.2 K and 323.2 K. Values from both these sources are close to those from Sciamanna's work. Wolfer (43) reported solubility data for polyethylene glycol methyl isopropyl ether. Mole fraction solubilities at 101.3 kPa in all these compounds are greater than in polyglycols having no alkoxy groups but the same number of ether links. Mole ratio solubilities plotted against the number of ether links lie close to a straight line passing through the solubility in diethyl ether which has one ether link (Fig 1).

Makranczy et al.(20) measured solubility in methoxytriethylene glycol acetate and butoxytriethylene glycol acetate. Makarov et al.(38) measured solubility in polyethylene glycol diacetate. No other measurements on these solvents are available for comparison. Data for the two monoacetates fall close to values for glycol ethers and diethers having the same number of ether linkages. The data for the diacetate lies closer to corresponding data for polyglycols (Fig. 1)

The limiting value of Henry's constant for dissolution in phenol at 323.2 K was measured by Lenoir et al.(21) using the gas-liquid chromatographic method. The mole fraction estimated for a partial pressure of 101.3 kPa is 0.00467 but this value is subject to the limitations associated with the method. Horvath et al.(44) measured solubility in 3-methylphenol at 300.5 K. The value of the mole fraction solubility at a partial pressure of 101.3 kPa is 0.00592. This value is compatible with the value for phenol at 323.2 K estimated from Lenoir's



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g - polyethylene glycol methyl isopropyl ether,
a - diethyl ether (31)
b - diethylene glycol dimethyl ether (41)
                                                                             ®Sepasolv (43)
c - triethylene glycol dimethyl ether(41) h - polyethylene glycol diethyl ether 336 (38)
d - triethylene glycol dimethyl ether(16)<sup>1</sup> i - polyethylene glycol dipropyl ether (38)
e - triethylene glycol diethyl ether (38) j - polyethylene glycol diethyl ether 456 (38)
f - tetraethylene glycol dimethyl ether (41) k - polyethylene glycol methyl propyl ether(38)
           Glycol monoethers and ethanol
                                                 n - diethylene glycol monomethyl ether(41)
1 - ethanol (smoothed value; see p.128)
m - ethylene glycol monomethyl ether (40) o - triethylene glycol butyl ether (41)
           Glycols
p - ethylene glycol<sup>2</sup> (37)
                                                 r - polyethylene glycol 280 (38)
                                                 s - polyethylene glycol 400 (38)
q - triethylene glycol (35)
           Glycol esters
t - methoxy triethylene glycol acetate(20) v - polyethylene glycol diacetate (38)
u - butoxy triethylene glycol acetate (20)
     <sup>1</sup> 298.15 K
                         <sup>2</sup> 297.1 K
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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

# **EVALUATOR:**

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measurements. Just (8) measured solubility in 2-methoxy-4-(2-propenyl)-phenol at 288.2 K to 298.2 K. Extrapolated values of solubility at a partial pressure of 101.3 kPa are much higher than the apparent solubilities in phenol and 3-methylphenol. This is due to the presence of the methoxy group in this compound. Solubility data for phenols must be accepted on a tentative basis until further measurements on these compounds have been carried out.

Kassim et al.(34) measured solubility in dihydro-2-(3H)-furenone at 303.2-333.2 K; 101.3 kPa. Mole fraction solubility is high compared with the reference line based on Raoult's law. These measurements may be accepted on a tentative basis until measurements on this or similar systems are available for comparison.

Selected values of mole fraction solubilities in solvents containing oxygen are shown in Table 1 and in Fig 2.

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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

# **EVALUATOR:**

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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

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July 1991

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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

# **EVALUATOR:**

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# CRITICAL EVALUATION:

Table 1.
Mole fraction solubilities of carbon dioxide at a partial pressure of 101.3 kPa in solvents containing carbon, hydrogen and oxygen

Solvent	T/K	<sup>x</sup> CO₂	Referenc
2-Propanone	298.15	0.0211	9
Cyclopentanone	298.15	0.01641	12
Cyclohexanone	298.15	0.0160	13
2,6-Dimethylcyclohexa	anone		
	298.15	0.0168	14
Benzaldehyde	298.15	0.0115 ±0.0006	*
4-Methyl-1,3-dioxolar	1-2-one		
-	298.15	0.01210 ±0.00060	*
Acetic acid	298.15	0.01120 ±0.00012	*
Propanoic acid	298.15	0.0123	8
Butanoic acid	298.15	0.0130	8
9-Octadecenoic acid	298.15	0.0157	28 †
Acetic anhydride	298.15	0.0199	8
Methyl acetate	298.15	0.0208	8
•	298.15	0.0226	9
Ethyl acetate	298.15	0.0230	1 ¶
Propyl acetate	298.15	0.0245	9
2-Methylpropyl acetat			
	298.15	0.0250	8
Pentyl acetate	298.15	0.02584 ±0.00056	*
Pentyl formate	298.15	0.0212	8
Ethyl stearate	307.15	0.0190	28 ¶
Methyl oleate	298.15	0.0269	30
Ethyl oleate	298.15	0.0277	30
Butyl oleate	298.15	0.0279	30
1,2,3-Propanetriol tr	ciacetate		
	298.15	0.0284	17
	298.15	0.0222	20
1,1'-Oxybisethane	288.15	0.0233	31
Tetrahydrofuran	298.15	0.027	32 ¶
1,4-Dioxane	298.15	0.02272	33
Oxybispropanol	298.15	0.00826	21
Triethylene glycol	298.15	0.00846	35
2-Methoxyethanol	298.15	0.0100	40 †
Phenol	323.15	0.0047	21
3-Methylphenol	300.15	0.0059	44

<sup>\*</sup> from the equation given by the evaluator on a previous page  $\dagger$  interpolated;  $~\P$  extrapolated

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents, other than Alcohols, Containing Carbon, Oxygen and Hydrogen

# **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K. July 1991

CRITICAL EVALUATION:

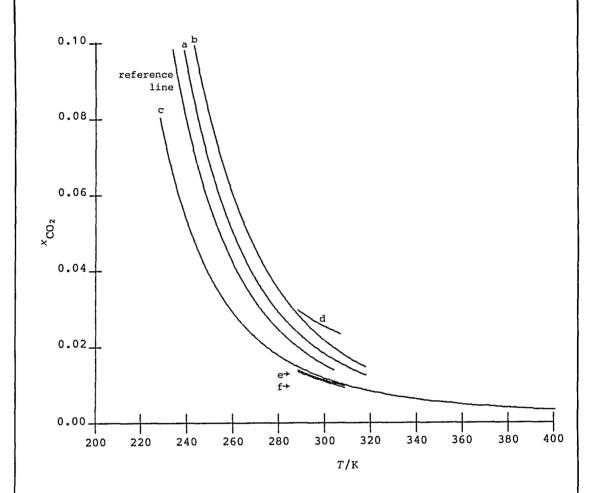


Fig. 2 Mole fraction solubility of carbon dioxide in various solvents containing carbon, oxygen and hydrogen at a partial pressure of gas of 101.3 kPa.

a - ethyl acetate

b - 2-propanone

c - 4-methyl-1,3-dioxolan-2-one (propylene carbonate)

d - pentyl acetate

e - benzaldehyde

f - acetic acid

The curves showing the variation of solubility with temperature correspond to equations derived by the evaluator.

A reference line corresponding to values from the Raoult's law equation is also shown.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Propanone or acetone; C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 293.15, 298.15  $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

TURE AUTHORS.			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
293.15	2.07	6.45	6.921
298.15	1.87	5 <b>.</b> 77	6.295

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 2-Propanone. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2-Propanone, (acetone); C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

Benzaldehyde; C<sub>7</sub>H<sub>6</sub>O; [100-52-7]

# ORIGINAL MEASUREMENTS:

Kunerth, W.

Phys. Rev. 1922, 19, 512-524.

### VARIABLES:

T/K = 291.15-307.15

P/kPa ≃ 101.3

PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	T/K	Ostwald coefficient L	$x_{\text{CO}_2}$ at $P_{\text{CO}_2} = 101.3 \text{ kPa*}$
2-Propanone	293.15	6.98	0.02103
	295.15	6.76	0.02031
	297.15	6.55	0.01961
	299.15	6.22	0.01857
	301.15	5.88	0.01751
	303.15	5.49	0.01631
	305.15	5.08	0.01506
	307.15	4.66	0.01378
Benzaldehyde	291.15	3.06	0.01292
	293.15	2.98	0.01252
	295.15	2.90	0.01213
	297.15	2.80	0.01166
	299.15	2.73	0.01131
	301.15	2.66	0.01097
	303.15	2.58	0.01059
	305.15	2.52	0.01030
	307.15	2.46	0.01001
	309.15	2.39	0.00968

<sup>\*</sup> calculated by the compiler

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The method is based upon that described by McDaniel (1). The apparatus consisted of a gas buret attached to a levelling tube containing mercury and to the absorption cell containing the solvent under test. The volume of gas absorbed by a measured volume of liquid was measured at a total pressure equal to barometric pressure. The mercury in the gas buret was covered with a layer of solvent so that the gas in the buret was saturated with solvent vapor. Buret and absorption cell were surrounded by heating wire and water jackets fitted with thermometers.

# SOURCE AND PURITY OF MATERIALS:

- produced by heating NaHCO<sub>3</sub>; dried with CaCl<sub>2</sub>; frozen in liquid air and volatile impurities pumped away; passed over P<sub>2</sub>O<sub>5</sub>.
- commercial sample; purity attested by boiling point and density.

# ESTIMATED ERROR:

 $\delta x_{\text{CO}_2} = \pm 5\%$  (compiler)

- 1. McDaniel, A.S.;
  - J. Phys. Chem. 1911, 15, 587.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Propanone or acetone; C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

# ORIGINAL MEASUREMENTS:

Felsing, W. A.; Durban, S. A.

J. Am. Chem. Soc. 1926, 48, 2885 - 2893.

VARIABLES:

T/K = 200.01 - 293.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

H. L. Clever

EXPERIMENT Tempe	MAL VALUES rature	: Carbon Dioxide Molality	Kuenen Coefficient <sup>1</sup>	Mol Fraction	Ostwald Coefficient
<i>t</i> /°C	<i>T</i> /K	m <sub>1</sub> /mol kg <sup>-1</sup>	10 <sup>3</sup> S/cm <sup>3</sup> (STP) g <sup>-1</sup>	<i>x</i> <sub>1</sub>	L/cm <sup>3</sup> cm <sup>-3</sup>
-73.14	200.01	13.94490	313,597.1	0.4475	-
-60.12	213.03	5.92017	132,710.1	0.2559	-
-45.14	228.01	2.79867	62,736.6	0.13982	-
-29.24	243.91	1.47773	33,125.1	0.07904	25.0
-13.55	259.60	0.90322	20,247.1	0.04984	15.9
- 2.54	270.61	0.62115	13,924.0	0.03482	11.3
+20.00	293.15	0.35537	7,966.2	0.02022	6.76

 $<sup>^1</sup>$  The authors labeled the solubility as cm  $^3$  (0  $^{\circ}\text{C}/760/\text{mmHg})$  per 1000 g of acetone. The compiler has labeled it 10  $^3$  x Kuenen coefficient.

The mole fraction and Ostwald coefficient values were calculated by the compiler.

The authors fitted the solubility data to the equation

 $\log m_1 = -18.085436 + 2615.017/(T/K) + 66.55546 \times 10^{-3}(T/K)$ 

- 79.07114 x  $10^{-6}$  (T/K) $^2$  for the molal solubility of carbon dioxide at a partial pressure of 760 mmHg.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of an absorption flask, a manometer, and a gas buret.

The absorption flask was in a cryostat with ethyl bromide as the fluid.

The gas buret appears to be water jacketed. It appears that the volume of dry carbon dioxide vapor was measured, but the authors do not make a statement to confirm the procedure.

The measurement was carried out at a total pressure equal to 760 mmHg  $\rm CO_2$  + the 2-propanone vapor pressure.

The authors used an ideal gas molar volume of  $22,416.55~{\rm cm}^3~{\rm mol}^{-1}$  to convert the gas volumes to moles.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not stated.
- (2) 2-Propanone. The best c.p. material available was distilled three times, converted to the NaI addition compound which was distilled and reformed several times. Density,  $\rho^{2.5}/g$  cm<sup>-3</sup> = 0.78612.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$ 

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Propanone or acetone; C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient α/cm³(STP)cm-³atm-1	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	2.12	6.48	7.07
	2.11	6.45	7.04
	2.11	6.43	7.02
	2.08	6.34	6.92
	2.12	6.49	7.08

The mole fraction and Ostwald coefficient values were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO<sub>2</sub>.
- (2) Acetone. Merck and Co. Fractionated by distillation. B.p. (760 mmHg)/°C = 56.12 - 56.14, refractive index n<sub>D</sub>(20°C) = 1.3588 - 1.3589.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. 1930, 52, 68.
- Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Propanone (acetone); C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

# ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. Univ. Strasbourg (France) 1954.

# VARIABLES:

T/K = 293.15p/kPa = 101.325 PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K <sup>b</sup>	Ostwald Coefficienta		Mole Fraction <sup>b</sup>
	L/cm <sup>3</sup> cm <sup>-3</sup>	α/cm³ (STP)cm <sup>-3</sup> atm <sup>-1</sup>	
293.15	6.88	6.40	0.0211

a Original data.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and below atmospheric.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) 2-Propanone (acetone). Research grade. Purity not given. Dried and distilled.

ESTIMATED ERROR:  $\delta T/K = \pm 0.2$  $\delta p/kPa = \pm 0.1$  $\delta L/L = \pm 0.02$  (compiler)

### REFERENCES:

Some data in the thesis have been published. See:

1. Maillard, A.; Rosenthal, W. Comp rend. 1952, 234, 2546-8.

D Calculated by compiler using real gas molar volumes.

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Bodor, E.; Bor, Gy.; Maleczkine, M.; Mesko, G.; Mohai, B.; 2. 2-Propanone (Acetone); Siposs, G. Veszpremi. Vegyip. Egyet. Kozlemen. $C_3H_6O;$ [67-64-1] <u>1957</u>, 1, 63-76. VARIABLES: PREPARED BY: T/K = 198-318.2C. L. Young P/kPa = 7.7-97.2EXPERIMENTAL VALUES: Mole fraction \* of Absorption<sup>†</sup> of gas /cm³g-1 carbon dioxide T/Kp/kPa p/mmHg in liquid, <sup>x</sup>co₂ 7.7 0.83 0.00215 318.2 58 18.9 0.00431 142 1.67 0.00415 148 19.7 1.61 28.5 0.00603 214 2.34 2.75 0.00708 246 32.8 295.2 176 23.5 2.54 0.00654 0.00746 216 28.8 2.90 254 33.9 3.88 0.00995 4.32 310 41.3 0.0111 0.0125 348 46.4 4.90 54.0 5.72 0.0146 405 59.7 6.40 448 0.0163 0.0185 514 68.5 7.27 69.6 522 7.25 0.0184 273.2 355 47.3 8.20 0.0208 386 51.5 8.12 0.0206 419 55.9 9.70 0.0245 469 62.5 9.87 0.0249 471 62.8 10.70 0.0270 73.6 552 11.60 0.0292 563 75.1 12.60 0.0316 81.1 608 12.70 0.0319 (cont.) AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 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). ESTIMATED ERROR: $\delta T/K = \pm 0.1;$ $\delta$ (absorption) = ±4% or less REFERENCES: Bodor, E.; Bor, G. J.; Mohai, B.; Siposs, G. Veszpremi. Vegyip. Egy. Kozl. 1957, 1, 55.

# ORIGINAL MEASUREMENTS:

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Propanone (Acetone);
  C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

Bodor, E.; Bor, Gy.; Maleczkine, M.; Mesko, G.; Mohai, B.; Siposs, G. Veszpremi. Vegyip. Egyet. Kozlemen. 1957, 1, 63-76.

EXPERIMEN	TAL VALUES:		Absorption	Mole fraction * of
T/K	p/mmHg	p/kPa	of gas /cm³g-1 +	carbon dioxide in liquid, <sup>x</sup> CO <sub>2</sub>
273.2	639	85.2	14.25	0.0356
	677	90.3	14.20	0.0355
	689	91.9	15.0	0.0374
	(760)	(101.3)	(16.5)	(0.0410)
248.2	88	11.7	5.8	0.0148
	219	29.2	8.8	0.0223
	351	46.8	12.8	0.0321
	470	62.7	16.6	0.0412
	566	75.5	21.0	0.0516
	712	94.9	27.0	0.0654
	(760)	(101.3)	(30)	(0.072)
223.2	225	30.0	26.8	0.0649
	258	34.4	29.6	0.0712
	395	52.7	42.1	0.0984
	568	75.7	59.3	0.133
	612	81.6	67.6	0.149
	726	96.8	82.9	0.177
	(760)	(101.3)	(90)	(0.189)
198 ± 2	(760) 151 246 540 632 729 (760)	20.1 32.8 72.0 84.3 97.2 (101.3)	74.3 118.2 310.3 421 509 (570)	0.161 0.234 0.446 0.522 0.569 (0.596)

Values in parentheses are extrapolated to 1 atmosphere.

<sup>†</sup> the volume of gas absorbed by one gram of solvent was corrected to 273.15 K and 101.3 kPa calculated by compiler.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alkanones

# ORIGINAL MEASUREMENTS:

Balog-Megyery, K.; Makranczy, J.;
Rusz, L.; Mate, E.

Hung. J. Ind. Chem. 1986, 14(1), 49-51.

### VARIABLES:

T/K = .298.15; P/kPa = 101.3

### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K = 298.15 Solvent	Bunsen coeff. a	* *
2-Propanone, (acetone); C <sub>3</sub> H <sub>6</sub> O; [67-64-1]	5.92	0.0192
3-Pentanone, (diethyl ketone); $C_5H_{10}O$ ; [96-22-0]	4.15	0.0194
4-Heptanone, (dipropy1 ketone); C <sub>7</sub> H <sub>14</sub> O; [123-19-3]	3.25	0.0200
5-Nonanone, (dibutyl ketone); C9H18O; [502-56-7]	2.62	0.0200
2-Butanone, (methyl ethyl ketone); C4H8O; [78-93-3	4.85	0.0191
2-Pentanone, (methyl propyl ketone); C <sub>5</sub> H <sub>10</sub> O; [107-	-87-9] 4.20	0.0197
2-Hexanone, (methyl butyl ketone); C <sub>6</sub> H <sub>12</sub> O; [591-78	3.53	0.0192

<sup>\*</sup> calculated by the compiler for a partial pressure of CO<sub>2</sub> of 101.3 kPa by use of densities of solvents given in ref.(1).

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Solubility measurements were made by a static method using apparatus described in earlier papers (2-4). A measured quantity of solvent was saturated with carbon dioxide and the volume of gas absorbed was measured when equilibrium was attained.

### SOURCE AND PURITY OF MATERIALS:

No information

# ESTIMATED ERROR:

- Weast, R.C.; Astle, M.J. CRC Handbook of Data on Organic Compounds 1985, CRC Press Inc., Boca Raton, Florida, U.S.A.
- Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. 1976, 4, 269.
- Makranczy, J.; Rusz, L.;
   Balog-Megyery, K.
   Hung. J. Ind. Chem. 1979, 7, 41.
- Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Alkanones

# ORIGINAL MEASUREMENTS:

Balog-Megyery, K.; Makranczy, J.;
Rusz, L.; Mate, E.

Hung. J. Ind. Chem. 1986, 14(1), 49-51.

# EXPERIMENTAL VALUES:

Solvent	Bunsen coeff.	Mole fraction* *CO2
3-Hexanone, (ethyl propyl ketone); C <sub>6</sub> H <sub>12</sub> O; [589-38-8]	3.62	0.0197
3-Heptanone, (ethyl butyl ketone); C7H14O; [106-35-4]	3.17	0.0195
3-Octanone, (ethyl pentyl ketone); C <sub>8</sub> H <sub>16</sub> O; [106-68-3]	2.91	0.0200
3-Nonanone, (ethyl hexyl ketone); C <sub>9</sub> H <sub>18</sub> O; [925-78-0]	2.63	0.0200
3-Decanone, (ethy1 hepty1 ketone); C <sub>10</sub> H <sub>20</sub> O; [928-80-3]	2.51	0.0209
2-Octanone, (methyl hexyl ketone); C <sub>8</sub> H <sub>16</sub> O; [111-13-7]	2.86	0.0197
2-Nonanone, (methyl heptyl ketone); C9H18O; [821-55-6]	2.60	0.0198
2-Decanone, (methyl octyl ketone); C <sub>10</sub> H <sub>20</sub> O; [693-54-9]	2.48	0.0207
2-Undecanone, (methyl nonyl ketone); C11H22O; [112-12-	9] 2.33	0.0212

 $<sup>^{</sup>st}$  calculated by the compiler using densities of liquids given in (1)

130		
COMPONENTS:		ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; 2. Compounds containing		Luhring, P.; Schumpe, A. <i>J. Chem. Eng. Data</i> , 1989, 34, 250-252.
VARIABLES:		PREPARED BY:
T/K = 293.2	}	C.L. Young
EXPERIMENTAL VALUES:		
T/K Henry /(Pa	's Constant <sup>†</sup> m³/mol <sup>-1</sup> )	Mole fraction of CO <sub>2</sub> at 101.3 kPa partial pressure*
Acetic	acid, ethyl e	ster; C <sub>4</sub> H <sub>8</sub> O; [141-78-6]
293.2	399	0.0248
Acetic	acid, butyl e	ster; C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> ; [141-78-6]
293.2	499	0.0267
2-Pr	copanone; C <sub>3</sub> H <sub>6</sub> O;	[67-64-1]
293.2	347	0.0215
1,4-	oioxane; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	; [123-91-1]
293.2	357	0.0242
Henry's constant mul *calculated by compiler	using density	data taken from ref.(1).
	AUXILIARY INFORM	ATION
METHOD/APPARATUS/PROCEDURE		SOURCE AND PURITY OF MATERIALS:
Little infomation given Method consisted of equi known amounts of degasse gas and measuring the ch pressure. Equilibration in 3 to 6 minutes. Some given in ref.(2).	librating d liquid and ange in was reached	Obtained from Merck at the highest available purity. No other details given.
		ESTIMATED ERROR:
		<ol> <li>Riddick, J.A.; Bunger, W.B.;1970         Organic Solvents, Wiley-         Interscience, New York.</li> <li>Schumpe, A.; Quiker, G.;         Decker, W.D.         Adv. Biochem. Eng., 1982, 24, 1.</li> </ol>

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Propanone; C<sub>3</sub>H<sub>6</sub>O; [67-64-1]
- 3. Ethyne; C<sub>2</sub>H<sub>2</sub>; [74-86-2]

VARIABLES: T/K = 217.17 $P_{\text{CO}_2}/\text{kPa} = 13.3-101.3$  $x_{\text{C}_2\text{H}_2} = 0.08-0.34$ 

### ORIGINAL MEASUREMENTS:

Shenderei, E.R.

Zhur. Prik1. Khim. 1965, 38(9), 2126-2128.

### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Conc.of ethyne* /cm <sup>3</sup> g <sup>-1</sup>	Mole fraction of ethyne,  *C2H2***	Pressure increase due to CO <sub>2</sub> , P tot O	Mole fraction of CO <sub>2</sub> ,	Solubility of CO <sub>2</sub> at P <sub>tot</sub> -P <sub>0</sub> * /cm <sup>3</sup> g <sup>-1</sup>
42.7	0.0978	100	0.0281	12.27
	0.0924 0.0865	300 500	0.0842 0.1402	37.90 69.32
	0.0003	760	0.1402	115.10
128	0.2451	100	0.0243	12.71
	0.2329	300	0.0730	40.13
	0.2207	500	0.1216	70.59
	0.2049	760	0.1848	115.62
207	0.3439	100	0.0222	13.35
	0.3283	300	0.0666	42.09
	0.3128	500	0.1109	73.43
	0.2926	760	0.1685	119.27
384	0.4919	100	0.0194	15.14
	0.4725	300	0.0582	47.29
	0.4530	500	0.0970	82.40
	0.4279	760	0.1475	132.37

\* concentrations are expressed at volume of gas, corrected to 273.15 K and 101.325 kPa, dissolved per gram of acetone \*\* calculated by the compiler

т/к	Mole fraction of ethyne		constant, H, ition of CO <sub>2</sub> /kPa**
217.17	0.10	3570	476
_ , , , ,	0.25	4115	549
	0.35	4505	601
	0.45	5150	687
$H = \frac{1}{2}$	$\lim_{x \to 0} \left( \frac{\delta P}{\delta x} \text{tot} \right)$	•	

calculated from measurements of the total pressure over the solution,  $P_{tot}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

The method is described in ref. (1).

No information

# ESTIMATED ERROR: $\delta x_{CO_2} = \pm 0.5\%$ (author)

# REFERENCES:

1. Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.N. Gaz. Prom. 1958, 12, 36.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Cyclopentanone; C<sub>5</sub>H<sub>8</sub>O; [120-92-3]

# VARIABLES:

T/K = 273.15-303.15 $P_{CO_2}/kPa = 101.33$ 

# ORIGINAL MEASUREMENTS:

Gallardo, M.A.; Lopez, M.C.;
Urieta, J.S.; Gutierrez Losa, C.

Fluid Phase Equilibria, 1989, 50, 223-233.

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

P <sub>CO<sub>2</sub></sub>	<i>T</i> /K	<sup>x</sup> CO₂
101.33	273.15	0.02750
	283.15	0.02205
	293.15	0.01810
	298.15	0.01641
	303.15	0.01495

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Details of the apparatus and procedure are given in refs. (1) and (2). The total pressure was chosen so that the partial pressure of carbon dioxide was about 101.33 kPa. The number of moles of carbon dioxide introduced into the vessel containing the solution was calculated from the volume and pressure of gas introduced, taking non-ideality into account. The number of moles remaining in the gas phase in the reaction vessel was then calculated and the number of moles dissolved in the known weight of solvent found by difference.

# SOURCE AND PURITY OF MATERIALS:

- Supplied by Sociedad Española del Oxigeno; purity 99.998 mol%.
- 2. Supplied by Fluka; GLC indicated a purity better than 99.5 mol.%;  $n_D^{20} = 1.43657$

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$  (authors)

- Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa C. J. Chim. Phys. 1983, 80, 621.
- Carnicer, J.; Gibanel, F.;
   Urieta, J.S.; Gutierrez Losa C.
   Rev. Acad. Cienc. (Zaragoza)
   1979, 34, 115.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Cyclohexanone; C<sub>6</sub>H<sub>10</sub>O; [108-94-1]

# ORIGINAL MEASUREMENTS:

Gallardo, M.A.; Melendo, J.M.; Urieta, J.S.; Gutierrez Losa, C.

Can. J. Chem.

1987, 65, 2198-2202.

### VARIABLES:

T/K = 283.15-303.15P/kPa = 101.3

### PREPARED BY:

C. L. Young

# EXPERIMENTAL VALUES:

$$T/K$$
 10<sup>4</sup> × Mole fraction of carbon dioxide at 1 atm partial pressure  $10^{+}x_{\rm CO_2}$ 

283.15	216
293.15	176
298.15	160 <sup>a</sup>
303.15	147

Smoothing equation given in source

$$\ln x_{\text{CO}_2} = -5.6368 \text{ ln } (T/\text{K}) + 27.986$$
(Std. dev. =  $0.882 \times 10^{-4}$ )

a Data reported previously in ref. (1).

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Solubility apparatus was similar to that used by Ben-Naim and Baer (2) consisting essentially of a gas buret, mercury manometer and solution vessel. The solvent was degassed in the solution vessel.

Measurements were carried out on the saturated gas. It appears that the mole fraction at a partial pressure of 1 atmosphere was estimated from the raw experimental data by assuming that Henry's law is obeyed and that the partial pressure of solvent in the gas phase is given by Raoult's law. Some details in ref. (3).

# SOURCE AND PURITY OF MATERIALS:

- Sociedad Española del Oxigeno sample, purity 99.998 mole per cent.
- Carla Erba sample, purity at least 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta x/x = \pm 0.01.$ 

- Melendo, J.M.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C. Acta Cient. Compostelana 1985, XXII, 269.
- 2. Ben-Naim, A.; Baer, S. Trans. Faraday Soc. 1963, 59, 2735.
- Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. J. Chim. Phys. <u>1981</u>, 78, 171.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2,6-Dimethylcyclohexanone;
   C<sub>B</sub>H<sub>1</sub>4O; [2816-57-1]

# ORIGINAL MEASUREMENTS:

Gallardo, M.A.; Lopez, M.C.;
Urieta, J.S.; Gutierrez Losa, C.

Can. J. Chem. 1990, 68, 435-439.

### VARIABLES:

T/K = 273.15-303.15 $P_{CO_2}/kPa = 101.33$ 

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

P <sub>CO<sub>2</sub></sub> /kPa	т/к	<sup>X</sup> CO₂
101.33	273.15	0.0267
	283.15	0.0218
	293.15	0.0181
	298.15	0.0168
	303.15	0.0154

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Details of the apparatus and procedure are given in refs. (1) and (2). The total pressure was chosen so that the partial pressure of carbon dioxide was about 101.33 kPa. The number of moles of carbon dioxide introduced into the vessel containing the solution was calculated from the volume and pressure of gas introduced, taking non-ideality into account. The number of moles remaining in the gas phase in the reaction vessel was then calculated and the number of moles dissolved in the known weight of solvent found by difference.

# SOURCE AND PURITY OF MATERIALS:

- Supplied by Sociedad Española del Oxigeno; purity 99.998 mol%.
- 2. Supplied by Fluka; GLC indicates a purity of 98.2%;  $n_{\rm D}^{\rm 20}$  = 1.44686

# ESTIMATED ERROR:

 $\delta x_{CO_2} = \pm 0.7\%$  (authors)

- Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa C. J. Chim. Phys. 1983, 80, 621.
- Carnicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa C. Rev. Acad. Cienc. (Zaragoza) 1979, 34, 115.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Methyl-5-(1-methylethenyl)-2-cyclohexen-1-one or carvon or carvol; C<sub>10</sub>H<sub>14</sub>O; [99-49-0]

# ORIGINAL MEASUREMENTS:

Just, Ģ.

Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2 x_1$	Bunsen Coefficient a/cm³(STP)cm-³atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	1.89	2.76	2.914
293.15	1.72	2.51	2.690
298.15	1.58	2.29	2.498

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 2-Methyl-5-(l-methylethenyl)-2-cyclohexen-l-one. No information.

## ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

### COMPONENTS: ORIGINAL MEASUREMENTS: Bodor, E.; Mohai, B.; Pfeifer, 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Gy. 2. Acetaldehyde; C<sub>2</sub>H<sub>4</sub>O; [75-07-0] Vespremi. Vegyip. Egyet. Kozlemen. 1959, 3, 205-210. **VARIABLES:** PREPARED BY: T/K = 198-248.2C. L. Young P/kPa = 33.2-97.2EXPERIMENTAL VALUES: Absorption <sup>†</sup> Mole fraction of of gas /cm<sup>3</sup>g<sup>-1</sup> carbon dioxide T/Kin liquid, p/mmHg p/kPa <sup>x</sup>CO₂ 4.8 0.0093 248.2 267 35.6 364 48.5 9.4 0.0181 455 60.7 11.8 0.0227 531 70.8 14.4 0.0275 632 84.3 19.9 0.0376 (25) (0.047)(760)(101.3)223.2 266 35.5 21.5 0.0405 40.5 27.3 0.0509 304 408 54.4 39.3 0.0717 70.0 53.3 525 0.0948 610 81.3 62.6 0.1096 75.6 0.1294 716 95.5 (760)(80) (101.3)(0.136)83.7 $198 \pm 2$ 249 33.2 0.1413 48.1 361 137.0 0.2121 460 61.3 194.5 0.2765 72.0 540 256.8 0.3354 629 83.9 302 0.3725 0.3977 97.2 336 729 (760)(101.3)(370)(0.4210)†volumes of gas corrected to 273.15 K and 101.3 kPa; \*calc. by compiler Values in parentheses are extrapolated to 1 atmosphere. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 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. ESTIMATED ERROR: Details in ref. (1). $\delta T/K = \pm 0.1;$ $\delta$ (absorption) = ±4% or less REFERENCES: 1. Bodor, E.; Bor, G. J.; Mohai, B.; Siposs, G. Veszpremi. Vegyip. Egy. Kozl. 1957, 1, 55.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzaldehyde; C<sub>7</sub>H<sub>6</sub>O; [100-52-7]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $\frac{10^3 x_1}{}$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	13.98	3.13	3.304
293.15	12.75	2.85	3.057
298.15	11.67	2.60	2.841

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Benzaldehyde. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

# 206 COMPONENTS: ORIGINAL MEASUREMENTS: Vilcu, R.; Perisanu, St.; Carbon dioxide; CO2; [124-38-9] Cucuiat, M. 1,3-Dioxolan-2-one, (ethylene carbonate); C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>; [96-49-1] Pol. J. Chem. 1980, 54, (10), 2043-2050. VARIABLES: PREPARED BY: P.G.T. Fogg T/K = 313.15P/kPa = 101.3EXPERIMENTAL VALUES: P/kPa T/KXCO2

101.3 313.15 0.00703

Solubilities in the pressure range 1520 to 3550 kPa are also given in the paper.

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Carbon dioxide was bubbled through 10-50 cm3 of solvent for "a sufficiently long time to attain saturation". The carbon dioxide was than stripped from solution by another gas and collected in a gas buret. The mixed gas in the buret was analysed by gas chromatography.

# SOURCE AND PURITY OF MATERIALS:

- 1. Purity better than 99%
- 2. Merck's p.a. grade reagent.

ESTIMATED ERROR:

$$\delta x_{\text{CO}_2} = \pm 5\%$$
 (authors)

- Carbon dioxide; CO₂; [124-38-9]
- 4-Methyl-1,3-dioxolan-2-one, (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>; [108-32-7]

# ORIGINAL MEASUREMENTS:

Makranczy, J.; Mohai, B.; Papp, S.; Rusz, L.

Veszpremi. Vegyip. Egyet. Kozlemen. 1964, 8, 225-234.

### VARIABLES:

T/K = 273.2-303.2P/kPa = 101.3

### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

P/kPa	T/K	Solubility* cm³g-1	<sup>×</sup> CO₂
101.3	273.15	3.50	0.0158
	283.15	4.55	0.0205
	293.15	6.00	0.0268
	303.15	8.30	0.0367

<sup>\*</sup> solubilities are defined as the volume of gas, reduced to 273.15 K and 101.325 kPa, absorbed by one gram of solvent at the temperature and pressure stated.

Solubilities at 506.6, 1013.3, 2533.1 and 5066.3 kPa are also given in the paper.

# AUXILIARY INFORMATION:

# METHOD/APPARATUS/PROCEDURE:

Apparatus and method described in ref. (1)

# SOURCE AND PURITY OF MATERIALS:

No information

# ESTIMATED ERROR:

 $\delta$ (solubility) =  $\pm 10$ %

# REFERENCES:

 Macranczy, J.; Mohai, B.; Papp, S.; Rusz, L. Veszpremi. Vegyip. Egyet. Kozlemen. 1964, 8, 213.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 4-Methyl-1,3-dioxolan-2-one,
   (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

# ORIGINAL MEASUREMENTS:

Shakhova, S.F.; Bondareva, T.I.; Zubchenko, Yu.P.

Khim. Prom. 1966, (10), 753-4.

# VARIABLES:

P/kPa = 101-1677T/K = 273-328

### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K	$/cm^3$ atm $mol^{-1}$	Henry's /mmHg	constant, H /kPa*	x <sub>CO<sub>2</sub></sub> (101.3 kPa)*
273.15	2500	36900	4920	0.0208
288.15	5800	53400	7120	0.0147
298.15	1000	64500	8600	0.0118
313.15	22000	85900	11450	0.0092
328.15		108500**	14465	0.0070

Solubility measurements at 223-1677 kPa and 273-313 K were given by the authors. These were used by the authors to calculate the limiting value of Henry's constant, H, from the Krichevsky-Il'inskaya equation in the following form:

$$RT \ln \frac{f_2}{x_2} = RT \ln H + \int_{P_0}^{P} \overline{V}_2 dP - A(1-x_1^2)$$

where  $f_2$  = fugacity of carbon dioxide

 $x_1$  and  $x_2$  mole fractions of carbon dioxide and solvent

 $\overline{V}_2$  = partial molar volume of carbon dioxide at  $x_2$  = 0

A = a coefficient

- \* calculated by the compiler.
- \*\* based on measurements at 101.3 kPa only.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Apparatus described in ref. (1).

# SOURCE AND PURITY OF MATERIALS:

2. Supplied by BNIIneftekhime.

# ESTIMATED ERROR:

 $\delta H = \pm 3-5\%$  (authors)

# REFERENCES:

 Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Khim. Prom. 1960, (5), 370.

- Carbon dioxide; CO<sub>2</sub>;
- 2. 4-Methyl-1,3-dioxolan-2-one,
   (Propylene Carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

# ORIGINAL MEASUREMENTS:

Lenoir, J-Y.; Renault, P.; Renon, H. J. Chem. Eng. Data, 1971, 16, 340-2.

# VARIABLES:

T/K = 298.2-343.2

PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

T/K	Henry's constant  HCO2/atm	Mole fraction at 101.3 kPa  **CO2 (1 atm)**
298.2	67.7	0.0148
323.2	103	0.00971
343.2	124	0.00806

\* Calculated by compiler assuming a linear function of  $^{P}_{CO_{2}}$  vs  $^{x}_{CO_{2}}$ , i.e.,  $^{x}_{CO_{2}}$  (1 atm) =  $^{1/H}_{CO_{2}}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

# SOURCE AND PURITY OF MATERIALS:

- (]) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. 4-Methyl-1,3-dioxolan-2-one;
   (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

# ORIGINAL MEASUREMENTS:

Zubchenko, Yu. P.; Shakhova, S. F. Ting Wei; Titel'man, L. I.; Kaplan, L. K.

Zh. Prikl. Khim. 1971, 44(9), 2044-2047.

### VARIABLES:

P/kPa = 334-12260T/K = 228-423

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Solubility measurements over a range of pressures to high pressures were reported. Solubility data were used to calculate the limiting value of Henry's law constant, H, at zero partial pressure of carbon dioxide.

T/K	/mmHg	/kPa*
228.15 243.15	9500 16700	1267 2226
263.15	28700	3826
343.15	144000	19198
373.15	196000	26131
423.15	247000	32931

$$H = \lim_{x_{\text{CO}_2} \to 0} \left( {P_{\text{CO}_2}} / x_{\text{CO}_2} \right)$$

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Apparatus described in ref.(1) was used for temperatures from 228 K to 313 K and pressures to 6080 kPa. Measurements at 343 K to 423 K were carried out in a high pressure apparatus described in refs.(2,3).

### SOURCE AND PURITY OF MATERIALS:

No information

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  $\delta P/kPa = \pm 30.3$ 

- Shenderei, E.R.;
   Zel'venskii, Ya.D.;
   Ivanovskii, F.P.
   Khim. Prom. 1960, (5), 370.
- Krichevskii, I.R.;
   Efremova, G.D.
   Zh. Fiz. Khim. 1959, 33, 1328.
- Tsiklis, D.S. High-pressure Physicochemical Investigation Techniques, 1958, Goskhimizdat, Moscow,

<sup>\*</sup> calculated by the compiler

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. 4-Methyl-1,3-dioxolan-2-one,
   (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

# ORIGINAL MEASUREMENTS:

Meder, A.P.; Tubolkin, A.F.; Tarat, E.Ya.; Durkina, A.G.

Zhur. Fiz. Khim. 1974, 48(8), 1985; Russian J. Phys. Chem. 1974, 48(8), 1172-1174.

# VARIABLES:

T/K = 293.2-343.2 $P_{CO_2}/kPa = 9.3-93$ 

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

:	T/K Pto	otal <sup>/kPa</sup> PC	O <sub>2</sub> /kPa V	CO <sub>2</sub> /cm³†	*CO <sub>2</sub>
2:	93.2	93.0	93.0	3.430	0.01306
	93.2				0.00225
2	93.2		27.9	0.357	0.00138
2	93.2	93.0	9.3	0.057	0.00022
3	03.2	91.8	91.8	2.750	0.01050
3	13.2	90.6	90.6	2.360	0.00902
3:	23.2	89.4	89.4	2.000	0.00766
3:	33.2	89.6	89.6	1.670	0.00640
3	49.2	87.2	87.2	1.140	0.00438

 $<sup>^{\</sup>dagger}$   $\rm \textit{V}_{\rm CO_2}$  is the volume of carbon dioxide absorbed by one cm³ of solvent.

The compiler has assumed that these volumes have been reduced to  $273.2~\mathrm{K}$  and a pressure of 101.3 kPa although this was not stated by the authors.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A static method, was used as described in ref. (1). The authors did not state what gas was used to reduce the partial pressure of carbon dioxide below the total pressure.

# SOURCE AND PURITY OF MATERIALS:

No information

ESTIMATED ERROR:

# REFERENCES:

 E.Ya. Tarat; V.V. Zubov; Yu.L. Ponomarev Izv. Vys. Ucheb. Zaved. Khim. i Khim. Tekhnol. 1963, No.4.

 $<sup>^{</sup>st}$  calculated by the compiler.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 4-Methyl-1,3-dioxolan-2-one,
   (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

# ORIGINAL MEASUREMENTS:

Isaacs, E.E.; Otto, F.D.; Mather, A.E.

Can. J. Chem. Eng. <u>1977</u>, 55, 751-2.

### VARIABLES:

T/K = 313.2,373.2P/kPa = 42.2-5768.9

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	P/kPa	mole ratio solubility	*CO <sub>2</sub> *	H/Mpa <sup>†</sup>	H/kPa*
313.15	0			11.8	11800
373.15	0			26.9	26900
	42.2	0.0017	0.0017		

<sup>\*</sup>Measurements were made at 313.15 K over the pressure range 415.8-5768.9 kPa and at 373.15 K over the pressure range 42.2-5739.8 kPa. The authors obtained the partial molar volume at the two temperatures from volumetric data given by Zubchenko et a1.(1) and then fitted the data for low partial pressures to the Krichevsky-Il'inskaya equation (2) to evaluate Henry's law constants given above.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The equilibrium cell consisted of a Jerguson gauge with a 250 cm<sup>3</sup> gas reservoir. Temperatures were measured be thermocouples and controlled to ±0.5K by an air-bath. Pressures were measured by a Heise Bourdon tube gauge. The cell was charged with solvent. CO2 was added to give an appropriate pressure. Nitrogen was added, when necessary, to ensure that total pressure  $>350\ \mathrm{kPa}$ . Gases were circulated by a magnetic pump for at least 8h. The gas phase was analysed by gas chromatography. Samples of the liquid phase were withdrawn, heated at barometric pressure and the quantity of gas evolved found from P-V-T values.

# SOURCE AND PURITY OF MATERIALS:

- 1. no information
- 2. from Eastman Kodak Co.; minimum
   purity 98%

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$   $\delta (\text{mole ratio}) = \pm 0.02 \text{ or } \pm 4\%$ whichever is the larger (authors).

- Zubchenko, Yu.P.; Shakhova, S.F.; Wei, T.; Titel'man, L.I.; Kaplan, L.K. Zhur. Prik1. Khim. 1971, 44(9), 2044
- Prausnitz, J.M. Molecular Themodynamics of Fluid-Phase Equilibria, 1969, Prentice-Hall, Englewood Cliffs, NJ, USA.

<sup>\*</sup> calculated by the compiler

# ORIGINAL MEASUREMENTS: COMPONENTS: Carbon dioxide; CO<sub>2</sub>; [124-38-9] Rivas, O.R.; Prausnitz, J.M. 4 - methyl-1,3-dioxolan-2-one, Ind. Eng. Chem. Fundam. 1979, 18, (propylene carbonate); C4H6O3; 289-292. [108-32-7]. VARIABLES: PREPARED BY: T/K = 278.15, 298.15C.L. Young EXPERIMENTAL VALUES: Mole fraction of CO2 T/KHenry's constant at 101.3 kPa (1 atm) partial pressure\* / atm 278.15 54.8 0.0183 298.15 82.8 0.0121 \* Calculated by compiler assuming mole fraction solubility linear with pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus with a fused quartz precision bourdon pressure No details given. gauge. Solubility apparatus carefully thermostatted. Solvent degassed in situ. Apparatus described in ref. (1) and modifications given in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05; \ \delta x_{CO_2} = \pm 1\%.$ REFERENCES: 1. Cukor, P.M.; Prausnitz, J.M. Ind. Eng. Chem. Fundam. 1971, 10, 638.

# COMPONENTS: ORIGINAL MEASUREMENTS: Rivas, O.R.; Prausnitz, J.M. 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Am. Inst. Chem. Engnrs. J. 4-Methyl-1,3-Dioxolan-2-one, (Propylene carbonate); <u>1979</u>, 25, 975-984. C4H6O3; [108-32-7] VARIABLES: PREPARED BY: T/K = 263.15-373.15C.L. Young EXPERIMENTAL VALUES: Mole fraction of + T/KHenry's constant, H carbon dioxide in /MPa liquid, $x_{CO_2}$ 0.0277 3.66 263.15 298.15 8.39 0.01208 0.00813 323.15 12.47 17.12 0.00592 348.15 0.00453 373.15 22.35 + at a partial pressure of 101.3 kPa calculated by compiler assuming Henry's law applies at that pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus with a fused 1. and 2. Purity at least quartz precision bourdon pressure 99 mole per cent. gauge. Solubility apparatus carefully thermostatted. Solvent degassed in situ. Apparatus described in ref. (1) and modifications given in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05$ ; $\delta x_{CO_2} = \pm 1\%$ . REFERENCES: 1. Cukor, P.M.; Prausnitz, J.M. Ind. Eng. Chem. Fundam. 1971, 10, 638.

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. 4-Methyl-1,3-dioxolan-2-one,
   (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

### ORIGINAL MEASUREMENTS:

Mantor, P.D.; Abib, O.; Song, K.Y. Kobayashi, R.

J. Chem. Eng. Data 1982, 27, 243-245.

### VARIABLES:

T/K = 299.9-377.6P/kPa = 1966-6900

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solubility measurements over a range of high pressures were reported. Variation of solubility with pressure could be correlated with the Krichevsky-Kasarnovsky equation i.e.

 $\log(f_1/x_1) = \log H + \overline{V}(P-P_2)/2.303RT$ 

where  $f_1$  is the fugacity of carbon dioxide in the vapor;  $x_1$  is the mole fraction of carbon dioxide in the liquid; H is the limiting value of Henry's law constant at zero partial \_pressure of carbon dioxide;  $\overline{V}$  is the partial molar volume of carbon dioxide in the liquid; P is the total pressure;

PP2 is the partial pressure of the solvent.

T/K	Partial molar vol. of CO <sub>2</sub> /cm <sup>3</sup> mol <sup>-1</sup>	Henry's /atm		Mole fraction of CO <sub>2</sub> at P <sub>CO<sub>2</sub></sub>	
299.9	-0.06786	81.7	8280	0.01224	

299.9	-0.06786	81.7	8280	0.01224
311.0	-0.04762	101.7	10310	0.009833
344.3	-0.01000	159.4	16150	0.006274
377.6	0.02273	227.8	23080	0.004390

\* calculated by the compiler from the Krichevsky-Kasarnovsky equation

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Equilibrium between gas and liquid phases was established in a high pressure cell which could be agitated. A mercury displacement pump was used to provide pressures greater than that in the carbon dioxide cylinder. Temperatures were maintained to ±0.6 K in an air bath. There was provision for withdrawal of samples of the gas from the top of the cell and of liquid from the bottom of the cell.

# SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Spencer Chemical
  Co.,; purity 99.6 mol%
- 2. Supplied by Jefferson Chemical Co., minimum purity 99 wt%

# ESTIMATED ERROR:

 $\delta H/H = \pm 0.06$  (estimated by compiler from the stated deviation from the K.-K. eqn.);  $\delta T/K = \pm 0.6$  (authors)

COMPONENTS:	ORIGINAL MEASUREMENTS:
	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Sweeney, C.W.
2. Polar solvents	Chromatographia <u>1984</u> , 18, 663-7
VARIABLES:	PREPARED BY:
T/K = 298.15; 323.15	P.G.T. Fogg
EXPERIMENTAL VALUES: Solvent	Henry's constant Henry's constant
	/bar /kPa 198.15 K 323.15 K 298.15 K 323.15 K
Phosphoric acid, tributyl ester (tributyl phosphate); C <sub>12</sub> H <sub>27</sub> PO <sub>4</sub> ; [126-73-8]	29.4 46.6 2940 4660
4-Methyl-1,3-dioxolan-2-one (propylene carbonate); C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> ; [108-32-7]	82.9 127.7 8290 12770
1-Methyl-2-pyrrolidinone (N-methylpyrrolidone); C <sub>5</sub> H <sub>9</sub> NO; [872-50-4]	69.8 110.9 6980 11090
2,5,8,11,14-Pentaoxapentadecane (tetraethylene glycol dimethyl ether) C <sub>10</sub> H <sub>22</sub> O <sub>5</sub> ; [143-24-8]	
The Henry's constant, H, was defined a	s:
$H = x_2 + 0 \begin{bmatrix} f_2 \\ \overline{x_2} \end{bmatrix}$	. ]
where $f_2$ is the fugacity of $CO_2$ in the fraction of $CO_2$ in the liquid phase.	gas phase and $x_2$ the mole
AUXILIARY I	NFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Henry's constants were calculated from retention volumes measured with a modified 204 Series Pye-Unicam gas chromatograph. Helium was used as carrier gas and the support material was PTFE. Further	1. from Cambrian Gases, London; 97.5 - 99.9% pure. 2. from Aldrich Chemicals, Gillingham, U.K.; re-distilled.
details are given in refs. 1 - 3.	ESTIMATED ERROR:
	$\delta T/K = \pm 0.05$ ; $\delta H/H = \pm 0.05$ (author)
	REFERENCES:
	1. Conder, J.R.; Young C.L.,  Physicochemical Measurements by  Gas Chromatography, 1979, Wiley,  Chichester, U.K.
	2. Ng, S.; Harris, H.G.; Prausnitz,J.M. J. Chem. Eng. Data 1969, 14, 482.
	3. Lin, P.J.; Parcher, J.F.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 4-Methyl-1,3-dioxolan-2-one,
   (propylene carbonate); C<sub>4</sub>H<sub>6</sub>O<sub>3</sub>;
   [108-32-7]

### VARIABLES:

T/K = 298.15-373.15P/kPa = 56.3-2228.7

# ORIGINAL MEASUREMENTS:

Murrieta-Guevara, F.; Romero-Martinez, A.; Trejo, A.

Fluid Phase Equilibria, 1988, 44, 105-115.

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K	P <sub>CO2</sub> /kPa	<sup>x</sup> CO₂
298.15	56.3	0.0064
313.15	147.5 54.7 139.9	0.0178 0.0056 0.0137
373.15	177.2 219.4	0.0168 0.0075

The authors have also given data for higher pressures

T/K	Henry's la H/MPa	aw constant H/kPa	<sup>x</sup> CO <sub>2</sub> (101.3 kPa)*
298.15	8.21	8210	0.01234
313.15 373.15	10.23 28.88	10230 28880	0.00990 0.00351

<sup>\*</sup> estimated by the compiler as  $P_{\rm CO_2}/H$ 

# AUXILIARY INFORMATION:

## METHOD/APPARATUS/PROCEDURE:

The apparatus and method of calculation have been described in previous publications (refs.1 and 2). The limiting values of Henry's law constant which are given above were found by fitting the experimental data to the Krichevsky-Kasarnovsky equation (3).

# SOURCE AND PURITY OF MATERIALS:

- Supplied by Infra S.A.; reported purity 99.7 mol%.
- 2. Purity better than 99.5 mol%.

# ESTIMATED ERROR

 $\delta T/K = \pm 0.02$  to 343 K;  $\pm 0.5$  at 373 K. (authors)  $\delta P/kPa = \pm 3.5$ 

- Murrieta-Guevara, F.; Trejo, A.,
   J. Chem. Eng. Data, 1984, 29, 456.
- 2. Gonzalez, R.;
   Murrieta-Guevara, F.; Parra, O.;
   Trejo, A., Fluid Phase
   Equilibria, 1987, 34, 69.
- 3. Prausnitz, J.M.; Lichtenthaler, R.N.; Gomes de Azevedo, E. Molecular Thermodynamics of Fluid-Phase Equilibria, 1986, Prentice-Hall, Englewood Cliffs, NJ, USA; Chap.7

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid; C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>; [64-19-7]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
288.15	1.34	5.32	5.614
293.15	1.21	4.78	5.129
298.15	1.09	4.29	4.679

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Acetic acid. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Acetic acid, C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>; [64-19-7] Acetic acid, pentyl ester,

(amy1 acetate);  $C_7H_{14}O_2$ ; [628-63-7]

### ORIGINAL MEASUREMENTS:

Kunerth, W.

Phys. Rev. 1922, 19, 512-524.

### VARIABLES:

T/K = 291.15-307.15 $P/kPa \simeq 101.3$ 

### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Solvent	T/K	Ostwald coefficient L	$x_{\text{CO}_2}$ at $P_{\text{CO}_2} = 101.3 \text{ kPa*}$
Acetic acid	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15 309.15	5.40 5.23 5.07 4.91 4.73 4.57 4.41 4.25 4.12 4.00	0.01283 0.01237 0.01194 0.01152 0.01105 0.01063 0.01022 0.00981 0.00947 0.00916
Amyl acetate	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15	4.79 4.65 4.55 4.44 4.35 4.24 4.14 4.10	0.02904 0.02803 0.02726 0.02645 0.02576 0.02496 0.02423 0.02385 0.02324

<sup>\*</sup> calculated by the compiler

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The method is based upon that described by McDaniel (1). apparatus consisted of a gas buret attached to a levelling tube containing mercury and to the absorption cell containing the solvent under test. The volume of gas absorbed by a measured volume of liquid was measured at a total pressure equal to barometric pressure. The mercury in the gas buret was covered with a layer of solvent so that the gas in the buret was saturated with solvent vapor. Buret and absorption cell were surrounded by heating wire and water jackets fitted with thermometers.

# SOURCE AND PURITY OF MATERIALS:

- produced by heating NaHCO<sub>3</sub>; dried with CaCl2; frozen in liquid air and volatile impurities pumped away; passed over P2O5.
- commercial sample; purity attested by boiling point and density.

# ESTIMATED ERROR:

 $\delta x_{CO_2} = \pm 5\%$ (compiler)

- 1. McDaniel, A.S.;
  - J. Phys. Chem. 1911, 15, 587.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Butanoic acid or butyric acid; C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>; [107-92-6]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

Mol Fraction	Bunsen	Ostwald
10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm $^{-1}$	Coefficient L/cm³cm-3
15.55	3.87	4.084
14.20	3.51	3.767
12.97	3.19	3.478
	10 <sup>3</sup> x <sub>1</sub> 15.55 14.20	

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Butanoic acid. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Propanoic acid; C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>; [79-09-4]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. <u>1901</u>, 32, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	14.79	4.54	4.787
293.15	13.51	4.12	4.417
298.15	12.34	3.74	4.078

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Propanoic acid. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. 9-Octadecenoic acid (Z), (oleic acid); C<sub>18</sub>H<sub>34</sub>O<sub>2</sub>; [112-80-1] VARIABLES: T/K = 296.2-335.2 P/kPa ~ 11-59 ORIGINAL MEASUREMENTS: Ouellet, C.; Dubois, J.-T. Can. J. Research 1948, 26B, 54-58.

EXPERIMENTAL VALUES:

т/к	Bunsen coef. α	$x_{\text{CO}_2}$ at $P_{\text{CO}_2}$ = 101.3 kPa
296.15	1.13	0.0160
316.15	0.90	0.0127
326.15	0.79	0.0112
335.15	0.69	0.0098

The authors published a graph showing variations of the volume of carbon dioxide, reduced to 273.15 K and 101.3 kPa, with variations in the partial pressure of carbon dioxide. The partial pressure range was approximately 11-59 kPa. There was linear variation at each of the four temperatures.

# AUXILIARY INFORMATION

## METHOD /APPARATUS / PROCEDURE:

The solvent was placed in a glass bulb held in a thermostat bath and connected by flexible copper tubing to a manometer, gas reservoir and vacuum line. Dissolved air was first pumped out of the liquid. The carbon dioxide was then put in contact with the liquid which was agitated for 10-20 min. The quantity of gas absorbed was calculated from the change in pressure and volume of the system. It was also shown that the process of absorption was completely reversible.

# SOURCE AND PURITY OF MATERIALS:

- prepared by heating magnesium carbonate to 350°C; dried by phosphorus pentoxide.
- 2. no information.

ESTIMATED ERROR:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid anhydride;  ${\rm C_4^H_6^O_3}$ ; [108-24-7]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

Mol Fraction	Bunsen	Ostwald
10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
24.3	5.89	6.218
22.1	5.33	5.720
19.9	4.77	5.206
	10 <sup>3</sup> x <sub>1</sub> 24.3 22.1	$ \begin{array}{ccc} 10^{3}x_{1} & & \text{Coefficient} \\  & \alpha/\text{cm}^{3} \text{ (STP) cm}^{-3} \text{ atm}^{-1} \\ 24.3 & & 5.89 \\ 22.1 & & 5.33 \end{array} $

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Acetic acid anhydride. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Formic acid, pentyl ester or amyl formate; C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [638-49-3]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

TAT ANTORS:			
T/K	Mol Fraction	Bunsen	Ostwald
	10³x_1	Coefficient α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	25.0	4.40	4.646
293.15	23.1	4.03	4.329
298.15	21.2	3.69	4.026

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Formic acid, pentyl ester. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W.
  - Z. Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid, methyl ester or methyl acetate; C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>; [79-20-9]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

T/K = 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction	Bunsen	Ostwald
	10³x	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient _L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	20.76	5.95	6.494

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Acetic acid, methyl ester. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) <u>1894</u>, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid, methyl ester or methyl acetate; C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>; [79-20-9]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	2.28	6.47	7.06
	2.25	6.39	6.97
	2.26	6.42	7.01

The mole fraction and Ostwald coefficient values were calculated by the compiler.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 99.9% CO<sub>2</sub>.
- (2) Acetic acid, methyl ester. Fractionated by distillation. B.p. (760 mmHg)/°C = 56.72 - 56.85, refractive index n<sub>D</sub>(20°C) = 1.3618.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- Gjaldbaek, J. C.
   Acta Chem. Scand. <u>1952</u>, 6, 623.

### 227 COMPONENTS: ORIGINAL MEASUREMENTS: Bodor, E.; Bor, Gy.; Maleczkine, M.; Mesko, G.; Mohai, G.; 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Acetic acid, ethyl ester (ethyl Siposs, G. acetate); C4H8O2; [141-78-6] Veszpremi. Vegyip. Egyet. Kozlemen. 1957, 1, 77-87. VARIABLES: PREPARED BY: T/K = 198-318.2C. L. Young P/kPa = 9.6-102.4EXPERIMENTAL VALUES: Absorption + Mole fraction of of gas /cm<sup>3</sup>g<sup>-1</sup> carbon dioxide in liquid, T/Kp/kPa p/mmHq xCO2 318.2 72 9.6 0.50 0.00196 0.00321 169 22.5 0.82 198 26.4 1.24 0.00485 0.00544 41.2 1.39 309 346 2.06 0.00803 46.1 0.00834 407 54.3 2.14 515 68.7 2.83 0.01100 0.00981 295.2 2.52 285 38.0 379 50.5 3.37 0.01308 3.23 59.5 0.0125 446 451 60.1 4.00 0.0155 0.0156 4.03 70.1 526 4.77 0.0184 538 71.7 4.95 0.0191 620 82.7 768 102.4 6.45 0.0247 (760)(101.3)(6.40)(0.0245)2.46 4.74 273.2 24.1 0.00958 181 327 43.6 0.0183 54.1 406 5.90 0.0227 6.95 482 64.3 0.0266 81.5 7.70 0.0294 611 (cont.) AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS:

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).

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;

 $\delta$ (absorption) = ±4% or less.

# REFERENCES:

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

# ORIGINAL MEASUREMENTS:

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Acetic acid, ethyl ester (ethyl
  acetate); C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>; [141-78-6]

Bodor, E.; Bor, Gy.; Maleczkine, M.; Mesko, G.; Mohai, G.; Siposs, G. Veszpremi. Vegyip. Egyet. Kozlemen. 1957, 1, 77-87.

EXPERIMEN	NTAL VALUES:			
T/K	p/mmHg	p/kPa	Absorption <sup>†</sup> of gas /cm³g-¹	Mole fraction <sup>*</sup> of carbon dioxide in liquid, <sup>x</sup> CO <sub>2</sub>
273.2	685	91.3	10.2	0.0386
	686	91.5	8.86	0.0337
	799	106.5	10.5	0.0396
248.2	(760)	(101.3)	(11)	(0.041)
	273	36.4	8.2	0.0312
	321	42.8	10.6	0.0400
	348	46.4	10.0	0.0378
	452	60.3	14.3	0.0532
	534	71.2	17.7	0.0651
	562	74.9	20.1	0.0732
	730	97.3	23.4	0.0842
	731	97.5	23.8	0.0856
	(760)	(101.3)	(25)	(0.089)
223.2	233	31.1	20.3	0.0739
	277	36.9	24.3	0.0872
	331	44.1	29.9	0.105
	407	54.3	30.8	0.108
	517	68.9	47.1	0.156
	557	74.3	48.8	0.161
	616	82.1	58.0	0.186
	734	97.9	61.8	0.195
198 ± 2	735	98.0	69.6	0.215
	(760)	(101.3)	(70)	(0.216)
	162	21.6	52.8	0.172
	188	25.1	63.5	0.200
	235	31.3	74.5	0.227
	303	40.4	106.0	0.294
	379	50.5	135.6	0.348
	481	64.1	180.0	0.414
	504	67.2	180.3	0.415
	577	76.9	218.8	0.462
	736	98.1	264.0	0.509
	(760)	(101.3)	(280)	(0.524)

Values in parentheses are extrapolated to 1 atmosphere.

the volume of gas absorbed by one gram of solvent was corrected to 273.15 K and 101.3 kPa. calculated by compiler.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid, propyl ester or propyl acetate; C<sub>5</sub>H<sub>10</sub>O<sub>2</sub>; [109-60-4]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³ (STP) cm-³atm-1	Ostwald Coefficient L/cm³cm-3
298.15	2.46	4.84	5.28
	2.44	4.80	5.24

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 99.9% CO<sub>2</sub>.
- (2) Acetic acid, propyl ester.
   Judex Chemicals. Fractionated
   by distillation. B.p.
   (760 mmHg)/°C = 101.66 101.70,
   refractive index n<sub>D</sub>(20°C) =
   1.3846.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid, 2-methylpropy1
   ester or isobutyl acetate;
   C<sub>6</sub>H<sub>12</sub>O<sub>2</sub>; [110-19-0]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 293.15, 298.15  $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

TUD AUTORD.			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
293.15	2.67	4.63	4.968
298.15	2.50	4.30	4.691

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Acetic acid, 2-methylpropyl ester. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Acetic acid, pentyl ester or amylacetate; C<sub>7</sub>H<sub>14</sub>O<sub>2</sub>; [628-63-7]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm3cm-3
288.15	2.95	4.60	4.850
293.15	2.66	4.11	4.411
298.15	2.46	3.77	4.119

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Acetic acid, pentyl ester. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. 1890, 6, 141.
- 2. Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52,
  275.

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Ouellet, C.; Dubois, J.-T. [124-38-9] Can. J. Research 1948, 26B, 54-58. Octadecanoic acid, ethyl ester, (ethyl stearate); C20H40O2; [111-61-5] VARIABLES: PREPARED BY: T/K = 307.15-347.15 $P/kPa \simeq 8-78$ P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Bunsen coef. a	${}^{x}_{\text{CO}_2}$ at ${}^{p}_{\text{CO}_2}$ = 101.3 kPa
307.15	1.15	0.0190
	1.05	0.0190
316.15		
325.15	0.94	0.0155
335.15	0.85	0.0140
347.15	0.76	0.0125

The authors published a graph showing variations of the volume of carbon dioxide absorbed, reduced to 273.15 K and 101.3 kPa, with variations in the partial pressure of carbon dioxide. The partial pressure range was approximately 8-78 kPa. There was linear variation at each of the five temperatures.

### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

The solvent was placed in a glass bulb held in a thermostat bath and connected by flexible copper tubing to a manometer, gas reservoir and vacuum line. Dissolved air was first pumped out of the liquid. carbon dioxide was then put in contact with the liquid which was agitated for 10-20 min. The quantity of gas absorbed was calculated from the change in pressure and volume of the system. It was also shown that the process of absorption was completely reversible.

# SOURCE AND PURITY OF MATERIALS:

- prepared by heating magnesium carbonate to 350°C; dried by phosphorus pentoxide.
  2. density at 40°C = 0.848 g cm<sup>-3</sup>;
- no further information.

ESTIMATED ERROR:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Octadecenoic acid, methyl ester, (methyl oleate); C<sub>19</sub>H<sub>36</sub>O<sub>2</sub> [27234-05-5]
   Octadecenoic acid, ethyl ester, (ethyl oleate); C<sub>20</sub>H<sub>38</sub>O<sub>2</sub>; [2855-06-8]
   Octadecenoic acid, butyl ester, (butyl oleate); C<sub>22</sub>H<sub>42</sub>O<sub>2</sub>; [142-77-8]

# ORIGINAL MEASUREMENTS:

Arai, C.; Yoshitama, T.; Nishihara, K.; Sano, Y.

Kagaku Kogaku Ronbunshu 1989, 15(6), 1193-5.

### VARIABLES:

T/K = 273.2-343.2 $P/kPa \approx 30-90$ 

## PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Solvent	T/K	Henry's o		x <sub>CO2</sub> at P <sub>CO2</sub> 101.3 kPa
Butyl oleate	273.2	2.42	2420	0.0419
	283.2	2.86	2860	0.0354
	293.2	3.37	3370	0.0301
	298.2	3.63	3630	0.0279
	303.2	3.93	3930	0.0258
	323.2	5.14	5140	0.0197
	343.2	6.45	6450	0.0157
Ethyl oleate	273.2	2.31	2310	0.0439
	298.2	3.66	3660	0.0277
	323.2	5.26	5260	0.0193
Methyl oleate	273.2	2.37	2370	0.0428
	298.2	3.77	3770	0.0269
	323.2	5.36	5360	0.0189

The authors fitted the following equation to the data for butyl oleate:

 $\ln H = 6700/(T/K) + 53.729\ln(T/K) - 0.08962(T/K) - 300.58$ 

standard deviation in values of H = 0.8%

# AUXILIARY INFORMATION

# A static method was used. The apparatus consisted of an absorption vessel connected to a gas buret and manometers. The system could be evacuated via a vacuum line. Gas was held in a storage bulb. The contents of the absorption vessel could be stirred magnetically and the temperature measured with a thermometer. The apparatus was held at constant temperature by a thermostat.

METHOD/APPARATUS/PROCEDURE:

# SOURCE AND PURITY OF MATERIALS:

No information

# ESTIMATED ERROR:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 1,2,3-Propanetriol, triacetate (glycerol triacetate); C9H14O6; [102-76-1]
  - 2-[2-(2-Methoxyethoxy)ethoxy]ethanol, acetate, (methoxy-triethyleneglycol acetate); C<sub>9</sub>H<sub>18</sub>O<sub>5</sub>; [3610-27-3]
  - 2-[2-(2-Butoxyethoxy)ethoxy]ethanol, acetate, (butoxy-triethyleneglycol acetate); C<sub>12</sub>H<sub>24</sub>O<sub>5</sub>; [3610-26-2]

# ORIGINAL MEASUREMENTS:

Makranczy, J.; Mohai, B.; Papp, S.; Rusz, L.

Veszpremi. Vegyip. Egyet. Kozlemen. 1964, 8, 225-234.

# VARIABLES:

P/kPa = 101.3T/K = 273.2-303.2

# PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Solvent	P/kPa	T/K	Solubility* cm³g-1	<sup>x</sup> co₂
Glycerol triacetate	101.3	273.15 283.15 293.15 303.15	4.40 3.45 2.65 1.98	0.0414 0.0327 0.0253 0.0190
Methoxytriethyleneglycol acetate	L 101.3	273.15 283.15 293.15 303.15	8.10 6.40 4.55 3.50	0.0698 0.0560 0.0405 0.0314
Butoxytriethyleneglycol acetate	101.3	273.15 283.15 293.15 303.15	4.60 3.70 2.95 2.38	0.0488 0.0397 0.0319 0.0259

<sup>\*</sup> solubilities are defined as the volume of gas, reduced to 273.15 K and 101.325 kPa, absorbed by one gram of solvent at the temperature and pressure stated.

Solubilities at 506.6, 1013.3, 2533.1 and 5066.3 kPa are also given in the paper.

# AUXILIARY INFORMATION

# Apparatus and method described in

METHOD/APPARATUS/PROCEDURE:

No information

ref. (1)

# ESTIMATED ERROR:

 $\delta(\text{solubility}) = \pm 10\%$ (compiler)

# REFERENCES:

1. Macranczy, J.; Mohai, B.; Papp, S.; Rusz, L. Veszpremi. Vegyip. Egyet. Kozlemen. 1964, 8, 213.

SOURCE AND PURITY OF MATERIALS:

# COMPONENTS: 1. Carbon dioxide; CO2; [124-38-9]

1,2,3-Propanetriol, triacetate, (triacetin); C9H14O6; [102-76-1]

# ORIGINAL MEASUREMENTS:

Shakhova, S.F.; Bondareva, T.I.; Zubchenko, Yu.P.

Khim. Prom. 1966, (10), 753-4.

# VARIABLES:

P/kPa = 101-1677T/K = 273-328

PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K	$/cm^3$ atm $mol^{-1}$	Henry's co	onstant, H /kPa*	*CO <sub>2</sub> (101.3 kPa)*
273.15	-4200	15700	2090	0.0466
288.15	-4500	21800	2910	0.0339
298.15	-2100	27100	3610	0.0284
308.15	2.00	32700**	4360	0.0232
313.15	-1200	34600	4610	0.0221
323.15		38900**	5190	0.0195
328.15		45800**	6110	0.0166

Solubility measurements at 223-1677 kPa and 273-313 K were given by the authors. These were used by the authors to calculate the limiting value of Henry's constant, H, from the Krichevsky-Il'inskaya equation in the following form:

RTln 
$$\frac{f_2}{x_2} = RTlnH + \int_{P_0^1}^{P} \overline{V}_2 dP - A(1-x_1^2)$$

where  $f_2$  = fugacity of carbon dioxide  $x_1$  and  $x_2$  mole fractions of solvent and carbon dioxide respectively.

 $\overline{V}_2$  = partial molar volume of carbon dioxide at  $x_2$  = 0

A = a coefficient

\* calculated by the compiler

METHOD /APPARATUS / PROCEDURE:

\*\* based on measurements at 101.3 kPa only

# AUXILIARY INFORMATION

Apparatus described in ref. (1).

2. Pure grade; distilled in vacuum.

ESTIMATED ERROR:

 $\delta H = \pm 3-5\%$  (authors)

SOURCE AND PURITY OF MATERIALS:

# REFERENCES:

 Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P. Khim. Prom. 1960, (5), 370.

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] Christoff, A. (2) 1,1'-Oxybisethane or diethyl ether; C<sub>4</sub>H<sub>10</sub>O; [60-29-7] VARIABLES: T/K = 273.15, 283.15 p<sub>1</sub>/kPa = atmospheric PRIGINAL MEASUREMENTS: Christoff, A. Z. Phys. Chem. 1912, 79, 456-60.

### EXPERIMENTAL VALUES:

Temp	perature T/K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
0	273.15	3.19	7.330	7.330
10	283.15	2.59	5.831	6.044
15	288.15	2.33	5.181	5.465

The mole fraction and Bunsen coefficient values were calculated by the compiler assuming ideal gas behavior.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus is an Ostwald type as described by Just (ref 1), and modified by Skirrow (ref 2). The apparatus consists of a thermostated gas buret and an absorption flask.

The modification involves the use of vapor free gas in the gas buret. A correction is made for the vapor pressure of the solvent. A steel capillary tube with a stopcock, which prevents the gas and the solvent vapor from mixing in the buret, is used to connect the absorption flask and the buret.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide.
   No information.
- (2) Diethyl ether. Merck. Stated to be pure and anhydrous.

# ESTIMATED ERROR:

 $\delta L/L = \pm 0.03$ 

- Just, G.
   Z. Phys. Chem. 1901, 37, 342.
- 2. Skirrow, F. W. Z. Phys. Chem. 1902, 41, 139.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Tetrahydrofuran; C<sub>4</sub>H<sub>8</sub>O; [109-99-9] VARIABLES: T/K = 198-318.2 P/kPa = 10.5-98.0 CORIGINAL MEASUREMENTS: Bodor, E.; Bor, Gy.; Maleczkine, M.; Mesko, G.; Mohai, B.; Siposs, G. Veszpremi. Vegyip. Egyet. Kozlemen. 1957, 1, 89-98. C. L. Young

p/mmHg 79 189 229 283	p/kPa 10.5 25.2 30.5	Absorption <sup>†</sup> of gas /cm³g-¹  0.51 1.57	Mole fraction of carbon dioxide in liquid,  **CO <sub>2</sub> 0.00164 0.00503
189 229 283	25.2		
283		1.80	0.00576
316 337	37.7 42.1 44.9	2.63 2.50	0.00839 0.00798 0.00984
270 298	36.0 39.7	2.72 3.26	0.00868 0.0104 0.0128
394 394 464	52.5 61.9	4.45 5.53	0.0141 0.0175
490 547	72.9	5.64	0.0161 0.0178 0.0213
585 430	78.0 57.3	6.07 7.12	0.0192 0.0224
527	70.3	7.67 9.30 8.65	0.0241 0.0291 0.0271
609 637	81.2 84.9	10.9 10.3	0.0339 0.0321
	337 270 298 394 394 464 490 547 569 585 430 441 527 541 609	337       44.9         270       36.0         298       39.7         394       52.5         394       52.5         464       61.9         490       65.3         547       72.9         569       75.9         585       78.0         430       57.3         441       58.8         527       70.3         541       72.1         609       81.2	337       44.9       3.09         270       36.0       2.72         298       39.7       3.26         394       52.5       4.02         394       52.5       4.45         464       61.9       5.53         490       65.3       5.08         547       72.9       5.64         569       75.9       6.75         585       78.0       6.07         430       57.3       7.12         441       58.8       7.67         527       70.3       9.30         541       72.1       8.65         609       81.2       10.9

# AUXILIARY INFORMATION

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METHOD	/APPAR	ATUS / PE	n	CEDURE	•

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:

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ 

 $\delta$ (absorption) =  $\pm 4%$  or less.

# REFERENCES:

1. Bodor, E.; Bor, G. J.;
Mohai, B.; Siposs, G.

Veszpremi. Vegyip. Egy. Kozl.

1957, 1, 55.

# ORIGINAL MEASUREMENTS:

1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]

2. Tetrahydrofuran; C<sub>4</sub>H<sub>8</sub>O; [109-99-9]

Bodor, E.; Bor, Gy.; Maleczkine, M.; Mesko, G.; Mohai, B.; Siposs, G. Veszpremi. Vegyip. Egyet. Kozlemen. 1957, 1, 89-98.

			Mole fraction * of carbon dioxide	
T/K	p/mmHg	p/kPa	of gas /cm³g-1	in liquid,  "CO <sub>2</sub>
273.2	728 735 (760)	97.1 98.0 (101.3)	11.7 12.9 (13)	0.0363 0.0399 (0.040)
248.2	111 222 345 412 420 518 526 622 722 722 722 (760)	14.8 29.6 46.0 54.9 56.0 69.1 70.1 82.9 96.3 96.3 (101.3)	2.6 5.0 8.1 10.4 11.5 14.9 14.1 16.8 20.8 21.4 (23)	0.0083 0.0158 0.0254 0.0324 0.0357 0.0458 0.0434 0.0513 0.0627 0.0644 (0.0689)
223.2	158 319 321 429 528 541 636 730 731 (760)	21.1 42.5 42.8 57.2 70.4 72.1 84.8 97.3 97.5 (101.3)	15.1 30.5 29.7 43.8 53.6 51.1 66.9 77.3 72.6 (80)	0.0463 0.0894 0.0872 0.124 0.147 0.141 0.177 0.199 0.189 (0.205)
198 ± 2	147 244 261 417 420 493 542 588 653 733 733 (760)	19.6 32.5 34.8 55.6 56.0 65.7 72.3 78.4 87.1 97.7 97.7	63.4 87.4 97.1 160.4 164.3 202.4 225.8 256.1 301.8 351.0 357.8 (375)	0.169 0.219 0.238 0.340 0.346 0.394 0.421 0.452 0.493 0.530 0.535 (0.547)

Values in parentheses are extrapolated to 1 atmosphere.

 $<sup>^{\</sup>dagger} the\ volume\ of\ gas\ absorbed\ by\ one\ gram\ of\ solvent\ was\ corrected\ to\ 273.15\ K\ and\ 101.3\ kPa$ 

<sup>\*</sup> calculated by compiler.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,4-Dioxane; C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>; [123-91-1]

#### ORIGINAL MEASUREMENTS:

Gallardo, M. A.; Urieta, J. S.;
Gutierrez Losa, C.

J. Chim. Phys. Phys.-Chim. Biol. 1983, 80, 621-25.

# VARIABLES:

T/K = 285.15 - 303.15 $p_1/kPa = 101$ 

# PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen Coefficient a/ cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³ cm-3
285.15	300.9	8.229	8.590
289.15	269.4	7.312	7.740
293.15	254.6	6.869	7.732
298.15	227.2	6.080	6.636
303.15	197.4	5.237	5.812

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior.

The authors fitted their data to the equation:

 $-\ln x_1 = 6.781 \ln (T/K) - 34.859$  from which they obtained.

 $\Delta H_1^2/kJ \text{ mol}^{-1} = -2.09$ , and  $\Delta S_1^2/J \text{ K}^{-1} \text{ mol}^{-1} = -62$  for the transfer

of one mole of carbon dioxide from the gas phase at 101 kPa to the hypothetical unit mole fraction solution.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to that of Ben-Naim and Baer (ref 1). It was described in detail in an earlier paper (ref 2).

The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on the solvent vapor saturated gas.

Literature 1,4-dioxane vapor pressure data were fitted to the equation

$$ln (p_2//kPa) =$$

$$-4591.3/(T/K) + 16.98.$$

#### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Sociedad Espanola del Oxigeno. Stated to be 99.998 %.
- (2) 1,4-Dioxane. Merck and Co. Purity checked by GLC to be ≥ 99 %.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$   $\delta p_1/kPa = \pm 1$  $\delta x_1/x_1 = \pm 0.01$ 

- Ben Naim, A.; Baer, S. Trans. Faraday Soc. <u>1963</u>, 59, 2735-38.
- Carniecer, J.; Gibanel, F.;
   Urieta, J.S.; Gutierrez Losa, C.
   Rev. Acad. Ciencieas Zaragoza
   1979, 34, 115-22.

240	
COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Kassim, D.M.; Zainel, H.A.; Al-Asof, S.A.; Talib, E.K.
2. 1,4-Dioxane; C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> ; [124-91-1]	Fluid Phase Equilibria
	<u>1988</u> , 41, 287-294.
VARIABLES:	PREPARED BY:
T/K = 303.15-333.15 P/kPa = 101.3	C. L. Young
EXPERIMENTAL VALUES:	
T/K Mole frac	tion of carbon dioxide in liquid, $x_{\mathrm{CO}_2}$
303.15 313.15 323.15 333.15	0.0192 0.0187 0.0182 0.0175
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Falling film flow apparatus similar to that of Morrison and Billet (1). Apparatus consisted of (i) degassing section in which solvent could be degassed by freezing and thawing under vacuum and (ii) absorption section. The latter consisted of a gas buret and absorption spiral. Mole fraction solubility corrected to 1 atm partial pressure by assuming Henry's law was valid.	<ol> <li>Purity 99.99 mole per cent.</li> <li>Fluka AG puriss grade sample, purity better than 99 mole per cent.</li> </ol>
	ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta x/x = \pm 0.02$ (estimated by compiler).  REFERENCES:  1. Morrison, T.J.; Billet, F.J.  J. Chem. Soc. 1948, 2033.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Lenior, J-Y.; Renault, P.; Renon, H.
2. Oxybispropanol, (Dipropylene glycol); C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> ; [25265-71-8]	J. Chem. Eng. Data, <u>1971</u> , 16, 340-2.
VARIABLES:	PREPARED BY:
T/K = 298.2-343.2	C. L. Young

#### EXPERIMENTAL VALUES:

T/K	Henry's constant  HCO2/atm	Mole fraction at 101.3 kPa  **CO2 (1 atm)**
298.2	121	0.00826
323.2 343.2	154 212	0.00649 0.00472

\* Calculated by compiler assuming a linear function of  $^{P}_{\text{CO}_{2}}$  vs  $^{x}_{\text{CO}_{2}}$ , i.e.,  $^{x}_{\text{CO}_{2}}$  (1 atm) =  $^{1/H}_{\text{CO}_{2}}$ .

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

#### SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2,2'-[1,2-Ethanediylbis(oxy)]bisethanol, (triethylene glycol);
  C<sub>6</sub>H<sub>1</sub>4O<sub>4</sub>; [112-27-6]

# BLES: PREPARED BY:

VARIABLES: P/kPa = 101.3 T/K = 273.2-303.2

PREPARED BI:

Rusz, L.

P.G.T. Fogg

ORIGINAL MEASUREMENTS:

Makranczy, J.; Mohai, B.; Papp, S.;

Veszpremi. Vegyip. Egyet. Kozlemen. 1964, 8, 213-224.

#### EXPERIMENTAL VALUES:

P/kPa	т/к	Solubility* cm³g-1	<sup>x</sup> CO₂
101.3	273.15	1.700	0.01134
	283.15	1.405	0.00939
	293.15	1.135	0.00760
	303.15	0.900	0.00604

<sup>\*</sup> solubilities are defined as the volume of gas, reduced to 273.15 K and 101.325 kPa, absorbed by one gram of solvent at the temperature and pressure stated.

Solubilities at 506.6, 1013.3, 2533.1 and 5066.3 kPa are also given in the paper.

# AUXILIARY INFORMATION

SOURCE AND PURITY OF MATERIALS:

Apparatus and method described in ref. (1)

ESTIMATED ERROR:

 $\delta$ (solubility) =  $\pm 10%$ 

#### REFERENCES:

 Macranczy, J.; Mohai, B.; Papp, S.; Rusz, L.

> Veszpremi. Vegyip. Egyet. Kozlemen. 1964, 8, 213.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2,2'[1,2-Ethanediylbis(oxy)]bisethanol, (triethylene glycol);
  C<sub>6</sub>H<sub>1</sub>4O<sub>4</sub>; [112-27-6]

# ORIGINAL MEASUREMENTS:

Jou, F-Y.; Deshmukh, R.D.; Otto, F.D.; Mather, A.E. Fluid Phase Equilibria 1987, 36, 121-140.

#### VARIABLES:

T/K = 298-398; P/kPa = 105-20250

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

Experimental data were used to calculate the parameters H,  $\overline{V}_2$  and A in Krichevsky-Il'inskaya equations of the form

$$RT \ln(f_2/x_2) = RT \ln H + \overline{V}_2(P-P_S) + A(x_1^2 - 1)$$

where  $f_2$  = fugacity of solute  $x_2$  = mole fraction of solute

 $\frac{H}{V_2}$  = Henry's constant of the solute at infinite dilution  $\frac{1}{V_2}$  = partial molar volume of the solute at infinite diution

A = Margules parameter

 $x_1$  = mole fraction of the solvent

 $P^{-}$  = total pressure  $P_{s}$  = partial pressure of the solvent

T/K	Henry's Constant, H /kPa	$\overline{V}_2/\text{cm}^3\text{mol}^{-1}$	A/RT	<sup>x</sup> <sub>CO₂</sub> at 101.3 kPa <sup>*</sup>
298.15 323.15 348.15 373.15 398.15	17440 23550 29850	36.50 38.14 40.03 42.23 44.82	0.229 0.228 0.229 0.232 0.237	0.008443 0.005792 0.004292 0.003388 0.002814

calculated by the compiler from the parameters for the Krichevsky-Il'inskaya equation

#### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

The solubility of carbon dioxide in triethylene glycol was measured at five temperatures over a partial pressure range of 105 kPa to 20250 kPa using apparatus and procedure described earlier (1). Where necessary nitrogen was added to maintain a total pressure above 200 kPa. The gas phase was analysed by gas chromatography. The liquid phase was analysed by absorption of dissolved gas in sodium hydroxide solution or barium hydroxide solution, addition of excess barium chloride solution and estimation of the barium carbonate which was precipitated. Relationships described by Bender et al. (2) were used to obtain parameters of the Krichevsky- Il'inskaya equation which are given above.

# SOURCE AND PURITY OF MATERIALS:

 from Aldrich Chemicals; water content reduced to less than
 6 mole percent by heating under vacuum to 120°C.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ 

 $\delta P/P = \pm 0.18$ 

- Jou, F-Y.; Mather, A.E.;
   Otto, F.D. Ind. Eng. Chem.
   Process Des. Dev. 1982, 21, 539.
- Bender, E.; Klein, U.; Schmitt, W.P.; Prausnitz, J.M.
   Fluid Phase Equilibria 1984, 15, 241.

#### COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Makarov, K.I.; Malyutin, S.P.; Sushkova, T.V. Soversh. Tekhn. i Tekhnol. Promysl. i Zavod. Obrab. Gaza. i Kondensata [124-38-9] 2. Polyethylene glycol Polyethylene glycol ethers na Mestorozhd. so Slozhn. Sostavov Gaza 1980, 106-115 Ref. Zh. Khim. Abstr. No 8530, 1981 The compiler consulted British $\overline{Gas}$ Polyethylene glycol diacetate Translation T6325/BG/LRS/LRST708/84 but was unable to see the original article. PREPARED BY: VARIABLES: P/kPa to about 4050 T/K = 293.2-323.2P.G.T. Fogg EXPERIMENTAL VALUES: T/KMole fraction Solvent Mean Runsen solubility relative coeff. molecular CO<sub>2</sub>=101.3 kPa\* a masst $\alpha$ -Hydro- $\omega$ -hydroxypoly(oxy-1,2-ethanediyl), (polyethylene glycol) \*\*; 293.15 1.3\*\*\* 280 0.014 $H(OC_2H_4)_6OH$ ; [25322-68-3] $\alpha$ -Hydro- $\omega$ -hydroxypoly(oxy-1,2-ethanediyl), (polyethylene glycol); 293.15 1.5 0.023 $H(OC_2H_4)_{8.7}OH; [25322-68-3]$ 3,6,9,12-Tetraoxatetradecane, (triethylene glycol diethyl 206 293.15 2.7 0.026 ether); C<sub>10</sub>H<sub>22</sub>O<sub>4</sub>; [4499-99-4] $\alpha$ -Ethyl- $\omega$ -ethoxypoly(oxy-1,2-ethanediyl), 336 293.15 2.9 (polyethylene glycol diethyl 0.041 ether); C<sub>2</sub>H<sub>5</sub>(C<sub>2</sub>H<sub>4</sub>O)<sub>5-7</sub>OC<sub>2</sub>H<sub>5</sub>; [53609-62-4] $\alpha\text{-Ethyl-}\omega\text{-ethoxypoly(oxy-1,2-ethanediyl)}$ (polyethylene glycol diethyl 456 293.15 2.6 0.049 ether) \*\*; C2H5 (C2H4O)8-9OC2H5; [53609-62-4] 456 2.2\*\*\* 308.15 0.042 456 1.6\*\*\* 323.15 0.031 $\alpha$ -Propyl- $\omega$ -propoxypoly(oxy-1,2-ethanediyl), 478 293.15 2.8 0.055 (polyethylene glycol dipropyl ether); $C_3H_7(C_2H_4O)_{8-9}OC_3H_7$ ; [60314-50-3] $\alpha$ -Methyl- $\omega$ -propoxypoly(oxy-1,2-ethanediyl), 2.8 0.058 (polyethylene glycol methyl- 514 293.15 propy1 ether); CH3 (C2H4O)10OC3H7 $\alpha$ -Acetyl- $\omega$ -(acetyloxy)poly(oxy-1,2-ethanediyl), 476 293.15 1.8 0.031 (polyethylene glycol diacetate); CH<sub>3</sub>CO(C<sub>2</sub>H<sub>4</sub>O)<sub>8-9</sub>OOCCH<sub>3</sub>; [27252-83-1] † It is not stated whether this represents a number average or a weight average. \* calculated by the compiler. The authors published a graph showing the variation of volume of

carbon dioxide absorbed (corrected to 1.014 bar and 273.15 K) per unit volume of solvent with the variation of partial pressure of carbon dioxide.

<sup>\*\*\*</sup> estimated from graphical data

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Polyethylene glycol Polyethylene glycol ethers Polyethylene glycol diacetate

#### ORIGINAL MEASUREMENTS:

Makarov, K.I.; Malyutin, S.P.; Sushkova, T.V. Soversh. Tekhn. i Tekhnol. Promysl. i Zavod. Obrab. Gaza. i Kondensata na Mestorozhd. so Slozhn. Sostavov Gaza 1980, 106-115

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Measurements were made over a range of pressures to a maximum of about 4050 kPa. Apparatus for use to about 98 kPa consisted of an absorption vessel fitted with a magnetic stirrer and connected to a surge tank and mercury pressure gage. The absorption vessel was held in a thermostat bath. The vessel was filled with gas under test and the solvent added with a syringe via a diaphragm. The quantity of gas absorbed was calculated from the difference between the final pressure, when the system had reached equilibrium, and the initial pressure. A steel bomb fitted with sampling devices was used for measurements at higher pressures. The bomb containing gas and solvent was rotated in a water bath for 4-5 h before samples of solution were withdrawn. Solubilities were published as Bunsen coefficients. A graph showing the variation of gas solubility with pressure in four of the solvents was also published.

# SOURCE AND PURITY OF MATERIALS:

Solvents were from various industrial sources. Densities and refractive indices at 293.15 K were as follows:

Solvent	Density /g cm <sup>-3</sup>	Refractive index
polyethylene glycol (RMM 280)	1.12	1.4625
polyethylene glycol (RMM 400)	1.125	1.4625
triethylene glycol diethyl ether	0.9567	1.4266
polyethylene glycol diethyl ether (RMM 336)	1.019	
polyethylene glycol diethyl ether (RMM 456)	1.04	
polyethylene glycol dipropyl ether	1.03	1.4505
polyethylene glycol methylpropyl ether	1.05	1.4539
polyethylene glycol diacetate	1.20	1.4560
RMM - relative molecular mass		

# ESTIMATED ERROR:

 $\delta x_{\text{CO}_2} = \pm 5\%$  (compiler)

COMPONENTS:			ORIGINAL MEASUREMENT	C+	
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9] 2. 2-Methoxyethanol (ethylene glycol			Bodor, E.; Bor, Gy.; Maleczkine, M.; Masko, G.; Mohai, B.; Siposs, G.		
	ethyl ether); C		Vesspremi. Vegy 1957, 1, 99-108	gip. Egyet. Kozlemen. 3.	
VARIABLES:		-	PREPARED BY:		
	T/K = 198-318.2 p/kPa = 30.3-102	. 9		C. L. Young	
EXPERIMENTAL	VALUES:				
T/K	p/mmHg	p/kPa	Absorption <sup>†</sup> of gas /cm³g-¹	Mole fraction tof carbon dioxide in liquid, "CO <sub>2</sub>	
318.2	297 443 532 651	39.6 59.1 70.9 86.8 (101.3)	0.72 1.06 1.41 1.72 (2.0)	0.00244 0.00359 0.00476 0.00581 (0.0067)	
295.2	(760) 563 674 731 (760)	75.1 89.9 97.5 (101.3)	(2.0) 2.29 2.84 3.11 (3.2)	0.0077 0.00772 0.00955 0.0104 (0.0107)	
273.2	(760) 605 658 703 772 (760)	80.7 87.7 93.7 102.9 (101.3)	4.15 4.55 4.95 5.45 (5.5)	0.0139 0.0152 0.0165 0.0182 (0.0183)	
248.2	227 346 411 610 744	30.3 46.1 54.8 81.3 99.2	3.5 6.7 7.9 10.7 12.8	0.0117 0.0222 0.0261 0.0351 0.0416	
223.2	(760) 266	(101.3) 35.5	16.3	(0.042) 0.0524 ont.)	
		AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:			SOURCE AND PURITY OF	MATERIALS:	
measured gas were a known vessel o Correction	when known amou added, in incre amount of liquid f known dimensio ons were made fo	ments, to in a ns. r the			
	pressure of solv in ref. (1).	ent.	ESTIMATED ERROR: $\delta T/K = \pm 0.1;$ $\delta (absorption)$	= ±4% or less.	
			REFERENCES:  1. Bodor, E.; Mohai, B.; Veszpremi. 1957, 1, 55	Siposs, G. Vegyip. Egy. Kozl.	

# ORIGINAL MEASUREMENTS:

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Methoxyethanol (ethylene glycol
  monomethyl ether); C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>
  [109-86-4]

Bodor, E.; Bor, Gy.; Maleczkine, M.; Masko, G.; Mohai, B.; Siposs, G. Veszpremi. Vegyip. Egyet. Kozlemen. 1957, 1, 99-108.

EXPERIMENTAL VALUES:			Absorption <sup>†</sup>	Mole fraction * of
T/K	p/mmHg	p/kPa	of gas /cm³g <sup>-1</sup>	carbon dioxide in liquid, <sup>©</sup> CO <sub>2</sub>
223.2	350	46.7	17.4	0.0558
	441	58.8	21.8	0.0689
	544 637	72.5 84.9	28.6 31.6	0.0885 0.0969
	744	99.2	37.0	0.0969
	(760)	(101.3)	(38)	(0.114)
198 ± 2	244	32.5	47.6	0.1391
±30 ± 2	326	43.5	60.5	0.1704
	410	54.7	74.5	0.2019
	552	73.6	104.0	0.2610
	744	99.2	139.7	0.3217
	(760)	(101.3)	(145)	(0.330)

 $<sup>^{\</sup>dagger} the\ volume\ of\ gas\ absorbed\ by\ one\ gram\ of\ solvent\ was\ corrected\ to\ 273.15\ K\ and\ 101.3\ kPa.$ 

Values in parentheses are extrapolated to 1 atmosphere.

<sup>\*</sup> calculated by compiler.

COMPONENTS:	ORIGINAL MEASUREMENTS:				
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> </ol>	Zubchenko, Yu.P.; Shakhova, S.F.				
<pre>2. 2,5,8,11,14-Pentaoxapentadecane;   (tetraethylene glycol dimethyl   ether); C<sub>10</sub>H<sub>22</sub>O<sub>5</sub>; [143-24-8]</pre>	Tr. Ni. Proekt. In-Ta. Azot. Prom. St. I. Productov. Organ. Sinteza <u>1975</u> , (33), 13-15.				
VARIABLES:	PREPARED BY:				
P/kPa = 101.3 T/K = 298.15	P.G.T. Fogg				
EXPERIMENTAL VALUES:					
	,				
T/K P/kPa vol.ga	s/vol.solvent* $x_{\text{CO}_2}^{T}$				
298.15 101.3	3.40 0.0323				
$^{*}$ the compiler has assumed the volume 101.3 kPa.	of gas was corrected to 273.15 K and				
† calculated by the compiler. The der the same as that of tetramethylene g	sity of the solvent was taken to be lycol, 1.0171 g cm <sup>-3</sup> at 293.2 K.				
AUXILIARY	INFORMATION				
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:				
	SOURCE AND FORTH OF IMPERIALS,				
The method was described in a previous publication (1).	No information				
	NCTIMATED COROL.				
	ESTIMATED ERROR:				
	REFERENCES:				
	1. Braude, G.E.; Shakhova, S.F.				
	Khim. Prom. <u>1961</u> , (3), 177.				

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Polyglycol ethers

# ORIGINAL MEASUREMENTS:

Sciamanna, S.F.; Lynn, S.

Ind. Eng. Chem. Res. 1988, 27, 492-499

VARIABLES:

P/kPa = 3-100T/K = 288.2-373.2 PREPARED BY:

P.G.T. Fogg

EXPERIMENTAL VALUES: Solvent	т/к	H/kPa <sup>†</sup>	* soln /kJ mol <sup>-1</sup>
1,1'-Oxybis(2-methoxyethane), (diethylene glycol dimethyl ether diglyme); C <sub>6</sub> H <sub>1</sub> 4O <sub>3</sub> ; [111-96-6]	298.15	3667.0	-11.46 ± 1.7%
2,5,8,11-Tetraoxadodecane, (triethylene glycol dimethyl ether triglyme); C <sub>8</sub> H <sub>18</sub> O <sub>4</sub> ; [112-49-2]	r;	3400.0	-11.40 ± 0.2%
2,5,8,11,14-Pentaoxapentadecane, (tetraethylene glycol dimethyl etitetraglyme); C <sub>10</sub> H <sub>22</sub> O <sub>5</sub> ; [143-24-8]	her;	3002.0	-11.39 ± 4.0%
2-(2-Methoxyethoxy)ethanol (diethylene glycol monomethyl ethe methyl carbitol); C <sub>5</sub> H <sub>12</sub> O <sub>3</sub> ; [111-73		6476.0	-10.40 ± 2.5%
3,6,9-Trioxatridecan-1-ol, (triethylene glycol butyl ether); C <sub>10</sub> H <sub>22</sub> O <sub>4</sub> ; [143-22-6]	· -•	3708.0	-10.33 ± 0.6%

Limiting values of Henry's constants, H, were found by use of a modified form of the Krichevsky-Il'inskaya equation i.e.

 $\ln(f_2/x_2) = \ln H + (A/RT)(x_1^2-1)$ 

where  $f_2$  is the fugacity of carbon dioxide

 $x_2$  is the mole fraction of carbon dioxide in the solution

 $x_1$  is the mole fraction of the solvent

A is a constant

A plot of  $\ln(f_2/x_2)$  against  $x_1^2-1$  has an intercept equal to  $\ln H$ .

Values of the heat of solution,  $\Delta H$ , fitted the equation

 $H = H^{\circ} \exp[(\Delta H_{soln}/R)(1/T - 1/T^{\circ})]$ 

where  $T^{\circ}$  = 298.15 K and  $H^{\circ}$  is the value of Henry's constant at 298.15 K.

# AUXILIARY INFORMATION:

#### METHOD/APPARATUS/PROCEDURE:

Dried solvent was added to a flask of known weight. The solvent was then heated, degassed, and the flask reweighed. Subsequent steps were automated and data stored in a computer. The solvent vapor pressure was recorded after each increment of temperature of 5 K from 288.2 to 373.2 K. The flask was then cooled, a predetermined mass of gas added and total pressures recorded at intervals of 5 K. The process was repeated with further additions of gas.

#### SOURCE AND PURITY OF MATERIALS:

Analysis of solvents after being degassed indicated a water content of about 0.1 wt%.
2-(2-Methoxyethoxy)ethanol was referred to by the trade name \*Dowanol DM;
3,6,9-Trioxatridecan-1-ol, by the trade name \*Dowanol TBH

# ESTIMATED ERROR:

As indicated above

#### REFERENCES:

1. Prausnitz, J.M.; Lichtenthaler, R.N.; de Azevedo, E.G.
Molecular Theromodynamics of Fluid-Phase Equilibria, Prentice-Hall, Englewood Cliffs, N.J. 1986, Chap.8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Sepasolv MPE<sup>†</sup></li> </ol>	Wolfer, W.; Schwarz, E.; Vodrazka, W.; Volkamer, K. Oil Gas J. 1980, 78(3), 66-70
VARIABLES: T/K = 268-393	PREPARED BY: P.G.T. Fogg

#### EXPERIMENTAL VALUES:

The authors stated that BASF had developed <code>Sepasolv MPE</code>, a special mixture of oligoethylene glycol methyl isopropyl ethers with a mean relative molecular mass of 316. Solubilities of several gases were presented on a small scale graph with solubility,  $\alpha$ , in units of  $\rm m^3/m^3$  bar, plotted against temperature. No experimental points were shown. The solubility of  $\rm CO_2$  was plotted over the temperature range -5°C to 120°C. The compiler found that the line plotted for this gas fits the equation:

$$log_{10}(\alpha bar) = -2.207 + 823.5K/T$$

The compiler considers that  $\alpha/\text{pressure}$  is the volume of gas absorbed, reduced to 273.15 K and 1 bar (or alternatively 1 atm), absorbed by one volume of solvent at the temperature of measurement.

The pressure and temperature at which measurements were made was not stated although the graphical information was intended to show behaviour of the solvent from low pressures to pressures greater than 1 bar. Use of the data implies an assumption that the reduced volume of gas absorbed is proportional to partial pressure of gas. The higher the pressure the greater the errors introduced by this assumption.

†Sepasolv MPE is a registered trademark of BASF.

# AUXILIARY INFORMATION $\begin{tabular}{lllll} \hline METHOD/APPARATUS/PROCEDURE: & SOURCE AND PURITY OF MATERIALS: \\ No information. & No information. \\ \hline \hline ESTIMATED ERROR: & $\delta \alpha/\alpha = \pm 10 \$ \\ & (estimated by the compiler) \\ \hline \hline REFERENCES: & \\ \hline \end{tabular}$

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Lenoir, J-Y,; Renault, P.; Renon, H. 2. Phenol; C<sub>6</sub>H<sub>6</sub>O; [108-95-2] J. Chem. Eng. Data, 1971, 16, 340-3. VARIABLES: PREPARED BY: T/K = 323.2 C. L. Young

# EXPERIMENTAL VALUES:

T/K	Henry's constant  HCO2/atm	Mole fraction at 101.3 kPa $^{x}$ CO <sub>2</sub> (1 atm)*
323.2	214	0.00467

\* Calculated by compiler assuming a linear function of  $P_{\text{CO}_2}$  vs  $x_{\text{CO}_2}$ , i.e.,  $x_{\text{CO}_2}$  (1 atm) =  $1/H_{\text{CO}_2}$ .

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

#### SOURCE AND PURITY OF MATERIALS:

- (]) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

252			
COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Horvath, M. J.; Sebastian, H. M.;		
<pre>2. 3-Methylphenol (m-cresol);</pre>	Chao, KC.		
C <sub>7</sub> H <sub>8</sub> O; [108-39-4]	Ind. Eng. Chem. Fundam.		
C/MgO/ [100 35 1]	1981, 20, 394-396.		
VARIABLES:	PREPARED BY:		
T/K = 300.5 P/kPa = 101.3	C. L. Young		
17,824 - 70110			
EXPERIMENTAL VALUES:			
T/K Henry's consta /atm	Mole fraction of ant carbon dioxide in liquid, $^x{ m CO}_2$		
300.5 168	0.00592		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Gas chromatographic analysis of a	1. No details given.		
saturated solution at barometric			
pressure. Henry's constants deter-	2. Purity 99.45 mole per cent.		
$H = (p - p_o)\phi(m + 1)/m$			
where p is the total pressure, p.			
the vapor pressure of the solvent	ESTIMATED ERROR:		
and $\phi$ is the fugacity coefficient of	$\delta T/K = \pm 0.25;  \delta H/atm = \pm 3\%$		
the gas. The mole ratio, m, is	(estimated by compiler).		
defined by	1		
Moles of carbon dioxide	1		
m = in gas phase	REFERENCES:		
	REFERENCES:		
Moles of carbon dioxide in liquid phase	REFERENCES:		
in liquid phase	REFERENCES:		

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Methoxy-4-(2-propenyl) phenol or eugenol; C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>;
   [97-53-0]

# ORIGINAL MEASUREMENTS:

Just, G.

2. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

) <b>:</b>			
Mol Fraction	Bunsen	Ostwald	
10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm³cm-3	
11.29	1.67	1.762	
10.45	1.54	1.653	
9.60	1.41	1.539	
	Mol Fraction  10 <sup>3</sup> x <sub>1</sub> 11.29 10.45	Mol Fraction Bunsen  10 $^3x_1$ Coefficient $\alpha/\text{cm}^3 \text{ (STP) cm}^{-3} \text{ atm}^{-1}$ 11.29 1.67 10.45 1.54	

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 2-Methyl-4-(2-propenyl)-phenol. No information.

#### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

# 254 COMPONENTS: ORIGINAL MEASUREMENTS: Kassim, D.M.; Zainel, H.A.; 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Al-Asof, S.A.; Talib, E.K. 2. Dihydro-2(3H)-furenone Fluid Phase Equilibria $(\gamma-butyrolactone)$ ; $C_4H_6O_2$ ; [96-48-0] 1988, 41, 287-294. **VARIABLES:** PREPARED BY: T/K = 303.15-333.15C. L. Young P/kPa = 101.3EXPERIMENTAL VALUES: Mole fraction of carbon dioxide T/K in liquid, x<sub>CO2</sub> 0.0160 303.15 0.0145 313.15 323.15 0.0130 0.0115 333.15 AUXILIARY INFORMATION METHOD / APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Falling film flow apparatus similar 1. Purity 99.99 mole per cent. to that of Morrison and Billet (1). 2. Fluka AG puriss grade sample, Apparatus consisted of (i) degassing purity better than 99 mole section in which solvent could be per cent. degassed by freezing and thawing

under vacuum and (ii) absorption section. The latter consisted of a gas buret and absorption spiral. Mole fraction solubility corrected at 1 atm partial pressure by assuming Henry's law was valid.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta x/x = \pm 0.02$ (estimated by compiler).

# REFERENCES:

1. Morrison, T.J.; Billet, F.J. J. Chem. Soc. 1948, 2033.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Compounds Containing Halogens

#### **EVALUATOR:**

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July 1991

#### CRITICAL EVALUATION:

The Solubility of carbon dioxide in solvents containing halogens

The solubility in tetrachloromethane measured by Gjaldbaek (1) at 298.2 K and about 101.3 kPa is close to a value measured by Horiuti (2) and is consistent with a value measured by Luhring and Schumpe (3) at 293.2 K. Just (4) made measurements from 288.2 K to 298.2 K. The values of the solubility are low compared with values from later work. The mole fraction solubility at 101.3 kPa and 298.2 K from Just's data is 0.00902 compared with 0.01048 (Horiuti) and 0.01070 (Gjaldbaek). A value of 0.00877 obtained by an indirect method by Takahashi et al. (5) can be disregarded. A value of 0.0106, the mean of Gjaldbaek and Horiuti's values, is provisionally recommended for mole fraction solubility at 298.2 K.

Kunerth (6) measured the solubility in trichloromethane at about 101.3 kPa from 291.2 K to 309.2 K. A plot of mole fraction solubility against temperature from these data is concave towards the solubility axis. This is not in agreement with the behaviour of other systems under similar conditions and may indicate incorrect allowance for the vapor pressure of solvent at the higher temperatures of measurement. Just (4) reported a solubility value at 298.2 K which is close to Kunerth's value at this temperature. Gjaldbaek (1) reported a solubility at 298.2 K which is high in comparison but is compatible with measurements by Woukoloff (7) at 286 K and of Koudelka (8) at 293.2 K. Values of mole fraction solubility at 298.2 K and 101.3 kPa are 0.0128 (Gjaldbaek); 0.01120 (Just); 0.0113 (Kunerth). Values at 293.2 K are 0.01375 (Koudelka); 0.0121 (Just); 0.01230 (Kunerth). The evaluator considers that the higher and more recent measurements by Gjaldbaek and by Koudelka may be more reliable than the earlier measurements by Just and Kunerth. These data can only be accepted on a provisional basis until the system is re-investigated.

Eldridge and co-workers (9,10) measured solubility in dichloromethane over pressure ranges from 310.9 K to 327.6 K. Dantzler et al. (11) measured solubilities in dichlorodifluoromethane and in trichlorofluoromethane over pressure ranges at 273.2 K to 310.9 K. These three sets of data seem to be reliable but measurements by other groups are not available for comparison.

The data which are available for 298.2 K and a partial pressure of carbon dioxide of 101.3 kPa show that the mole fraction solubility of gas increases when the hydrogens in dichloromethane or trichloromethane are replaced by fluorine atoms but decreases when they are replaced by chlorine atoms (see Table 1).

Solubility in 1,2-dibromoethane was measured at about 101.3 kPa by Gjaldbaek and Andersen (12), Begley et al.(13), Just (4) and Kunerth (6). There is very good agreement between the sets of data. The greatest discrepancy between values of mole fraction solubility is less than 4% i.e 0.00642 at 309.2 K (Kunerth); 0.00618 at 308.8 K (Begley). The following equation based on data from the four papers is recommended.

$$\ln x_{CO_2} = 324.89 - 13552.2/(T/K) - 49.902ln(T/K)$$

temperature range = 288.2-319.5 K standard deviation in  $x_{CO_2}$  = 9.3 × 10<sup>-5</sup>

Just (4) measured solubility in 1,2-dichloroethane at about 101.3 kPa from 288.2 K to 298.2 K. Luhring and Schumpe (3) measured solubility at 293.2 K and confirmed Just's value at this temperature. Values of mole

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Compounds Containing Halogens

**EVALUATOR:** 

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July 1991

CRITICAL EVALUATION:

fraction solubility at 101.3 kPa fit the following equation.

$$\ln x_{CO_2} = -9.120 + 1384.9/(T/K)$$

temperature range = 288.2-298.2 K standard deviation in  $x_{\rm CO_2}$  = 3.6 × 10<sup>-5</sup>

Just (4) also measured solubilities in 1-bromopentane, 1-chloropentane, 1-chloro-2-methylpropane and 1,2-dibromopropane under the same conditions of temperature and pressure as in 1,2-dichloroethane. Hiraoka and Hildebrand (14) measured solubility in trichlorotrifluoroethane at 101.3 kPa from 276.1 K to 308.5 K. Dantzler et al.(11) measured solubility in 1,2-dichloro-1,1,2,2-tetrafluoroethane over pressure ranges from 273.2 K to 310.9 K. Begley et al.(13) measured solubility in a mixture of 1-bromo-2-chloropropane and 2-bromo-1-chloropropane. There is no reason to doubt the reliability of any of these measurements but no other data for these systems are available for comparison.

Kobatake and Hildebrand (15) measured the solubility in hexadecafluoroheptane at 101.3 kPa and from 292.2 K to 303.2 K. The measurements are consistent with an earlier measurement of the solubility at 298.25 by Gjaldbaek (1) and may therefore be accepted as reliable. Solubility data for a partial pressure of gas of 101.3 kPa from the two papers fit the following equation

$$\ln x_{CO_2} = -7.413 + 1056.2/(T/K)$$

temperature range = 292.2-303.2 K standard deviation in  $x_{\rm CO_2}$  = 8.5 × 10<sup>-5</sup>

Mole fraction solubilities at a partial pressure of 101.3 kPa for various halogenated alkanes are given in Table 1. and are shown in Fig 1. The available data show that the relative effects of halogen in enhancing the solubility of carbon dioxide are fluorine > chlorine > bromine.

Solubility in L-1822 has been measured by Sargent and Seffl (16) at 101.3 kPa; 298.2 K and 310.2 K and reported as Ostwald coefficients and also as weight fractions. This solvent is reported to be mostly a mixture of 10-carbon linear, branched and cyclic fluorocarbons. The relative molecular mass of a C-10 linear or branched perfluorinated alkane is 538. If this is taken to be the approximate average relative molecular mass of L-1822 then the solubility data correspond to a mole fraction solubility of about 0.0186. The mole fraction solubility in hexadecafluoroheptane at this temperature and pressure is 0.0209. The data reported by Sargent and Seffl are therefore consistent with the nature of the solvent under test.

The solubility in three fluorinated ethers has been studied. FC-80 is mostly a mixture of isomers of heptafluorotetrahydro(nonafluorobutyl) -furan ( $C_8F_{16}O$ ). Solubilility in this solvent at 101.3 kPa has been measured by Tham et al.(17) from 298.2 K to 323.2 K. These data are supported by the measurements of Navari et al.(18) from 1.3 kPa to 101.3 kPa at 310.2 K. Solubility values at 298.2 K and 310.2 K; 101.3 kPa from Sargent and Seffl (16) are very low in comparison with Tham's values.

Values of  $x_{CO_2}$  for FC-80 at 101.3 kPa.

298.2 K	310.2 K
0.0223	0.0186
	0.0186
0.0181	0.0150
	0.0223

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. Compounds Containing Halogens

# **EVALUATOR:**

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July 1991

# CRITICAL EVALUATION:

Solubility in 1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6- [1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethoxy]-hexane ( $C_9F_{2,0}O$ ) was measured by Tham et al.(17) at 298.2 K to 323.2 K; 101.3 kPa. Values are higher than those given by Nychka and Eiback (19). Tham's data are probably the more reliable but confirmation is needed.

# $x_{\rm CO_2}$ at 101.3 kPa in $\rm C_9F_{20}O$

***************************************	298.2 K	310.2 K
Tham et al.	0.0250	0.0232
Nychka and Eiback	0.0223	0.0198

Tham et al.(17) also measured solubility in 1,1,2,2,3,3,4,4-octafluoro-1,4- bis[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethoxy]-butane ( $C_{10}F_{22}O_{2}$ ) at 298.2 K to 323.2 K; 101.3 kPa. There is no reason to doubt the reliability of this work but no other data on the system are available for comparison.

López et al.(20) measured solubilities in chlorocyclohexane and bromocyclohexane at 263.2 K to 303.2 K; 101.3 kPa. The work is self-consistent but no other data on these systems are available for Comparison. Mole fraction solubilities increase in the order chlorocyclohexane > bromocyclohexane > cyclohexane under these conditions.

Just (4) measured the solubility in 1,3-dichloro-2-propanol from 288.2 K to 298.2 K at 99.5 kPa. The corresponding values of the mole fraction solubility at 101.3 kPa are greater than values for 2-propanol (see Table 1). No other work on the system is available for comparison.

López et al.(23) measured solubility in chlorobenzene from 263.2 K to 303.2 K at 101.3 kPa. The measurements are consistent with those of Gjaldbaek and Anderson (12) at 298.2 and about 5% higher than those of Just (4) in the temperature range of 288.2 K to 298.2 K. The following equation for the mole fraction solubility at a partial pressure of 101.3 kPa, based upon the first two sets of data, is recommended.

$$\ln x_{CO_2} = 4.2360 + 756.71/(T/K) - 2.0001 \ln(T/K)$$

temperature range = 263.2-303.2 Kstandard deviation in  $x_{\text{CO}_2} = 3 \times 10^{-5}$ 

López et al.(23) also measured solubility in bromobenzene under the same conditions of temperature and pressure. These measurements are consistent with those of Just (4) in the range 288.2 K to 298.2 K. The following equation for mole fraction solubility at a partial pressure of 101.3 kPa, based upon the two sets of data, is recommended.

$$\ln x_{CO_2} = -5.2127 + 1189.1/(T/K) - 0.63508 \ln(T/K)$$

temperature range = 263.2-303.2 Kstandard deviation in  $x_{\text{CO}_2} = 4 \times 10^{-5}$ 

Just also measured solubility in iodobenzene from 288.2 K to 298.2 K at 101.3 kPa. No other measurements on this system are available for Comparison. Mole fraction solubilities at 298.2 K and a partial pressure of 101.3 kPa are in the order chlorobenzene > bromobenzene > iodobenzene. Solubility in chlorobenzene is close to that in benzene.

Evans and Battino (21) published the solubility in hexafluorobenzene at 297.7 K and 298.0 K; 101.3 kPa. Mole fraction solubility in this solvent is higher than in chlorobenzene. There is no reason to doubt the reliability of this work which can be accepted on a provisional basis.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Compounds Containing Halogens

#### **EVALUATOR:**

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July 1991

#### CRITICAL EVALUATION:

Just (4) measured solubilities in (chloromethyl)-benzene and in (trichloromethyl)-benzene. No other data on these systems are available. The data indicate that substitution of chlorine into the methyl group of methylbenzene lowers the mole fraction solubility at 298.2 K; 101.3 kPa (see Table 1).

- 1. Gjaldbaek, J.C. Acta Chem. Scand. 1953, 7, 537-544.
- Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125-256.
- 3. Luhring, P.; Schumpe, A. J. Chem. Eng. Data 1989, 34, 250-252.
- 4. Just, W. Z. Phys. Chem. 1901, 37, 342-367.
- Takahashi, M.; Kobayashi, Y.; Takeuchi, H. J. Chem. Eng. Data 1982, 27, 328-331
- 6. Kunerth, W. Phys. Rev. 1922, 19, 512-524.
- 7. Woukoloff, Comptes Rendu 1889, 109, 61-63.
- 8. Koudelka, L. Chem. Zvesti 1964, 18, 178-185
- 9. Buell, D.S.; Eldridge, J.W. J. Chem. Eng. Data 1962, 7, 187-189.
- 10. Vonderheiden, F.H.; Eldridge, J.W. J. Chem. Eng. Data 1963, 8, 20-21.
- 11. Dantzler, E.M.; Holler, F.C.; Smith, P.T. Soap Chem. Specialties 1965, 41(1), 125-6; 146; 151.
- 12. Gjaldbaek, J.C.; Andersen, E.K. Acta Chem. Scand. 1954, 8, 1398-1413.
- Begley, J.W.; Maget, J.R.; Williams, B. J. Chem. Eng. Data 1965, 10, 4-8.
- 14. Hiraoka, H.; Hildebrand, J.H. J. Phys. Chem. 1964, 68, 213-214.
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- 16. Sargent, J.W.; Seffl, R.J. Fed. Proc. 1970, 29, 1699-1703.
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- Navari, R.M.; Rosenblum, W.I.; Kontos, H.A.; Patterson, J.L. Res. Exp. Med. <u>1977</u>, 170, 169-180.
- Nychka, H.R.; Eiback, R.E. Ger. Offen. 2253534 (C1.C07c,C01b,A61m)
   May 1973.
- López, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutiérrez Losa, C.;
   J. Chem. Eng. Data 1987, 32, 472-474.
- 21. Evans, D.F.; Battino, R. J. Chem. Thermodyn. 1971, 3, 753-760.
- 22. Tokunaga, J. J. Chem. Eng. Data 1975, 20, 41-46.
- López, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutiérrez Losa, Y.C. Rev. Acad. Ciencias Zaragoza 1988, 43, 183-189.

COMP	ONENTS:	EVALUATOR:
1.	Carbon dioxide; CO₂; [124-38-9] Compounds Containing Halogens	Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.
		July 1991

CRITICAL EVALUATION:

Table 1.
Mole fraction solubilities of carbon dioxide at a partial pressure of 101.3 kPa in solvents containing halogens.

Solvent	T/K	<sup>x</sup> co₂	Reference
Trichloromethane	298.15	0.0128	1
Tetrachloromethane	298.15	0.0107	i
10024020200040	298.15	0.0105	4
Dichloromethane	298.15	0.0125	9,10 ¶
Dichlorodifluorometh		****	- /
	297.04	0.019	11
Trichlorofluorometha			
	297.04	0.016	11
1,2-Dichloro-1,1,2,2			
.,	297.04	0.021	11
1,2-Dibromoethane	298.15	0.007553 ±0.000093	*
1,2-Dichloroethane	298.15	0.01139 ±0.00004	*
1-Chloro-2-methylpro			
	298.15	0.0133	4
1-Chloropentane	298.15	0.0142	4
1-Bromopentane	298.15	0.0123	4
1,2-Dibromopropane	298.15	0.00976	4
Hexadecafluoroheptan		0.02085 ±0.00009	*
1,1,2-Trichloro-1,2,			
.,.,_	298.07	0.01823	14 ¶
Heptafluorotetrahydr		probutyl)-furan or FO	280
<u></u>	298.15	0.0223	17
	310.15	0.0186	17
	310.15	0.0186	18
1,1,2,2,3,3,4,4-Octa	fluoro-1.	4-bis(tetrafluoro-1-	
(trifluoromethyl)-et	hoxy)-buta	ane or Caroxin-D	
•	298.15	0.0248	17
	310.15	0.0227	17
1.1.1.2.2.3.3.4.4.5.		decafluoro-6-(1,2,2,	2-tetrafluo
-1-(trifluoromethyl)	ethoxy)-he	exane or Caroxin-F	- 000-42-40
,	298.15	0.0250	17
,	310.15	0.0232	17
Chlorocyclohexane	298.15	0.0108	20
Bromocyclohexane	298.15	0.0092	20
Chlorobenzene	298.15	0.00984 ±0.00003	*
Bromobenzene	298.15	0.00788 ±0.00004	*
Iodobenzene	298.15	0.00592	4
Hexafluorobenzene	297.98	0.0232	21
(Chloromethyl)-benze			~ .
, , , ,	298.15	0.00907	4
(Trichloromethyl)-be			*
,,,,,,,,,,	298.15	0.00950	4
1,3-Dichloro-2-propa		0.0000	•
.,	298.15	0.00705	4 †
			• '

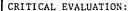
<sup>\*</sup> from the equation given by the evaluator on a previous page  $\dagger$  may be 2,3-dichloro-1-propanol; see page 294  $\P$  interpolated

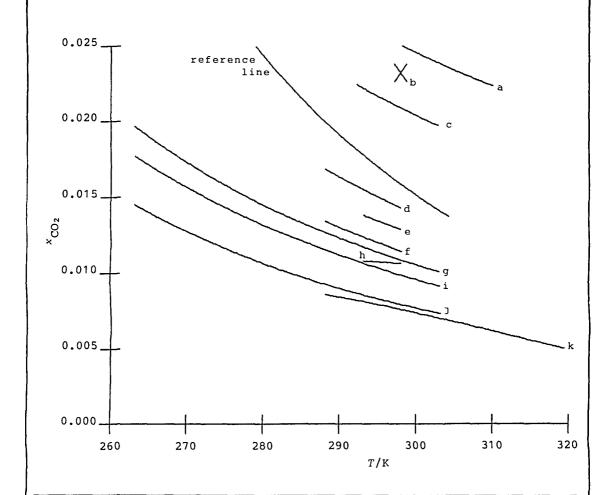
- Carbon dioxide; CO2; [124-38-9]
- Compounds Containing Halogens 2.

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991





Mole fraction solubility of carbon dioxide in various solvents containing halogens at a partial pressure of gas of 101.3 kPa. Fig. 1

```
a - perfluoro-1-isopropoxyhexane, C<sub>9</sub>F<sub>20</sub>O (17)
```

k - 1,2-dibromoethane (4,6,12,13)

A reference line corresponding to values from the Raoult's law equation is also shown.

b - hexafluorobenzene (21)

c - hexadecafluoroheptane (1,15)

d - 1-chloropentane (4)

e - trichloromethane (1,8)

f - 1,2-dichloroethane (3,4)

g - chlorocyclohexane (20)

h - tetrachloromethane (1,2,3) i - chlorobenzene (12,23)

j - bromobenzene (4,23)

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Tetrachloromethane or carbon tetrachloride; CCl<sub>4</sub>; [56-23-5]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient α/cm³ (STP)cm-³atm-1	Coefficient L/cm3cm-3
288.15	10.45	2.47	2.603
293.15	9.94	2.33	2.502
298.15	9.02	2.10	2.294

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Tetrachloromethane. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Tetrachloromethane or carbon tetrachloride; CCl<sub>4</sub>; [56-23-5]

# ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125 - 256.

VARIABLES:

T/K: 298.15

p<sub>1</sub>/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick

H. L. Clever

EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	1.048	2.444	2.668

The mole fraction and Bunsen coefficient values were calculated by the compiler with the assumption the gas is ideal and that Henry's law is obeyed.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret, a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption pipet.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared by the reaction of Na<sub>2</sub>CO<sub>3</sub> and H<sub>2</sub>SO<sub>4</sub>. Contamination by air was less than 0.004 per cent.
- (2) Tetrachloromethane. Kahlbaum. Dried over P<sub>2</sub>O<sub>5</sub> and distilled. Boiling point (760 mmHg) 76.74°C.

ESTIMATED ERROR:

$$\delta T/K = 0.05$$

$$\delta x_1/x_1 = 0.01$$

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Tetrachloromethane; CCl<sub>4</sub>;
  [56-23-5]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.

Acta Chem. Scand. 1953, 7, 537 - 544.

### VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

# PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

T/K	Carbon Dioxide Pressure p <sub>1</sub> /mmHg	Mol Fraction <sup>1</sup> 10 <sup>2</sup> x <sub>1</sub>	Bunsen Coefficient a/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	613.5 652.1	1.07	2.47 2.46	2.70 2.68

<sup>&</sup>lt;sup>1</sup>Mole fraction solubility values adjusted to a gas partial pressure of 101.325 kPa (1 atm) by the compiler assuming Henry's law is obeyed.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as confining liquid. The solvent was degassed in the apparatus.

The absorbed volume of gas is calculated from the initial and final amounts, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury.

The mole fraction solubility values are at 1 atm assuming Henry's law is obeyed.

Details of the apparatus and procedure are given in ref. 1 and 2.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate (analytical reagent) and concentrated sulfuric acid. 99.9 per cent CO<sub>2</sub>.
- (2) Tetrachloromethane. Riedel-E.
   de Haen. Analytical reagent.
   B.p. (759 mmHg)/°C = 76.80.
   n<sub>D</sub>(25°C) = 1.4573.

#### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. 1930, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

# 264 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Luhring, P.; Schumpe, A. 2. Tetrachloromethane, (carbon tetrachloride); CCl<sub>4</sub>; [56-23-5] J. Chem. Eng. Data, 1989, 34, 250-252. or 1,2-Dichloroethane; C2H4Cl2; [107-06-2] VARIABLES: PREPARED BY: T/K = 293.2C.L. Young EXPERIMENTAL VALUES: Henry's Constant<sup>†</sup> /(Pa m³/mol<sup>-1</sup>) T/K Mole fraction of CO<sub>2</sub> at 101.3 kPa partial pressure\* Tetrachloromethane 293.2 909 0.01076 1,2-Dichloroethane 293.2 0.01231 650 †referred to as Henry's constant in source but appears to be usual Henry's constant multiplied by molar volume. \*calculated by compiler using density data taken from ref.(1).

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE

Little infomation given in source. Method consisted of equilibrating known amounts of degassed liquid and gas and measuring the change in pressure. Equilibration was reached in 3 to 6 minutes. Some details given in ref. (2).

# SOURCE AND PURITY OF MATERIALS:

Obtained from Merck at the highest available purity. No other details given.

ESTIMATED ERROR:  $\delta T/K = \pm 0.1$  (authors)  $\delta x/x = \pm 0.01$  to 0.15 (compiler)

- Riddick, J.A.; Bunger, W.B.;1970 Organic Solvents, Wiley-Interscience, New York.
- Schumpe, A.; Quiker, G.; Decker, W.D. Adv. Biochem. Eng., 1982, 24, 1.

- (1) Carbon dioxide; CO2; [124-38-9]
- (2) Trichloromethane or chloroform; CHCl<sub>3</sub>; [67-66-3]

# ORIGINAL MEASUREMENTS:

Woukoloff, (No initial given)

Comptes rendu 1889, 109, 61 - 63.

VARIABLES:

$$T/K = 286$$
  
 $p_1/kPa = 4.88 - 101.59$   
 $(36.57 - 762 \text{ mmHg})$ 

PREPARED BY:

H. L. Clever

EXPERIMENTAL	VALUES:
--------------	---------

KPERIMENTA	L VALUES:			
Tempe	rature T/K	Carbon Dioxide Pressure p <sub>1</sub> /mmHg	Carbon Dioxide Absorption A/cm3 cm-3)1	Bunsen Coefficient α/cm³(STP)cm-3atm-1
13	286	36.57	0.20376	4.043
		73.22	0.40927	4.055
		109.62	0.62016	4.105
		144.93	0.83034	4.156
		182.75	1.0449	4.148
		218.95	1.25608	4.162
		255.48	1.4675	4.168
		293.15	1.6847	4.169
		330.1	1.89917	4.174
		367.64	2.1156	4.174
		404.4	2.33103	4.182
		441.95	2.5486	4.177
		479.29	2.758	4.174
		515.39	2.96986	4.180
		552.13	3.17998	4.178
		589.2	3.39003	4.174
		625.29	3.6006	4.177
		660.9	3.81068	4.183
		694.98	4.01633	4.192
		730.31	4.22446	4.196
		762	4.43757	4.225

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solvent was degassed by vacuum.

The solvent and the gas were brought into contact and a reading of the amount of gas absorbed was made. The readings were repeated after 24 and 48 hours.

In the author's earlier paper, Comptes rendu 1889, 108, 674, he stated the absorbed gas volume was reduced to the standard temperature and pressure of 0 °C and 760 mmHg. In the present paper the absorbed gas volume is measured at 13 °C and 760 mmHg.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information.
- (2) Chloroform. Specified as 891gr,075.

ESTIMATED ERROR:

REFERENCES:

1 The absorbed gas volume is at a temperature of 286 K and the partial pressure of the carbon dioxide. The Bunsen coefficient values were calculated by the compiler.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Trichloromethane or chloroform; CHCl<sub>3</sub>; [67-66-3]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

# PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

TAL VALUES:			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
288.15	1.315	3.75	3.956
293.15	1.21	3.43	3.681
298.15	1.12	3.14	3.430

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Trichloromethane. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Trichloromethane or chloroform; CHCl<sub>2</sub>; [67-66-3]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

J. Chr. Gjaldbaek

EXPERIMENTAL VALUES:

····	VALUES.			
T/K		Mol Fraction	Bunsen	Ostwald
		10 <sup>2</sup> x <sub>1</sub>	Coefficient a/cm³ (STP) cm-³ atm-1	Coefficient L/cm³cm-3
	298.15	1.28 1.28	3.59 3.58	3.92 3.91
		1.40	3.30	3.91

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1,2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO<sub>2</sub>.
- (2) Trichloromethane. Merck.
  Analytical reagent. Fractionated
  by distillation. B.p.
  (760 mmHg)/°C = 61.15 61.16,
  refractive index n
  D(20°C) =
  1.4460 1.4461.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Trichloromethane, (chloroform);
   CHCl<sub>3</sub>; [67-66-3]

1,2-Dibromoethane, (ethylene dibromide); C<sub>2</sub>H<sub>4</sub>Br<sub>2</sub>; [106-93-4]

# ORIGINAL MEASUREMENTS:

Kunerth, W.

Phys. Rev. 1922, 19, 512-524.

#### VARIABLES:

T/K = 291-15-309.15 P/kPa = 101.3

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

ENI DETENDENTAL VARIOUS	•		
Solvent	T/K	Ostwald coefficient L	*CO2 at PCO2 = 101.3 kPa*
Trichloromethane	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15 309.15	3.83 3.71 3.60 3.50 3.39 3.26 3.11 2.94 2.81 2.68	0.01275 0.01230 0.01189 0.01152 0.01111 0.01065 0.01012 0.00954 0.00909 0.00864
1,2-Dibromoethane	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15 309.15	2.32 2.27 2.22 2.16 2.12 2.07 2.03 1.97 1.92 1.86	0.00834 0.00812 0.00791 0.00766 0.00748 0.00727 0.00710 0.00686 0.00666

<sup>\*</sup> calculated by the compiler

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The method is based upon that described by McDaniel (1). The apparatus consisted of a gas buret attached to a levelling tube containing mercury and to the absorption cell containing the solvent under test. The volume of gas absorbed by a measured volume of liquid was measured at a total pressure equal to barometric pressure. The mercury in the gas buret was covered with a layer of solvent so that the gas in the buret was saturated with solvent vapor. Buret and absorption cell were surrounded by heating wire and water jackets fitted with thermometers.

# SOURCE AND PURITY OF MATERIALS:

- produced by heating NaHCO<sub>3</sub>; dried with CaCl<sub>2</sub>; frozen in liquid air and volatile impurities pumped away; passed over P<sub>2</sub>O<sub>5</sub>.
- commercial sample; purity attested by boiling point and density.

# ESTIMATED ERROR:

 $\delta x_{\text{CO}_2} = \pm 5\%$  (compiler)

- 1. McDaniel, A.S.;
  - J. Phys. Chem. 1911, 15, 587.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Dichloromethane; CH<sub>2</sub>Cl<sub>2</sub>; [75-09-2]

#### VARIABLES:

T/K = 294.3P/kPa = 103-2068

# ORIGINAL MEASUREMENTS:

Buell, D.S.; Eldridge, J.W.

J. Chem. Eng. Data 1962, 7, 187-189.

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/°F T/K*		Henry's la	w constant, H,	Mole fraction	
		/lbf in <sup>-2</sup>	/kPa*	solubility, $x_{CO_2}$ at $P_{CO_2} = 101.3 \text{ kPa*}$	
70	294.3	1085 ±5	7481 ±34	0.0135	

\* calculated by the compiler.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Measurements of solubility were made at pressures from 103 to 2068  $\ensuremath{kPa}$ using a specially designed cell. Dichloromethane was transferred to the cell and carbon dioxide introduced from a storage cylinder. The cell was rocked in a thermostatted bath until constant pressure was attained. A sample of the liquid phase was then isolated under pressure, withdrawn and weighed. The sample was then allowed to expand and the carbon dioxide estimated by absorption in sodium hydroxide solution and subsequent titration with hydrochloric acid. The partial pressure of dichloromethane in the cell was taken to be proportional to the mole fraction in the liquid. The partial pressure of carbon dioxide was the total pressure minus the partial pressure of dichloromethane. It was found that the mole fraction of carbon dioxide in the liquid was proportional to partial pressure of carbon dioxide to a pressure of about 1000 kPa.

# SOURCE AND PURITY OF MATERIALS:

- 1. Obtained from a cylinder.
- Technical grade, degassed by distillation.

# ESTIMATED ERROR:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Dichloromethane; CH<sub>2</sub>Cl<sub>2</sub>; [75-09-2]

#### ORIGINAL MEASUREMENTS:

Vonderheiden F.H.; Eldridge, J.W.

J. Chem. Eng. Data 1963, 8, 20-21.

# VARIABLES:

P/kPa = 103-2068T/K = 310.9, 327.6

# PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/°F	т/к*	Henry's law co /lbf in <sup>-2</sup>	nstant, H, /kPa*	Mole fraction solubility, ${}^{x}_{CO_{2}}$ , at ${}^{p}_{CO_{2}}$ = 101.3 kPa*
100	310.9	1505	10377	0.00976
130	327.6	2015	13893	0.00729
	i	$H = P_{CO} / x_{CO}$		

 $H = P_{\text{CO}_2}/x_{\text{CO}_2}$ 

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Measurements of solubility were made at pressures from 103 to 2068 kPa using a specially designed cell described previously (1). Dichloromethane was transferred to the cell and carbon dioxide introduced from a storage cylinder. The cell was rocked in a thermostatted bath until constant pressure was attained. A sample of the liquid phase was then isolated under pressure, withdrawn and weighed. The sample was then allowed to expand and the carbon dioxide estimated by absorption in sodium hydroxide solution and subsequent titration with hydrochloric acid. The partial pressure of dichloromethane in the cell was taken to be proportional to the mole fraction in the liquid. The partial pressure of carbon dioxide was the total pressure minus the partial pressure of dichloromethane. It was found that the mole fraction of carbon dioxide in the liquid was proportional to partial pressure of carbon dioxide to a pressure of about 1076 kPa at 373.2 K and to about 1310 kPa at 403.2 K.

# SOURCE AND PURITY OF MATERIALS:

- 1. Obtained from a cylinder.
- Technical grade, degassed by distillation.

# ESTIMATED ERROR:

- 1. Buell, D.S.; Eldridge, J.W.
  - J. Chem. Eng. Data 1962, 7, 187.

<sup>\*</sup> calculated by the compiler.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Fluorocarbons

# ORIGINAL MEASUREMENTS:

Dantzler, E.M.; Holler, F.C.; Smith, P.T.

Soap Chem. Specialties 1965, 41(1), 125-6; 146; 151.

# VARIABLES:

 $P_{\text{CO}_2}/\text{kPa} = 87-711$  T/K = 273.2-310.9

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Solvent	T∕°F	T/K"	<sup>P</sup> total /psig	<sup>P</sup> total /kPa*	mol% CO <sub>2</sub>	*CO <sub>2</sub>	PCO <sub>2</sub> /kPa*
Dichlorod	ifluoro	methane;	CCl <sub>2</sub> F <sub>2</sub> ;	[75-71-8]			
	32 32 32 32	273.15 273.15 273.15 273.15	40 55 90	377 481 722	2.07 5.31 12.90	0.0207 0.0531 0.1290 0.0250†	87 200 464 101.3
	70 70 75	294.26 294.26 297.04	90	722	3.05 1.9	0.0305 0.0200† 0.019	154 101.3 101.3

<sup>\*</sup> estimated by the compiler.

$$\log(P_{\text{CO}_2}/x_{\text{CO}_2}) = \log H - \beta(1-x_s^2)$$

where  ${\it H}$  is Henry's constant,  ${\it \beta}$  is a constant and  ${\it x}$  is the mole fraction of solvent in solution.

# AUXILIARY INFORMATION:

# METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 3 ounce aerosol compatibility tube connected via copper and nylon pressure tubing to a vacuum line, gas cylinder liquid phase sampling valve, gas phase sampling, valve and pressure gauge. The aerosol compatibility tube served as the absorption cell' and its temperature could be controlled to ±0.1 K by a constant temperature bath. A sample of the fluorocarbon was transferred from the gas cylinder and frozen in the absorbtion cell by liquid nitrogen. It was purified by repeated melting, refreezing and evacuation. Carbon dioxide was then admitted to the liquid fluorocarbon through a metering valve until the desired pressure was attained. The cell was mechanically shaken until the equilibrium pressure was reached. Samples of the gas phase and of the liquid phase were withdrawn and analysed with a gas chromatograph which had been previously calibrated with synthetic mixture of carbon dioxide and fluorocarbon.

# SOURCE AND PURITY OF MATERIALS:

- 1. Minimum purity 99.15-99.8%
- 2. Fluorocarbons refered to as P11 (trichlorfluoromethane) P12 (dichlorodifluoromethane) P114 (1,2-dichlorotetrafluoroethane) Analysis by gas chromatography indicated a purity of at least 99%

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.1$$
  $\delta P_{\text{total}}/\text{psig} = \pm 0.5$   
 $\delta x_{\text{CO}_2} = \pm 3\%$  (40-90 psig)  
(authors)  
 $\delta x_{\text{CO}_2} = \pm 5\%$  (101.3 kPa)  
(compiler)

# REFERENCES:

Krichevsky, I.R.; Il'inskaya,
 A.A. Acta Physicochim. URSS 1945,
 20, 327.

<sup>†</sup> extrapolated values estimated by the compiler. In the extrapolation it was assumed that data approximated to the Krichevsky-Il'inskaya equation in the form:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Fluorocarbons

# ORIGINAL MEASUREMENTS:

Dantzler, E.M.; Holler, F.C.; Smith, P.T.

Soap Chem. Specialties 1965, 41(1), 125-6; 146; 151.

EXPE	RIME	NTAL	VA	LUES:

Solvent	T/°F	T/K*	Ptotal /psig	Ptotal /kPa*	mol%	*CO2*	PCO <sub>2</sub> */kPa*
Trichloro	fluorom	ethane;	CCl <sub>3</sub> F; [75	-69-4]			
	32 32 32 70 70 70 70 75 100 100	273.15 273.15 273.15 294.26 294.26 294.26 294.26 297.04 310.93 310.93	40 55 90 40 55 90 40 55 90	377 481 722 377 481 722 377 481 722	7.70 10.10 15.30 4.83 6.50 10.50 1.6 3.18 4.56 7.92	0.0770 0.1010 0.1530 0.0234† 0.0483 0.0650 0.1050 0.0170† 0.016 0.0318 0.0456 0.0792 0.0146†	340 445 688 101.3 289 394 639 101.3 202 327 574 101.3
1,2-Dichl	oro-1,1	,2,2-tet	rafluoroet	hane; C <sub>2</sub> (	Cl <sub>2</sub> F <sub>4</sub> ;	[76-14-2]	
	32 32 32 70 70 70 70 75 100 100	273.15 273.15 273.15 273.15 294.26 294.26 294.26 294.26 297.04 310.93 310.93 310.93	40 55 90 40 55 90 40 55 90	377 481 722 377 481 722 377 481 722	9.54 12.90 20.70 4.27 6.63 12.10 2.1 1.04 3.06 7.70	0.0954 0.1290 0.2070 0.0341† 0.0427 0.0663 0.1210 0.0222† 0.021 0.0104 0.0306 0.0770 0.0136†	302 408 711 101.3 195 303 555 101.3 101.3 84 193 448

<sup>\*</sup> estimated by the compiler.

$$log(P_{CO_2}/x_{CO_2}) = logH - \beta(1-x_s^2)$$

where H is Henry's constant,  $\beta$  is a constant and x  $_{\rm S}$  is the mole fraction of solvent in solution.

 $<sup>^\</sup>dagger$  extrapolated values estimated by the compiler. In the extrapolation it was assumed that data approximated to the Krichevsky-Il'inskaya equation in the form:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2-Dibromoethane;  $C_2^H_4^Br_2^F_1$ ; [106-93-4]

# ORIGINAL MEASUREMENTS:

Just. G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

INT AUTORD.			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	8.69	2.30	2.424
293.15	8.16	2.14	2.294
298.15	7.61	1.98	2.157

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using ma ble and hydrochloric acid.
- (2) 1,2-Dibromoethane. No information.

#### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- 2. Steiner, P.

  Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2-Dibromoethane; C<sub>2</sub>H<sub>4</sub>Br<sub>2</sub>; [106-93-4]

## ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

J. Chr. Gjaldbaek

## EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^3 x_{1}$	Bunsen Coefficient a/cm³ (STP) cm-³ atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	7.72	2.00	2.18
	7.72	2.00	2.18

The mole fraction and Ostwald coefficient values were calculated by the compiler.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO<sub>2</sub>.
- (2) 1,2-Dibromoethane. Merck and Co. Purified by fractional freezing. M.p./°C = 9.5 9.8, refractive index,  $n_D(20^{\circ}C) = 1.5390$ , density  $\rho(20.6^{\circ}C)/g \text{ dm}^{-3} = 2.179$ .

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. 1930, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. <u>1952</u>, 6, 623.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1,2-Dibromoethane; C<sub>2</sub>H<sub>4</sub>Br<sub>2</sub>;
  [106-93-4]

# ORIGINAL MEASUREMENTS:

Begley, J.W.; Maget, J.R.;
Williams, B.

J. Chem. Eng. Data 1965, 10, 4-8.

# VARIABLES:

P/kPa = 101.3T/K = 293.45-319.45

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

т/к	Ostwald coefficient $\it L$	Mole fraction solubility ${}^{x}_{CO_{2}}$ at ${}^{p}_{CO_{2}}$ = 101.3 kPa $^{*}$
293.45	2.224	0.00795
299.75	2.067	0.00728
305.05	1.905	0.00664
308.75	1.789	0.00618
311.25	1.728	0.00594
315.15	1.617	0.00551
319.45	1.495	0.00505
5,5,15		

<sup>\*</sup>calculated by the compiler using the expression for the density of the solvent given in The International Critical Tables.

# AUXILIARY INFORMATION

# METHOD APPARATUS / PROCEDURE:

The solvent was boiled to remove any gases in solution and was then introduced into the absorption vessel without coming into contact With the air. The volume of carbon dioxide absorbed by the liquid from gas buret was then measured. The composition of the solution after equilibrium was attained was measured by chemical analysis. enabled a check to be made of solubility as calculated from the volume of gas absorbed. The absorption vessel and the gas buret Were kept at constant temperature by Circulation of water from a thermostat bath.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide 99.99% pure, from a cylinder supplied by Mathiesen Chemical Company.
- 2. 1,2-Dibromoethane supplied by Dow Chemical Company

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  Solubility measurements reproducible to about  $\pm 0.5\%$  (authors).

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2-Dichloroethane or ethylene chloride; C<sub>2</sub>H<sub>A</sub>Cl<sub>2</sub>; [107-06-2]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

## PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	13.30	3.85	4.061
293.15	12.31	3.54	3.795
298.15	11.32	3.23	3.525

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1,2-Dichloroethane. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Bromopentane or amyl bromide; C<sub>5</sub>H<sub>11</sub>Br; [110-53-2]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

WE AWTOES!			
T/K	Mol Fraction	Bunsen	Ostwald
-	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3 \text{ (STP) cm}^{-3} \text{atm}^{-1}$	Coefficient L/cm³cm-3
288.15	14.43	2.66	2.803
293.15	13.42	2.46	2.638
298.15	12.34	2.25	2.455

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

## SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1-Bromopentane. No information.

## ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) l-Chloropentane; C<sub>5</sub>H<sub>11</sub>Cl; [543-59-9]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_{1}/kPa = 101.325$  (1 atm)

PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

IND ANDORD.			
T/K	Mol Fraction	Bunsen	Ostwald
****	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm $^{-1}$	Coefficient L/cm³cm-3
288.15	16.81	3.19	3.363
293.15	15.47	2.91	3.127
298.15	14.25	2.67	2.910

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1-Chloropentane. No information.

#### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Chloro-2-methylpropane; C<sub>A</sub>H<sub>Q</sub>C1; [513-36-0]

## ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

#### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

WF AWPOES:			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient _L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	15.97	3.47	3.659
293.15	14.65	3.16	3.388
298.15	13.30	2.84	3.105

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1-Chloro-2-methylpropane. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,2-Dibromopropane or propylene bromide; C<sub>3</sub>H<sub>6</sub>Br<sub>2</sub>; [78-75-1]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

#### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

## PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

IND ANDORD.			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
288.15	11.27	2.45	2.586
293.15	10.54	2.29	2.453
298.15	9.76	2.11	2.301

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1,2-Dibromopropane. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) <u>1894</u>, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,1,2-Trichloro-1,2,2-trifluoroethane; C<sub>2</sub>Cl<sub>3</sub>F<sub>3</sub>; [76-13-1]

# ORIGINAL MEASUREMENTS:

Hiraoka, H.; Hildebrand, J. H.

J. Phys. Chem. 1964, 68, 213-214.

# VARIABLES:

T/K = 276.05 - 308.50 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

		HU.			
_	Temperature		Mol Fraction	Bunsen	Ostwald
	t/°C	<i>T</i> /K	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm $^{-1}$	Coefficient L/cm³cm-3
	2.90	276.05	2.514	4.98	5.03
	13.03	286.18	2.317	4.51	4.72
	24.92	298.07	1.823	3.47	3.79
	35.35	308.50	1.560	2.92	3.30

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior.

Smoothed Data: For use between 276.05 and 308.50 K.

 $\ln x_1 = -8.3717 + 13.0336/(T/100 K)$ 

The standard error about the regression line is  $1.04 \times 10^{-3}$ .

<i>T</i> /K	Mol Fraction 10 <sup>2</sup> x <sub>1</sub>
278.15	2.508
288.15	2.131
298.15	1.831
308.15	1.589

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25°C, the pipet at any temperature from 5 to 30°C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, evacuating, then boiling with a heat lamp. degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that the solvent never comes in contact with stopcock grease. The liquid in the Pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the volume of mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by P-V measurements in the buret before and after

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Western Gas Inc. Gas passed through a cold trap.
- (2) 1,1,2-Trichloro-1,2,2-trifluoroethane. Union Carbide Co. Distilled, purity checked by ultraviolet absorbance.

## ESTIMATED ERROR:

$$\delta T/K = 0.02$$
  
 $\delta x_1/x_1 = 0.003$ 

#### REFERENCES:

 Kobatake, Y.; Hildebrand, J. H. J. Phys. Chem. <u>1961</u>, 65, 331.

introduction of the gas into the pipet. The stirrer is set in motion. Equilibrium is attained within 24 hours.

- 1. Carbon dioxide; CO2; [124-38-9]
- 2. 1-Bromo-2-chloropropane; C3H6BrCl;
- [3017-96-7]
- 3. 2-Bromo-1-chloropropane; C3H6BrCl; [3017-95-6]

# ORIGINAL MEASUREMENTS:

Begley, J.W.; Maget, J.R.; Williams, B.

J. Chem. Eng. Data 1965, 10, 4-8.

#### VARIABLES:

P/kPa = 101.3T/K = 293.35-315.25

#### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

The solvent was a mixture of 1-chloro-2-bromopropane and 2-chloro-1-bromopropane.

T/K	Ostwald coefficient $\it L$	Mole fraction $x_{CO_2}$ at $P_{CO_2} = 101.3$	_
293.35	2.930	0.01258	
297.15	2.660	0.01134	
298.05	2.525	0.01075	
306.55	2.325	0.00972	
310.35	2.065	0.00857	
310.95	2.025	0.00839	
315.25	1.816	0.00746	

 $<sup>^</sup>st$ calculated by the compiler using densities given by the authors.

## AUXILIARY INFORMATION

#### METHOD APPARATUS / PROCEDURE:

The solvent was boiled to remove any gases in solution and was then introduced into the absorption vessel without coming into contact with the air. The volume of carbon dioxide absorbed by the liquid from gas buret was then measured. The composition of the solution after equilibrium was attained was measured by chemical analysis. enabled a check to be made of solubility as calculated from the volume of gas absorbed. The absorption vessel and the gas buret were kept at constant temperature by circulation of water from a thermostat bath. Densities of solvent were also measured by the authors.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Carbon dioxide 99.99% pure, from a cylinder supplied by Mathiesen Chemical Company.
- 2. 1-Bromo-2-chloropropane and 2-Bromo-1-chloropropane Technical mixture of the two sold as propylene chlorobromide

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ Solubility measurements reproducible to about ±0.5% (authors).

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Hexadecafluoroheptane or perfluoroheptane; C<sub>7</sub>F<sub>16</sub>; [335-57-9]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.

Acta Chem. Scand. 1953, 7, 537 - 544.

# VARIABLES:

$$T/K = 298.25$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

T/K	Carbon Dioxide Pressure p <sub>1</sub> /mmHg	Mol Fraction <sup>1</sup> 10 <sup>2</sup> x <sub>1</sub>	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
298.25	669.3 686.4	2.09	2.09	2.28

The mole fraction solubility values adjusted to a gas partial pressure of 101.325 kPa (1 atm) by the compiler assuming Henry's law is obeyed.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as confining liquid. The solvent was degassed in the apparatus.

The absorbed volume of gas is calculated from the initial and final amounts, both saturated with solvent Vapor. The amount of solvent is determined by the weight of displaced mercury.

The mole fraction solubility values are at 1 atm assuming Henry's law is obeyed.

Details of the apparatus and procedure are given in ref. 1 and 2.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate (analytical reagent) and concentrated sulfuric acid. 99.9 per cent CO<sub>2</sub>.
- (2) Hexadecafluoroheptane. E. I. duPont Co. B.p. (753.7 mmHg)/°C = 82.3 - 82.4.

## ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- Gjaldbaek, J. C.
   Acta Chem. Scand. 1952, 6, 623.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Hexadecafluoroheptane or perfluoroheptane; C<sub>7</sub>F<sub>16</sub>; [335-57-9]

# ORIGINAL MEASUREMENTS:

Kobatake, Y.; Hildebrand, J. H.

J. Phys. Chem. 1961, 65, 331 - 335.

VARIABLES:

T/K: 292.15 - 303.15 P/kPa: 101.325 (1 atm) PREPARED BY:

M. E. Derrick

H. L. Clever

EX	PERIMENTA	L VALUES:			
_	Temper	rature	Mol Fraction	Bunsen	Ostwald
	t/°C	T/K	10 <sup>2</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm3 cm-3
	19.00	292.15	2.231	2.282	2.441
	22.01	295.16	2.1685	2.206	2.384
	25.00	298.15	2.088 <sup>1</sup>	2.113	2.307
	26.02	299.17	2.059	2.079	2.277
_	30.00	303.15	1.959	1.964	2.179

<sup>1</sup> Probably a smoothed solubility value of the authors.

The Bunsen and Ostwald coefficients were calculated by the compiler. Smoothed Data: For use between 292.15 and 303.15 K.

 $\ln x_7 = -7.4216 + 10.5851/(T/100K)$ 

The standard error about the regression line is  $8.81 \times 10^{-5}$ .

T/K	Mol Fraction 10 <sup>2</sup> x <sub>1</sub>
293.15	2.213
298.15	2.083
303.15	1.965

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. buret is thermostated at 25°C, the pipet at any temperature from 5 to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. pure solvent is degassed by freezing with liquid nitrogen, evacuating, then boiling with a heat lamp. degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that the solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the volume of mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by P-V measurements in the buret before and after.

SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. California Dry Ice Co. Standard grade. Dried by passing through a trap at dry ice-acetone temperature, and tubes containing CaCl<sub>2</sub> then P<sub>2</sub>O<sub>5</sub>. The dried gas was distilled at liquid N<sub>2</sub> temperature several times.
- (2) Hexadecafluoroheptane. Source not given. Purified by method of Glew and Reeves, J. Phys. Chem. 1956, 60, 615.

ESTIMATED ERROR:

$$\delta T/K = 0.02$$
  
 $\delta x_1/x_1 = 0.003$ 

REFERENCES:

introduction of the gas into the pipet. The stirrer is set in motion. Equilibrium is attained within 24 hours.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) L-1822, which is a mixture of mostly 10-carbon fluorocarbons, including cyclic, open chain, and branched molecules.

## ORIGINAL MEASUREMENTS:

Sargent, J. W.; Seffl, R. J.

Fed. Proc. 1970, 29, 1699-1703.

# VARIABLES:

T/K: 298.15, 310.15 Total P/kPa: 101.325 (1 atm)

#### PREPARED BY:

A. L. Cramer H. L. Clever

## EXPERIMENTAL VALUES:

-	rature T/K		dioxide Solubility g <sup>-1</sup> cm <sup>3</sup> CO <sub>2</sub> 100 cm <sup>-3</sup>
25	298.15	1.55	164.0
37	310.15	1.31	143.0

The authors solubility, cm<sup>3</sup> CO<sub>2</sub> 100 cm<sup>-3</sup>, appears to be the Ostwald coefficient times 100.

# AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The equilibrium apparatus is a 50 cm<sup>3</sup> three neck flask equipped with a water condenser, a thermometer, and a gas dispersing tube extending below the fluid surface level. Between 25 and 35 cm<sup>3</sup> of solvent are placed in the flask. Gas is bubbled through the solvent for 2 - 3 h. An 80 microliter sample is slowly taken into a gas tight syringe. The sample is injected into a gas chromatograph. The results of three sampling and analyses are averaged.

The chromatograph is an F and M Model 720 equipped with a thermal conductivity detector at 320 °C, and a 6' by ¼" stainless steel column packed with 50/80 mesh Parapak-P at room temperature. The apparatus is calibrated with pure gas samples.

Details of the procedure were furnished by R. D. Danielson of the 3 M Co.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not given. Commercial cylinder, or dry ice.
- (2) L-1822. Minnesota Mining and Manufacturing Co. All H in an organic compound are replaced by F by Simons electrochemical process (1)

#### ESTIMATED ERROR:

 $\delta T/K = 0.1$ 

 $\delta c/c = 0.01$  (reproducibility)

= 0.05 (absolute)

(c = concentration of CO<sub>2</sub>)

#### REFERENCES:

Simons, J. H., Editor
 Fluorine Chemistry
 Academic Press, New York, 1950.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) FC-80, which is mostly a mixture of isomers of perfluorobutyltetrahydrofuran. For example 2,2,3,3,4,4,5-heptafluorotetrahydro-5 (nonafluorobutyl) furan; C<sub>8</sub>F<sub>16</sub>O; [335-36-4]

# ORIGINAL MEASUREMENTS:

Sargent, J. W.; Seffl, R. J.

Fed. Proc. 1970, 29, 1699-1703.

## VARIABLES:

298.15, 310.15 101.325 (1 atm) T/K: Total P/kPa:

#### PREPARED BY:

A. L. Cramer H. L. Clever

#### EXPERIMENTAL VALUES:

Tempe	rature	Carbon 1	Dioxide Solubility
t/°C	T/K	g CO <sub>2</sub> 1000	$g^{-1}$ cm <sup>3</sup> CO <sub>2</sub> 100 cm <sup>-3</sup>
25	298.15	1.95	192.0
37	310.15	1.61	160.0

The authors solubility,  $\mathrm{cm}^3$   $\mathrm{CO}_2$  100  $\mathrm{cm}^{-3}$ , appears to be the Ostwald coefficient times 100.

## AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The equilibrium apparatus is a 50 cm three neck flask equipped with a water condenser, a thermometer, and a gas dispersing tube extending below the fluid surface level. Between 25 and 35 cm<sup>3</sup> of solvent are placed in the flask. Gas is bubbled through the solvent for 2 - 3 h. An 80 microliter sample is slowly taken into a gas tight syringe. The sample is injected into a gas chromatograph. The results of three sampling and analyses are averaged.

The chromatograph is an F and M Model 720 equipped with a thermal conductivity detector at 320 °C, and a 6' by 4" stainless steel column packed with 50/80 mesh Parapak-P at room temperature. The apparatus is calibrated with pure gas samples.

Details of the procedure were furnished by R. D. Danielson of the 3 M Co.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source not given. Commercial cylinder, or dry ice.
- (2) FC-80. Minnesota Mining and Manufacturing Co. All H in an organic compound are replaced by F by Simons electrochemical process (1)

# ESTIMATED ERROR:

 $\delta T/K = 0.1$ 

δc/c = 0.01 (reproducibility) = 0.05 (absolute)

(c = concentration of CO2)

#### REFERENCES:

1. Simons, J. H., Editor Fluorine Chemistry Academic Press, New York, 1950.

- 1. Carbon Dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Heptafluorotetrahydro (nonafluorobutyl)-furan or Perfluorobutyl perfluorotetrahydrofuran or FC-80, C<sub>8</sub>F<sub>16</sub>O; [40464-54-8]

# ORIGINAL MEASUREMENTS:

Tham, M. K.; Walker, R. D. Jr.; Modell, J. H.

J. Chem. Eng. Data 1973, 18, 385-386.

VARIABLES: T/K: 298.15 - 323.15 Total P/kPa: 101.325 (1 atm)

#### PREPARED BY:

T. D. Kittredge H. L. Clever

# EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction  *1 × 10 <sup>3</sup>	Bunsen Coefficient a	Ostwald Coefficient $\stackrel{L}{L}$
298.15	22.3	2.17	2.37
303.15	21.0	2.02	2.24
310.15	18.6	1.77	2.01
313.15	17.72	1.68	1.93
323.15	15.50	1.44	1.70

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior. If the real carbon dioxide molar volume is used the values are decreased by about 0.5 per cent.

Smoothed Data:  $\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \ln x_{1} = -11938 + 71.604 T/K$ 

Std. dev.  $\Delta G^{O} = 19.9$ , Coef. corr. = 0.9996

 $\Delta H^{\circ}/J \text{ mol}^{-1} = -11938, \Delta S^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1} = -71.604$ 

T/K	Mol Fraction	$\Delta G^{O}/J \text{ mol}^{-1}$
	× <sub>1</sub> × 10 <sup>3</sup>	
298.15	22.4	9,410.9
303.15	20.7	9,768.9
308.15	19.2	10,127
313.15	17.8	10,485
318.15	16.6	10,843
323.15	15.5	11,201

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure described by Shoor, Walker and Gubbins (1) were used. The solvent was placed in a saturator immersed in a constant temperature bath. The gas was dispersed through the liquid by a fritted glass disk at a rate of about 40 cm<sup>3</sup> m-1. After an initial equilibration period of 30 minutes, samples were withdrawn with a Hamilton microliter syringe at 15 minute intervals and analyzed chromatographically (Perkin-Elmer 900 gas chromatograph with thermal conductivity detector). The solubility at one atmosphere partial pressure of the gas was the mean value of three consecutive samples which agreed within the limits of experimental error.

# SOURCE AND PURITY OF MATERIALS:

- 1. Carbon Dioxide. Source not given. Minimum purity 99.6 per cent.
- 2. FC-80. Minnesota Minning and Manufacturing Co. A mixture of several isomers. The authors also measured the density and viscosity of the solvent at several temperatures. At 298.15 K the density is 1.7657 g cm<sup>-3</sup> and the viscosity is 1.3957 centipoise.

#### ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
$$\delta x_1/x_1 = 0.005 \text{ (Compiler)}$$

#### REFERENCES:

 Shoor, S. K.; Walker, R. D. Jr.; Gubbins, K. E. J. Phys. Chem. 1969, 73, 312.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) FC-80 or heptafluorotetrahydro
   (nonafluorobutyl)-furan; C<sub>8</sub>F<sub>16</sub>O;
  [40464-54-8]

# ORIGINAL MEASUREMENTS:

Navari, R. M.; Rosenblum, W. I.; Kontos, H. A.; Patterson, J. L.

Res. Exp. Med. 1977, 170, 169 - 180.

VARIABLES: T/K: 310.15

P/kPa: 1.333 - 101.325 (10 - 760 mmHg) PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Carbon Dioxide p/mmHg	Carbon Dioxide Solubility <sup>1</sup> cm <sup>3</sup> CO <sub>2</sub> /cm <sup>3</sup>	Diffusion Coefficient <sup>2</sup> 10 <sup>-5</sup> D/cm <sup>3</sup> s <sup>-1</sup>
310.15	10 25 50 75 100 150 760	0.023 ± 0.002 0.059 ± 0.003 0.117 ± 0.007 0.176 ± 0.010 0.235 ± 0.013 0.353 ± 0.015 1.793 ± 0.031	$\begin{array}{r} 4.34 \ + \ 0.15 \\ 4.46 \ + \ 0.17 \\ 4.35 \ + \ 0.15 \\ 4.43 \ + \ 0.18 \\ 4.39 \ + \ 0.16 \\ 4.49 \ + \ 0.19 \\ 4.61 \ + \ 0.17 \\ \end{array}$

<sup>1</sup> Mean of five determinations + standard deviation.

The author's solubility coefficient is probably a Bunsen coefficient.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The solubilities were measured by the gas chromatograph method of Shoor  $et\ al$ . (1). The gas, presaturated with solvent vapor, was passed through the degassed liquid in the saturation cell at a rate of

50 ml m<sup>-1</sup>. Twenty microliter samples of the gas-saturated liquid were withdrawn and analyzed chromatographically at 15 m intervals. When readings remained constant for one hour the solution was assumed to be saturated. The time for saturation was less than 2 hours. The apparatus was calibrated with pure dry oxygen.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information.
- (2) FC-80. Minnesota Mining and Manufacturing Co.

ESTIMATED ERROR:

#### REFERENCES:

 Shoor, S. K.; Walker, R. D. Jr.; Gubbins, K. E. J. Phys. Chem. <u>1969</u>, 73, 312.

<sup>&</sup>lt;sup>2</sup> Mean of three determinations  $\pm$  standard deviation.

- 1. Carbon Dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1,1,1,2,2,3,3,4,4,5,5,6,6-Trideca-fluoro-6-[1,2,2,2-tetrafluoro-1-(trifluoromethyl)ethoxy]-hexane or Perfluoro-1-isopropoxy hexane or Caroxin-F; C<sub>9</sub>F<sub>20</sub>O; [37340-18-4] or [41719-16-8]

# ORIGINAL MEASUREMENTS:

Tham, M. K.; Walker, R. D. Jr.; Modell, J. H.

J. Chem. Eng. Data 1973, 18, 385-386.

# VARIABLES:

T/K: 298.15 - 323.15 Total P/kPa: 101.325 (1 atm)

#### PREPARED BY:

T. D. Kittredge H. L. Clever

# EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $x_1 \times 10^3$	Bunsen Coefficient a	Ostwald Coefficient L
298.15 303.15 310.15 313.15	25.0 24.3 23.2 22.8	1.99 1.92 1.81 1.77	2.17 2.13 2.05 2.03
323.15	21.4	1.63	1.93

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior. If the real carbon dioxide molar volume is used the values are decreased by about 0.5 per cent.

Smoothed Data:  $\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \ln x_1 = -5018.1 + 47.477 T$ 

Std. dev.  $\Delta G^{\circ} = 5.7$ , Coef. corr. = 0.9999

 $\Delta H^{\circ}/J \text{ mol}^{-1} = -5018.1, \Delta S^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1} = -47.477$ 

<i>T</i> /K	Mol Fraction	$\Delta G^{\circ}/J \text{ mol}^{-1}$
	$x_1 \times 10^3$	
298.15	25.0	9,137.1
303.15	24.2	9,374.5
308.15	23.5	9,611.9
313.15	22.8	9,849.3
318.15	22.1	10,087
323.15	21.4	10,324

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure described by Shoor, Walker and Gubbins (1) were used. The solvent was placed in a saturator immersed in a constant temperature bath. The gas was dispersed through the liquid by a fritted glass disk at a rate of about 40 cm<sup>3</sup> m<sup>-1</sup>. After an initial equilibration period of 30 minutes, samples were withdrawn with a Hamilton microliter syringe at 15 minute intervals and analyzed chromatographically (Perkin-Elmer 900 gas chromatograph with thermal conductivity detector). The solubility at one atmosphere partial pressure of the gas was the mean value of three consecutive samples which agreed within the limits of experimental error.

- SOURCE AND PURITY OF MATERIALS:
  1. Carbon Dioxide. Source not
  given. Minimum purity 99.6
  per cent.
  - 2. Caroxin-F. Allied Chemical Corp. Purity > 99.9 per cent as supplied. The authors also measured the density and viscosity of the solvent at several temperatures. At 298.15 K the density is 1.7449 g cm<sup>-3</sup> and the viscosity is 1.5405 centipoise.

# ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
$$\delta x_1/x_1 = 0.005 \text{ (Compiler)}$$

#### REFERENCES:

 Shoor, S. K.; Walker, R. D. Jr.; Gubbins, K. E. J. Phys. Chem. <u>1969</u>, 73, 312.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1,1,1,2,2,3,3,4,4,5,5,6,6Tridecafluoro-6-[1,2,2,2tetrafluoro-1-(trifluoromethy1)ethoxy]-hexane, (perfluoro-1isopropoxyhexane); C<sub>9</sub>F<sub>20</sub>O;
  [41719-16-8]

#### ORIGINAL MEASUREMENTS:

Nychka, H.R.; Eiback, R.E.

Ger. Offen. 2253534 (C1.CO7c,CO1b,
A61m) 10 May 1973

#### VARIABLES:

 $P/kPa \simeq 101.3$ T/K = 298.2; 310.2

#### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Volume of gas/cm $^3$ , reduced to 101.3 kPa and 273.15 K absorbed by 100 cm $^3$ of solvent at $^2$ CO $_2$ = 101.3 kPa	Bunsen coefficient* a	*CO2 at PCO2 = 101.3 kPa*
298.15	173.4 <sup>†</sup>	1.734	0.02232
310.15	151.1	1.511	0.01984

 $<sup>^\</sup>dagger$  The author also states elsewhere in the patent specification that the volume of gas absorbed at 298.15 K is 137.4 cm³. The compiler considers that this is a typing error. Carbon dioxide is unlikely to show an increase in solubility with increase in temperature under these conditions.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The authors used a method described by Reilly and Rae (1). The solvent was saturated with carbon dioxide and the solution subsequently analysed.

# SOURCE AND PURITY OF MATERIALS:

- 1. No information
- 2. Prepared by reaction of antimony pentafluoride with Perfluoroisopropylhexyl ether. Vapor pressure 45.6 mmHg at 37°C

t/°C	Density/g cm <sup>-3</sup>
20	1.732
25	1.721
30	1.709
35	1.696
40	1.683
45	1.661

## ESTIMATED ERROR:

 $\delta x_{\text{CO}_2} = \pm 10\%$  (compiler)

#### REFERENCES:

1. Reilly, J.; Rae, W.N.

Physico-Chemical Methods, Vol.III, D. van Nostrand and Co., Princeton, New Jersey 1948, 145-148.

<sup>\*</sup> Calculated by the compiler using absorption and density data given in the patent specification.

- 1. Carbon Dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1,1,2,2,3,3,4,4-Octafluoro-1,4bis(1,2,2,2-tetrafluoro-1-(trifluoromethy1)ethoxy) butane or
  Perfluoro-1,4-diisopropoxy butane
  or Caroxin-D; C<sub>10</sub>F<sub>22</sub>O<sub>2</sub>; [2322890-2]

## ORIGINAL MEASUREMENTS:

Tham, M. K.; Walker, R. D. Jr.; Modell, J. H.

J. Chem. Eng. Data 1973, 18, 385-386.

#### VARIABLES:

T/K: 298.15 - 323.15 Total P/kPa: 101.325 (1 atm)

# PREPARED BY:

T. D. Kittredge H. L. Clever

# EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $x_1 \times 10^3$	Bunsen Coefficient a	Ostwald Coefficient L
298.15	24.8	1.75	1.91
303.15	23.8	1.66	1.84
310.15	22.7	1.57	1.78
313.15	22.4	1.54	1.77
323.15	20.6	1.39	1.64

The Bunsen and Ostwald coefficients were calculated by the compiler assuming ideal gas behavior. The real carbon dioxide molar volume results in values smaller by  $0.5~\mathrm{per}$  cent.

Smoothed Data:  $\Delta G^{\circ}/J \text{ mol}^{-1} = -RT \ln x_1 = -5828.2 + 50.273 T$ 

Std. dev.  $\Delta G^{O} = 15.0$ , Coef. corr. = 0.9997

 $\Delta H^{\circ}/J \text{ mol}^{-1} = -5828.2, \Delta S^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1} = -50.273$ 

т/к	Mol Fraction  x <sub>1</sub> × 10 <sup>3</sup>	$\Delta G^{O}/J \text{ mol}^{-1}$
298.15	24.8	9,160.7
303.15	23.9	9,412.0
308.15	23.0	9,663.4
313.15	22.2	9,914.8
318.15	21.4	10,166
323.15	20.7	10,417

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure described by Shoor, Walker and Gubbins (1) were used. The solvent was placed in a saturator immersed in a constant temperature bath. The gas was dispersed through the liquid by a fritted glass disk at a rate of about 40 cm<sup>3</sup> m<sup>-1</sup>. After an initial equilibration period of 30 minutes, samples were withdrawn with a Hamilton microliter syringe at 15 minute intervals and analyzed chromatographically (Perkin-Elmer 900 gas chromatograph with thermal conductivity detector). The solubility at one atmosphere partial pressure of the gas was the mean value of three consecutive samples which agreed within the limits of experimental error.

# SOURCE AND PURITY OF MATERIALS:

- Carbon Dioxide. Source not given. Minimum purity 99.6 per cent.
- 2. Caroxin-D. Allied Chemical Corp. Purity > 99.9 per cent as supplied. The authors also measured the density and viscosity of the solvent. At 298.15 K the density is 1.7465 g cm<sup>-3</sup> and the viscosity is 2.0579 centipoise.

# ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
$$\delta x_1/x_1 = 0.005 \text{ (Compiler)}$$

# REFERENCES:

 Shoor, S. K.; Walker, R. D.; Gubbins, K. E. J. Phys. Chem. 1969, 73, 312.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Chlorocyclohexane; C<sub>6</sub>H<sub>11</sub>Cl; [542-18-7] VARIABLES: T/K = 263.15 -303.15 ORIGINAL MEASUREMENTS: López, M. C.; Gallardo, M. A.; Urieta, J. S.; Gutiérrez Losa, C.; J. Chem. Eng. Data, 1987, 32, 472-474.

P/kPa = 101.3
EXPERIMENTAL VALUES:

T/K	10 Mole fraction of carbon dioxide
263.15	197
273.15	163
283.15	137
293.15	117
303.15	101

Mole fraction solubility given by

 $\ln x$ , = -15.3774 + (1608.8/(T/K)) + 0.95751n(T/K)

# AUXILIARY INFORMATION

#### METHOD APPARATUS / PROCEDURE:

Solubility apparatus was similar to that used by Ben-Naim and Baer (1) consisting essentially of a gas buret, mercury manometer and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed that the mole fraction of the solvent in the gas phase was that corresponding to the vapor pressure of pure solvent. It appears that the mole fraction at a partial pressure of 1 atmosphere was estimated from raw experimental data assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- Obtained from Sociedad Española del Oxigeno, S.A.; purity 99.99 mole per cent.
- 2. Merck sample purity 98.5 mole per cent main impurity (0.4 mole per cent) cyclohexane.

## ESTIMATED ERROR:

 $\partial T/K = \pm 0.1 \ \partial x/x = \pm 0.015$ 

## REFERENCES:

 Ben-Naim, A.; Baer, S. Trans. Raraday Soc., 1963, 59, 2735.

Carbon dioxide; CO<sub>2</sub>; [124-38-9]
 Bromocyclohexane; C<sub>6</sub>H<sub>11</sub>Br; [108-85-0]

.91

Lopez, M. C.; Gallardo, M. A.; Urieta, J. S.; Gutierrez Losa, C. J. Chem. Eng. Data, 1989, 34,198-200.

VARIABLES:

PREPARED BY:

T/K = 263.15-303.15; p/kPa = 101.3

C.L. Young

ORIGINAL MEASUREMENTS:

#### EXPERIMENTAL VALUES:

T/K	10 <sup>4</sup> .Mole fraction of carbon dioxide in liquid at partial pressure of 101.3 kPa
263.15	162
273.15	135.5
283.15	114.7
293.15	98.4
303.15	85.7

## AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Solubility apparatus was similar to that used by Ben-Naim and Baer (1) consisting, essentially of a gas buret, mercury manometer and solution vessel. The solvent was degassed in the solution vessel. Measurements were carried out on the saturated gas. It was assumed that the mole fraction of the solvent in the gas phase was that corresponding to the vapor pressure of pure solvent. It appears that the mole fraction at a partial pressure of 1 atmosphere was estimated from raw experimental data assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- Obtained from Sociedad Espanola del Oxigeno, S.A.; purity 99.998 mole per cent.
- Fluka sample purity 99+ mole per cent as determined by gas chromatography.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta x_1/x_1 = \pm 0.015$ 

# REFERENCES:

1. Ben-Naim, A.; Baer, S. Trans. Faraday Soc., 1963, 59, 2735.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,3-Dichloro-2-propanol or α-dichlorohydrin; C<sub>3</sub>H<sub>6</sub>Cl<sub>2</sub>O; [96-23-1]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

## VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

<i>T/</i> K	Mol Fraction $10^3 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
288.15	8.05	1.915	2.020
293.15	7.55	1.79	1.917
298.15	7.05	1.66	1.810

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas. There is a possibility the solvent may be 2,3-dichloro-1-propanol or  $\beta$ -dichlorohydrin; [616-23-9].

# AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 1,3-Dichloro-2-propanol. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) <u>1894</u>, 52, 275.

(1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]

(2) Chlorobenzene; C<sub>6</sub>H<sub>5</sub>Cl; [108-90-7]

Bromobenzene; C<sub>6</sub>H<sub>5</sub>Br; [108-86-1]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

Solvent	T/K	Mole fraction	Bunsen Coefficient a/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm <sup>-3</sup>
Chlorobenzer	ie			
	288.15	10.93	2.45	2.581
	293.15	10.13	2.25	2.420
	298.15	9.38	2.08	2.265
Bromobenzene	<b>.</b>			
	288.15	9.17	1.98	2.092
	293.15	8.50	1.83	1.964
	298.15	7.88	1.69	1.842

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Chlorobenzene. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Chlorobenzene; C<sub>6</sub>H<sub>5</sub>Cl; [108-90-7]

## ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

J. Chr. Gjaldbaek

## EXPERIMENTAL VALUES:

IAL ANTOES:			
T/K	Mol Fraction $10^3 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	9.81 9.86 9.91 9.71 <sup>1</sup> 9.81 <sup>1</sup>	2.16 2.17 2.18 2.14 2.16	2.36 2.37 2.38 2.34 2.36

Results obtained by titration, see the paper.

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO<sub>2</sub>.
- (2) Chlorobenzene. Fractionated by
   distillation. B.p.
   (760 mmHg)/°C = 131.95 131.98,
   refractive index n<sub>D</sub>(20°C) =
   1.3840 1.3841.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. 1930, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Chlorobenzene; C<sub>6</sub>H<sub>5</sub>Cl; [108-90-7]
   Bromobenzene; C<sub>6</sub>H<sub>5</sub>Br; [108-86-1]

#### ORIGINAL MEASUREMENTS:

Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa Y.C. Rev. Acad. Ciencias Zaragoza 1988, 43, 183-189.

#### VARIABLES:

T/K = 263.15-303.15 $P_{CO_2}/kPa = 101.3 kPa$ 

#### PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Solvent	т/к	P <sub>CO₂</sub> /kPa	Mole fraction of CO <sub>2</sub>
Chlorobenzen	e		
	263.15	101.3	0.0177
	273.15		0.0148
	283.15		0.01247
	293.15		0.01060
	303.15		0.00910
Bromobenzene			
	263.15	101.3	0.0145
	273.15		0.01203
	283.15		0.01012
	293.15		0.00856
	303.15		0.00733

The authors gave the following smoothing equations for the mole fraction solubility of carbon dioxide:

Chlorobenzene

 $\ln x_{CO_2} = -0.2467 + 950.7321/(T/K) - 1.3279 \ln(T/K)$ 

Bromobenzene

 $\ln x_{CO_2} = -3.1678 + 1093.8344/(T/K) - 0.9371 \ln(T/K)$ 

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus was similar to that used by Ben Naim and Baer (1) which consisted essentially of a gas buret, mercury manometer and absorption vessel. The apparatus used for these measurements was described in an earlier publication (2).

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide supplied by Sociedad Española del Oxigeno, S.A.; purity 99.998%
- 2. Chlorobenzene supplied by Merck.

Merck.
Bromobenzene - supplied by

Fluka.
Purity of each liquid at least
99.5% as indicated by refractive
indices and analysis by gasliquid chromatography.

# ESTIMATED ERROR:

$$\delta x_{\text{CO}_2}/x_{\text{CO}_2}$$
 < 0.01 (authors)

- Ben-Naim, A.; Baer, S. Trans. Faraday Soc. 1963, 59, 2735.
- Carnicer, J.; Gibanel, F.;
   Urieta, J.S.; Gutierrez Losa, C.
   Rev. Acad. Ciencias Zaragoza,
   1979, 34, 115.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Iodobenzene; C<sub>6</sub>H<sub>5</sub>I; [591-50-4]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

Mol Fraction	Bunsen	Ostwald
10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
6.71	1.365	1.440
6.31	1.28	1.371
5.92	1.19	1.301
	$\frac{10^3 x_1}{6.71}$ 6.71 6.31	$ \begin{array}{ccc} 10^{3}x_{1} & & \text{Coefficient} \\ \alpha/\text{cm}^{3} \text{ (STP) cm}^{-3} \text{ atm}^{-1} \\ 6.71 & & 1.365 \\ 6.31 & & 1.28 \end{array} $

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Iodobenzene. No information.

## ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52,
   275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Hexafluorobenzene; C<sub>6</sub>F<sub>6</sub>;

# ORIGINAL MEASUREMENTS:

Evans, F. D.; Battino, R.

J. Chem. Thermodyn. 1971, 3, 753-760.

[392-56-3]

VARIABLES:

297.66, 297.98 101.325 (1 atm) T/K:  $p_1/kPa$ :

PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

t/°C	T/K	Mol Fraction $10^2 x_1$	Bunsen Coefficient a/cm³ (STP) cm⁻³atm⁻¹	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
	297.66	2.326	4.57	4.98
	297.98	2.322	4.44	4.84

The Bunsen coefficients were calculated by the compiler.

The solubility values were adjusted to an oxygen partial pressure of 101.325 kPa (1 atm) by Henry's law.

#### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans, and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to  $500~{\rm cm}^3$  of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid N<sub>2</sub> trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

## SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Either Air Products and Chemicals Inc. or the Matheson Co., Inc. Purest grade available. Minimum purity 99.0 mole per cent (usually > 99.9 mole per cent).
- (2) Hexafluorobenzene. Imperiel Smelting Co., Avnomouth, U.K. GC purity 99.7%, density,  $\rho_{298.15} = 1.60596 \text{ g cm}^{-3}$ . Purification described Anal. Chem. 1968, 40, 224.

ESTIMATED ERROR:  $\delta T/K = 0.03$  $\delta p/\text{mmHg} = 0.5$  $\delta x_1/x_1 = 0.005$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F.D.; Danforth, W.F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) (Chloromethyl)-benzene or benzyl chloride; C<sub>7</sub>H<sub>7</sub>Cl; [100-44-7]

## ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

## PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

E9:		
K Mol Fraction	Bunsen	Ostwald
10³x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3 \text{ (STP) cm}^{-3} \text{atm}^{-1}$	Coefficient L/cm³cm-3
15 10.46	2.07	2.180
15 9.82	1.93	2.072
15 9.07	1.775	1.938
	K Mol Fraction	K Mol Fraction Bunsen Coefficient $\alpha/\text{cm}^3(\text{STP}) \text{ cm}^{-3} \text{ atm}^{-1}$ 15 10.46 2.07 15 9.82 1.93

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

## SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) (Chloromethyl)-benzene. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. 1890, 6, 141.
- Steiner, P.
   *Ann. Phys. (Leipzig)* 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) (Trichloromethyl)benzene or benzotrichloride; C<sub>7</sub>H<sub>5</sub>Cl<sub>3</sub>; [98-07-7]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	T			
	+	Mol Fraction	Bunsen	Ostwald
		10 <sup>3</sup> x <sub>1</sub>	Coefficient α/cm <sup>3</sup> (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	298	9.50	1.505	1.643
298.15	298		· · · · · · · · · · · · · · · · · · ·	

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Trichloromethylbenzene. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) <u>1894</u>, 52, 275.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Solvents Containing Nitrogen

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

## CRITICAL EVALUATION:

Solubility of carbon dioxide in solvents containing nitrogen

Solubility in benzenamine was measured at or near to 101.3 kPa by Just (1) from 288.2 K to 298.2 K, by Kunerth (2) from 293.2 K to 309.2 K, by Gjaldbaek and Andersen (3) at 298.2 K and by Luhring and Schumpe (4) at 293.2 K. There is good correlation between these measurements with a maximum discrepancy of about 3.5%. Values of the mole fraction solubility based on data at 293.2 K are 0.005426 (Luhring) and 0.00524 (Kunerth). Lenoir et al.(5) published a limiting value of Henry's constant from chromatographic measurements at 298.2 K. The mole fraction solubility at a partial pressure of 101.3 kPa estimated from this value is clearly too large (0.0079). The following smoothing equation is based upon data from Just, Kunerth, and from Gjalbaek and Andersen.

$$\ln x_{CO_2} = -193.85 + 9531.6/(T/K) + 27.478ln(T/K)$$

temperature range = 288.2-309.2 K standard deviation in  $x_{\rm CO_2}$  = 4.2 × 10<sup>-5</sup>

Just (1) measured solubility in 2-methylbenzenamine and in 3-methylbenzenamine at 101.3 kPa and 288.2 K to 298.2 K. The measurements indicate a greater mole fraction solubility in these solvents than in benzenamine under the same conditions. These measurements can be accepted on a provisional basis until they are confirmed by other workers.

Just (1), Kunerth (2) and also Gjaldbaek and Andersen (3) measured solubility in pyridine at about 101.3 kPa. There is good correlation between the different measurements. The following smoothing equation for a partial pressure of 101.3 kPa is based upon these measurements.

$$\ln x_{CO_2} = 23.871 + 54.519/(T/K) - 5.0006\ln(T/K)$$

temperature range = 291.2-309.2 Kstandard deviation in  $x_{CO_2} = 0.00013$ 

Henry's constants for solubility in quinoline have been measured by Horvath et al.(6) at 300 K and by Chai and Paulaitis (7) from 298.6 K to 330.2 K. The measurements by Chai and Paulaitis are self consistent and can be provisionally recommended. Values of mole fraction solubility at a partial pressure of 101.3 kPa from these measurements fit the equation below.

$$\ln x_{CO_2} = -76.227 + 4508.7/(T/K) + 9.9003ln(T/K)$$

temperature range = 298.6-330.2 K standard deviation in  $x_{CO_2}$  = 6.0 × 10<sup>-5</sup>

The value of the mole fraction solubility at 300 K from this equation is 0.00884 compared with 0.00939 from Horvath's data.

Solubility in perfluorotributylamine was measured by Kobatake and Hildebrand (8) at 101.3 kPa and 277.2 K to 304.3 K. Sargent and Seffl (9) measured solubility at 298.2 K and 310.2 K but the purity of the solvent in this case is uncertain. The values of the mole fraction solubility at a pressure of 101.3 kPa and 298.2 K are 0.0200 (Kobatake) and 0.0218 (Sargent). Data from Kobatake and Hildebrand are likely to be a better measure of the solubility in the pure solvent.

Jou et al.(10) measured solubility in N-formyl morpholine at partial pressures of gas of 0.452 kPa to 7090 kPa at 298.2 K to 403.15 K. The data are self-consistent. Kassim et al.(11) measured solubilities at pressures of about 101.3 kPa from 303.2 K to 333.2 K. Mole fraction

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. Solvents Containing Nitrogen

## **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

solubilities at a partial pressure of 101.3 kPa from the two sources do not agree. Values for 313.2 K are 0.0114 (Jou) and 0.0137 (Kassim). Data from Jou et al. extend over a wider temperature and pressure range than those published by Kassim et al. The evaluator considers Jou's data are more likely to be reliable but confirmation is desirable.

Solubilities in 3-methyl-1*H*-pyrazole and *N*-substituted pyrazoles at 24 kPa to 2533 kPa at 273.2 K to 313.2 K have been reported by Egorova *et al.*(12) in a deposited document. Substitution on a nitrogen increases mole fraction solubility under these conditions. No other measurements on these systems are available for comparison.

Solubility in p-azoxyphenetole was measured by Homfray (13) at 407.2 K to 442.2 K and 118 kPa. There was an apparent decrease in solubility from 418.7 K to 422.2 K followed by a small increase from 429.7 K to 439.7 K. At this temperature there was a marked increase as the solvent changed from a nematic liquid to an isotropic liquid. The solubility then decreased with rise in temperature. Values of the mole fraction solubility at 439.7 K, estimated from the data are 0.00401 (nematic phase) and 0.00549 (isotropic phase). No other work on this system is available for confirmation of these findings.

Solubility in 1-methyl-2-pyrrolidinone has been measured by at least fourteen groups (5,11,14-25) over various temperature ranges. Measurements by Demidova et al.(14) and by Murrieta-Guevara et al.(15) extended to 1026 kPa and 1439 kPa respectively. Values of mole fractions solubility for a partial pressure of 101.3 kPa are scattered. Usyukin et al.(16) reported measurements from 253.2 K to 293.2 K. These measurements do not seem to be compatible with data given in the later paper from the same group (14). The evaluator considers that the most reliable measurements are those published in references (11,15,17, 19-23,25) over the temperature range 263.2 K to 393.2 K. Mole fraction solubility at a partial pressure of 101.3 kPa from these sources fit the equation

$$\ln x_{CO_2} = -14.820 + 1888.2/(T/K) + 0.7623\ln(T/K)$$

temperature range = 263.15-393.15 K standard deviation in  $x_{CO_2} = 0.0011$ 

The solubility in N,N-dimethylformamide at 27 kPa to 120 kPa from 278 K to 313 K has been published by Haidegger et al.(26). Braude et al.(27) also made measurements over a pressure range at 298.15 K to 353.15 K and reported limiting values of Henry's constant. Rosenthal (28) measured the solubility at 293.2 K and a partial pressure of 101.3 kPa and Byeseda et al.(17) at 297.1 K and 101.6 kPa. A value of the Bunsen coefficient at 298.2 K has been published by du Pont (29). Bunsen coefficients for 213.2 K to 293.2 K have been published by Usyukin and Shleynikov (16). The following equations (I) and (II) are based upon the available data for a partial pressure of 101.3 kPa.

$$\ln x_{CO_2} = 47.613 - 159.64/(T/K) - 9.0213ln(T/K)$$
 (I)

temperature range = 213.15-353.15 K standard deviation in  $x_{CO_2} = 0.0026$ 

$$\ln x = -123.79 + 6771.8/(T/K) + 16.994\ln(T/K)$$
 (II)

temperature range = 273.15-353.15 K standard deviation in  $x_{CO_2} = 0.0014$ 

Shenderei (30) measured the solubility of carbon dioxide in solutions of ethyne in N, N-dimethylformamide at 218.15 K and pressures of carbon

- Carbon dioxide; CO₂;
   [124-38-9]
- 2. Solvents Containing Nitrogen

#### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

dioxide from 13.3 kPa to 101.3 kPa. Extrapolation of the data to zero concentration of ethyne gives a mole fraction solubility of carbon dioxide of 0.169 at a partial pressure of 101.3 kPa. The corresponding value from equation (I) above is  $0.1827 \pm 0.0026$ .

Solubility in nitrobenzene has been measured at pressures close to 101.3 kPa by Gjaldbaek and Andersen (3) at 298.2 K, by Luhring and Schumpe (4) at 293.2 K and by Just (1) from 288.2 K to 298.2 K. Lenoir et al.(5) published a limiting value from chromatographic measurements at 298.2 K. The value of the mole fraction solubility at 298.2 K and a partial pressure of 101.3 kPa from Gjalbaek's data is 0.01015 and from Just's data is 0.0103. The value from Lenoir's data is 0.0130 and is subject to uncertainty because of the possibility of surface adsorption during the chromatographic process. Values at 293.2 K are 0.0112 (Just) and 0.0114 (Luhring). A smoothing equation based upon work by Gjalbaek and Andersen, Just and by Luhring and Schumpe can be recommended for the limited temperature range covered.

$$\ln x_{CO_2} = -9.583 + 1492.6/(T/K)$$

temperature range = 288.2-298.2 Kstandard deviation in  $\times_{CO_2} = 0.00016$ 

Solubility in hydrogen cyanide (31) and various nitriles (3,32,33) have been measured. A selection of values of solubilities at a partial pressure of 101.3 kPa are shown in Table 1. No estimation of the reliability of these measurements can be given.

Wehner et al.(34) reported the solubility of carbon dioxide in N-methyl- $\varepsilon$ -caprolactam at 293.2 K. Mole fraction solubility at a partial pressure of 101.3 kPa calculated from the data is close to that for dissolution in propanenitrile at 298.2 K reported by Gjaldbaek and Andersen (3) but no estimation of the reliability of the measurement can be made.

The solubility in formamide at 298 K has been given by Takahashi  $et\ al.(35)$ . The indirect method which was used is of uncertain reliability.

Selected values of mole fraction solubilities at a partial pressure of 101.3 kPa in compounds containing nitrogen are shown in Table 1 and Fig 1.

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342-367.
- 2. Kunerth, W. Phys. Rev. 1922, 19, 512-524.
- 3. Gjaldbaek, J.C.; Andersen, E.K. Acta Chem. Scand. 1954, 8, 1398-1413.
- 4. Luhring, P.; Schumpe, A. J. Chem. Eng. Data 1989, 34, 250-252.
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- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Solvents Containing Nitrogen

## **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

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	COMPONENTS:		EVALUATOR:
	1.	Carbon dioxide; CO₂; [124-38-9] Solvents Containing Nitrogen	Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.
-			July 1991

#### CRITICAL EVALUATION:

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Table 1. Mole fraction solubilities of carbon dioxide at a partial pressure of 101.3 kPa in solvents containing nitrogen

Solvent	T/K	<sup>x</sup> co₂	Refer	cence
Benzenamine	298.15	0.00488	±0.00004	*
2-Methylbenzenamine	298.15	0.00605		1
3-Methylbenzenamine	298.15	0.00634		1
Pyridine	298.15	0.01182	±0.00013	*
Quinoline	298.15	0.00912		7 †
1,1,2,2,3,3,4,4,4-None	afluoro-N	N-bis(no	onafluorobutyl)-1-	<del>-</del>
butanamine		0.0200	_	8
N-Formyl morpholine	298.15	0.01475		10
3-Methyl-1H-pyrazole	298.15	0.0063		12
1,3-Dimethyl-1H-pyraze				
	298.15	0.0092		12
1-Ethyl-3-methyl-1H-py	yrazole			12
	298.15	0.0166		
Methyl(1-methylethyl)		ole		12
	298.15	0.0166		
Methyl(3-methylbutyl)		ole		12
	298.15	0.0136		
1-Methyl-2-pyrroliding				
	298.15	0.0159		*
N, N-Dimethylformamide		0.0142		*
Nitrobenzene	298.15		±0.00016	*
Propanenitrile	298.15	0.0169		3 3
Benzeneacetonitrile		0.0105		3
Hexanedinitrile	298.15	0.01368		32
3-(Dimethylamino)prop				
	303.15	0.0289		33
Hexahydro-1-methyl-2H-a				
	293.15	0.0166		34

<sup>†</sup> extrapolated

<sup>\*</sup> from the equation given by the evaluator on a previous page

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Solvents Containing Nitrogen

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991



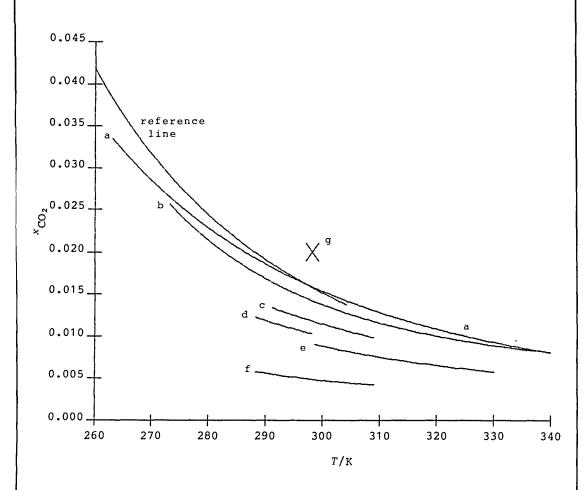


Fig. 1 Mole fraction solubility of carbon dioxide in various solvents containing nitrogen at a partial pressure of gas of 101.3 kPa.

- a 1-methyl-2-pyrrolidinone
- b N, N-dimethylformamide
- c pyridine
- d nitrobenzene
- e quinoline

is also shown.

- f benzenamine
- g perfluorotributylamine (8)

The curves showing the variation of solubility with temperature correspond to equations derived by the evaluator.

A reference line corresponding to values from the Raoult's law equation

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzenamine or aniline; C<sub>6</sub>H<sub>7</sub>N; [62-53-3]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

## VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

ITAL	AWTOE2:			
	T/K	Mol Fraction	Bunsen	Ostwald
_		10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm3cm-3
:	288.15	5.84	1.45	1.531
:	293.15	5.40	1.34	1.434
:	298.15	4.93	1.21	1.324

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Benzenamine. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) <u>1894</u>, 52, 275.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Pyridine, C<sub>5</sub>H<sub>5</sub>N; [110-86-1] Benzenamine (aniline); C<sub>6</sub>H<sub>7</sub>N; [62-53-3]

# VARIABLES:

T/K = 291.15-309.15  $P/kPa \approx 101.3$ 

# ORIGINAL MEASUREMENTS:

Kunerth, W.

Phys. Rev. 1922, 19, 512-524.

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

	*********		
Solvent	T/K	Ostwald coefficient L	$x_{CO_2}$ at $P_{CO_2} = 101.3 \text{ kPa}^*$
Pyridine	291.15 293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15 309.15	3.95 3.85 3.75 3.63 3.53 3.45 3.33 3.25 3.13	0.01320 0.01281 0.01242 0.01197 0.01159 0.01128 0.01084 0.01053 0.01010
Benzenamine	293.15 295.15 297.15 299.15 301.15 303.15 305.15 307.15 309.15	1.38 1.35 1.32 1.29 1.25 1.22 1.21 1.19	0.00524 0.00510 0.00496 0.00483 0.00465 0.00452 0.00446 0.00437

<sup>\*</sup> calculated by the compiler

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The method is based upon that described by McDaniel (1). The apparatus consisted of a gas buret attached to a levelling tube containing mercury and to the absorption cell containing the solvent under test. The volume of gas absorbed by a measured volume of liquid was measured at a total pressure equal to barometric pressure. The mercury in the gas buret was covered with a layer of solvent so that the gas in the buret was saturated with solvent vapor. Buret and absorption cell were surrounded by heating wire and water jackets fitted with thermometers.

# SOURCE AND PURITY OF MATERIALS:

- produced by heating NaHCO<sub>3</sub>; dried with CaCl<sub>2</sub>; frozen in liquid air and volatile impurities pumped away; passed over P<sub>2</sub>O<sub>5</sub>.
- commercial sample; purity attested by boiling point and density.

## ESTIMATED ERROR:

 $\delta x_{\rm CO_2} = \pm 5\%$  (compiler)

- 1. McDaniel, A.S.;
  - J. Phys. Chem. 1911, 15, 587.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzenamine or aniline; C<sub>6</sub>H<sub>7</sub>N; [62-53-3]

### ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

### VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

J. Chr. Gjaldbaek

### EXPERIMENTAL VALUES:

TAT AWTOES	•		
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient α/cm <sup>3</sup> (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm³cm-3
298.15	4.99	1.22	1.33
	4.83	1.18	1.29

The mole fraction and Ostwald coefficient values were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO<sub>2</sub>.
- (2) Benzenamine. Merck and Co.
  Puriss. Fractional distillation
  in vacuum. B.p. (760 mmHg)/°C =
  184.32 184.34, refractive index
  n<sub>D</sub>(20°C) = 1.5864.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. 1930, 52, 68.
- Gjaldbaek, J. C.
   Acta Chem. Scand. 1952, 6, 623.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Benzenamine, (aniline); C<sub>6</sub>H<sub>7</sub>N; [62-53-3]

### ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1971, 16, 340-2.

### VARIABLES:

T/K = 298.2

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Henry's con /atm	stant, H /kPa	$^{x}_{CO_{2}}$ at $^{p}_{CO_{2}}$ = 101.3 k	:Pa*
298.2	127	12868	0.00787	

\* calculated by the compiler assuming that  $x_{\text{CO}_2} = P_{\text{CO}_2}/H$ 

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

A conventional gas-liquid chromatographic unit was used with helium as carrier gas. Values of Henry's Constant were calculated from retention times extrapolated to zero sample size. Values correspond to very low partial pressure of carbon dioxide. Surface adsorption can cause appreciable errors in this method of measuring Henry's law constants.

### SOURCE AND PURITY OF MATERIALS:

- 1. Sample from L'Air Liquide; minimum purity 99.9 mol%
- 2. Sample from Touzart and Matignon or from Serlabo of purity 99 mol%

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  (estimated by compiler)

# 312 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; $CO_2$ ; [124-38-9] 2. Nitrobenzene; $C_6H_5NO_2$ ; [98-95-3] Luhring, P.; Schumpe, A. J. Chem. Eng. Data, 1989, 34, 250-252. or Benzenamine, (aniline); C6H7N; [62-53-3] VARIABLES: PREPARED BY: T/K = 293.2C.L. Young EXPERIMENTAL VALUES: Henry's Constant<sup>†</sup> / (Pa m³/mol<sup>-1</sup>) T/KMole fraction of CO2 at 101.3 kPa (1 atm) partial pressure\* Nitrobenzene; C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>; [98-95-3] 293.2 0.01146 Benzenamine, (aniline); C<sub>6</sub>H<sub>7</sub>N; [62-53-3] 293.2 1702 0.005426 †referred to as Henry's constant in source but appears to be usual Henry's constant multiplied by molar volume. \*calculated by compiler using density data taken from ref.(1). AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE SOURCE AND PURITY OF MATERIALS:

Little infomation given in source. Method consisted of equilibrating known amounts of degassed liquid and gas and measuring the change in pressure. Equilibration was reached in 3 to 6 minutes. Some details given in ref

Obtained from Merck at the highest available purity. No other details given.

ESTIMATED ERROR:  $\delta T/K = \pm \ 0.1$  (authors)  $\delta x/x = \pm \ 0.01$  to 0.15 (compiler)

- Riddick, J.A.; Bunger, W.B.;1970 Organic Solvents, Wiley-Interscience, New York.
   Schumpe, A.; Quiker, G.;
- Decker, W.D.

  Adv. Biochem. Eng., 1982, 24, 1.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 3-Methyl-benzenamine or m-toluidine; C<sub>7</sub>H<sub>9</sub>N; [108-44-1]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

$$T/K = 288.15 - 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

IND VALUES.			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm³cm-3
288.15	7.83	1.64	1.730
293.15	7.07	1.47	1.581
298.15	6.34	1.32	1.436

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas burct. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 3-Methyl-benzenamine. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Methyl-benzenamine or o-toluidine; C<sub>7</sub>H<sub>9</sub>N; [95-53-4]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

Mol Fraction	Bunsen	Ostwald
10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm $^{-1}$	Coefficient L/cm3cm-3
6.91	1.46	1.539
6.53	1.37	1.473
6.05	1.27	1.381
	10 <sup>3</sup> x <sub>1</sub> 6.91 6.53	$ \begin{array}{ccc}  & & & & \text{Coefficient} \\  & \alpha / \text{cm}^3 \text{ (STP) cm}^{-3} \text{ atm}^{-1} \\  & 6.91 & & 1.46 \\  & 6.53 & & 1.37 \end{array} $

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) 2-Methyl-benzenamine. No information.

### ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Pyridine; C<sub>5</sub>H<sub>5</sub>N; [110-86-1]

### ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

 T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>3</sup> x <sub>1</sub>	Coefficient $\alpha/\text{cm}^3$ (STP) $\text{cm}^{-3}$ atm <sup>-1</sup>	Coefficient L/cm3cm-3
288.15	14.32	4.07	4.291
293.15	12.75	3.60	3.862
298.15	11.94	3.35	3.656

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Pyridine. No information.

ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Pyridine; C<sub>5</sub>H<sub>5</sub>N; [110-86-1]

### ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

### VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

### PREPARED BY:

J. Chr. Gjaldbaek

### EXPERIMENTAL VALUES:

<i>T</i> /K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP) cm-³atm-1	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	1.22	3.38	3.69
	1.20	3.34	3.65

The mole fraction and Ostwald coefficient values were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. The solvent is added and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9 % CO<sub>2</sub>.
- (2) Pyridine. Fractionated by distillation. B.p. (760 mmHg)/  $^{\circ}\text{C} = 115.51 115.55$ , refractive index  $n_{D}(20 \ ^{\circ}\text{C}) = 1.5100 1.5101$ .

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. <u>1952</u>, 6, 623.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Horvath, M. J.; Sebastian, H. M.; Chao, K.-C. 2. Quinoline; C9H7N; [91-22-5] Ind. Eng. Chem. Fundam. 1981, 20, 394-396. VARIABLES: PREPARED BY: T/K = 300P/kPa = 101.3C. L. Young EXPERIMENTAL VALUES: Mole fraction of Henry's constant carbon dioxide in liquid, T/K /atm <sup>x</sup>co₂ † 106 0.00939 300 T at a partial pressure of carbon dioxide of 101.3 kPa calculated by compiler assuming $\phi = 0.995$ . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:

Gas chromatographic analysis of a saturated solution at barometric Henry's constants deterpressure. mined from formula

$$H = (p - p_o)\phi(m + 1)/m$$

where p is the total pressure, p. the vapor pressure of the solvent and  $\phi$  is the fugacity coefficient of the gas. The mole ratio, m, is defined by

Moles of carbon dioxide in gas phase m = Moles of carbon dioxide in liquid phase

- 1. No details given.
- 2. Purity 99.75 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.25$ ;  $\delta H/atm = \pm 3$ % (estimated by compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Quinoline; C<sub>9</sub>H<sub>7</sub>N; [91-22-5]</li> </ol>	Chai, C-P.; Paulaitis, M. E.;  J. Chem. Eng. Data, <u>1981</u> , 26,
	277-279.
VARIABLES:	PREPARED BY:
T/K = 298.6-330.2	C. L. Young

EXPERIMENTAL VALUES:

<u> </u>	· · · · · · · · · · · · · · · · · · ·				
T/K	Henry's constant /atm	Mole fraction a of carbon dioxide	T/K	Henry´s nstant /atm	Mole fraction a of carbon dioxide
298.6	110.51	0.0090490	316.2	146.97	0.0068041
298.6	111.66	0.0089558	316.2	144.79	0.0069066
302.7	118.36	0.0084488	320.2	153.72	0.0065053
302.7	117.17	0.0085346	320.2	151.20	0.0066138
302.7	118.09	0.0084681	320.2	152.81	0.0065440
307.1	127.15	0.0078647	323.6	160.83	0.0062177
307.1	128.68	0.0077712	323.6	162.81	0.0061421
311.0	134.52	0.0074338	323.6	160.03	0.0062488
311.0	133.06	0.0075154	330.2	172.07	0.0058116
311.0	134.57	0.0074310			
316.2	144.74	0.0069089			

<sup>&</sup>lt;sup>a</sup> Calculated by compiler for a partial pressure of

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus similar to that described in ref.(1). Known amount of carbon dioxide brought into contact with known amount of solvent. Reduction in pressure measured.

- SOURCE AND PURITY OF MATERIALS:
  - 1. Linde "bone dry" grade.
  - 2. Fisher certified grade.

ESTIMATED ERROR:

### REFERENCES:

 Dymond, J. H.; Hildebrand, J. H.; Ind. Eng. Chem. Fundam., 1967, 6, 130.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1,1,2,2,3,3,4,4,4-Nonafluoro-N,
  N-bis(nonafluorobutyl)-1butanamine or perfluorotributylamine;
  [311-89-7]

### ORIGINAL MEASUREMENTS:

Kobatake, Y.; Hildebrand, J. H.

J. Phys. Chem. 1961, 65, 331 - 335.

### VARIABLES:

T/K: 277.16 - 304.30 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

KIMENIAL V	ALUED:			
Tempe	rature	Mol Fraction	Bunsen	Ostwald
t/°C	T/K	10 <sup>2</sup> x <sub>1</sub>	Coefficient α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
4.01	277.16	2.606	1.76	1.79
9.52	282.67	2.363	1.57	1.62
17.98	291.13	2.179	1.42	1.51
24.87	298.02	2.000	1.28	1.40
25.00	298.15	2.000	1.28	1.40
31.15	304.30	1.850	1.17	1.30

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: For use between 277.16 and 304.30 K.

 $\ln x_1 = -7.3441 + 10.2213/(T/100K)$ 

The standard error about the regression line is  $2.54 \times 10^{-4}$ .

T/K	Mol Fraction
	10 <sup>2</sup> x <sub>1</sub>
278.15	2.549
283.15	2.389
288.15	2.244
293.15	2.112
298.15	1.992
303.15	1.883

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The a reservoir for the solvent. The buret is thermostated at 25°C, the pipet at any temperature from 5 to 30 °C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, evacuating, then boiling with a heat lamp. degassing process is repeated three The solvent is flowed into times. the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that the solvent never comes in contact with stopcock grease. The liquid in the pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the volume of mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by P-V measurements in the buret before and after introduction of the gas into the pipet.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. California Dry Ice Co. Standard grade. Dried by passing through a trap at dry ice-acetone temperature, and tubes containing CaCl<sub>2</sub> then P<sub>2</sub>O<sub>5</sub>. The dried gas was distilled at liquid N<sub>2</sub> temperature several times.
- (2) Perfluorotributylamine. Minnesota Mining and Manufacturing Co. Dried, fractionated, boiling point 178.5 - 179.0°C. Density, ρ/g cm<sup>-3</sup> = 1.872.

ESTIMATED ERROR:

$$\delta T/K = 0.02$$
  
 $\delta x_1/x_1 = 0.003$ 

REFERENCES:

introduction of the gas into the pipet. The stirrer is set in motion. Equilibrium is attained within 24 hours.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) FC-47, which is largely perfluorotributylamine or 1,1,2,2, 3,3,4,4,4-nonafluoro-N,N-bis (nonafluorobutyl)-1-butanamine; C<sub>12</sub>F<sub>27</sub>N; [311-89-7]

### ORIGINAL MEASUREMENTS:

Sargent, J. W.; Seffl, R. J.

Fed. Proc. 1970, 29, 1699 - 1703.

### VARIABLES:

T/K: 298.15, 310.15 Total P/kPa: 101.325 (1 atm)

### PREPARED BY:

A. L. Cramer H. L. Clever

### EXPERIMENTAL VALUES:

-	rature T/K		de Solubility cm <sup>3</sup> CO <sub>2</sub> 100 cm <sup>-3</sup>
25	298.15	1.46	152.0
37	310.15	1.34	142.0

The authors solubility, cm<sup>3</sup> CO<sub>2</sub> 100 cm<sup>-3</sup>, appears to be the Ostwald coefficient times 100.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The equilibrium apparatus is a 50 cm<sup>3</sup> three neck flask equipped with a water condenser, a thermometer, and a gas dispersing tube extending below the fluid surface level. Between 25 and 35 cm<sup>3</sup> of solvent are placed in the flask. Gas is bubbled through the solvent for 2 - 3 h. An 80 microliter sample is slowly taken into a gas tight syringe. The sample is injected into a gas chromatograph. The results of three sampling and analyses are averaged.

The chromatograph is an F and M Model 720 equipped with a thermal conductivity detector at 320 °C, and a 6' by 4" stainless steel column packed with 50/80 mesh Parapak-P at room temperature. The apparatus is calibrated with pure gas samples.

Details of the procedure were furnished by R. D. Danielson of the 3 M Co.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not given. Commercial cylinder, or dry ice.
- (2) FC-47. Minnesota Mining and Manufacturing Co. All H in an organic compound are replaced by F by Simons electrochemical process (1)

### ESTIMATED ERROR:

 $\delta T/K = 0.1$ 

 $\delta c/c = 0.01$  (reproducibility)

0.05 (absolute)

(c = concentration of carbon dioxide)

### REFERENCES:

Simons, J. H., Editor
 Fluorine Chemistry
 Academic Press, New York, 1950.

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 4-Morpholinecarboxaldehyde
   (4-formylmorpholine); C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>;
   [4394-85-8]

### ORIGINAL MEASUREMENTS:

Kassim, D.M.; Zainel, H.A.;
Al-Asof, S.A.; Talib, E.K.

Fluid Phase Equilibria

1988, 41, 287-294.

### VARIABLES:

T/K = 303.15-333.15P/kPa = 101.3

### PREPARED BY:

C. L. Young

### **EXPERIMENTAL VALUES:**

Mole fraction of carbon dioxide in liquid,  $x_{CO_2}$ , at  $P_{CO_2} = 101.3$  kPa

303.15	0.0157
313.15	0.0137
323.15	0.0120
333.15	0.0098

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Falling film flow apparatus similar to that of Morrison and Billet (1). Apparatus consisted of (i) degassing section in which solvent could be degassed by freezing and thawing under vacuum and (ii) absorption section. The latter consisted of a gas buret and absorption spiral. Mole fraction solubility corrected to 1 atm partial pressure by assuming Henry's law was valid.

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.99 mole per cent.
- Fluka AG puriss grade sample, purity better than 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta x/x = \pm 0.02$  (estimated by compiler).

### REFERENCES:

Morrison, T.J.; Billet, F.J.
 J. Chem. Soc. <u>1948</u>, 2033.

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 4-Morpholinecarboxaldehyde, (N-formy1 morpholine); C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>; [4394-85-8]

### ORIGINAL MEASUREMENTS:

Jou, F-Y.; Deshmukh, R.D.; Otto, F.D.; Mather, A.E. J. Chem. Soc. Faraday Trans. 1, 1989, 85, 2675-2682.

### VARIABLES:

P/kPa = 0.8-7000T/K = 398.15-403.15

### PREPARED BY:

P.G.T. Fogg

### **EXPERIMENTAL VALUES:**

T/K	Henry's Constant H <sub>21</sub> /kPa	$\overline{\it V}^{\infty}/{\rm cm}^3{\rm mol}^{-1}$	A/RT	<sup>x</sup> CO <sub>2</sub> at 101.3 kPa*
298.15	6890	35.55	0.099	0.01475
313.15	8920	36.60	0.105	0.01139
343.15	13800	38.93	0.121	0.00735
373.15	19600	41.60	0.142	0.00518
403.15	25900	44.69	0.168	0.00392

<sup>\*</sup> calculated by the compiler from the parameters for the Krichevsky-Il'inskaya equation given above.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility of carbon dioxide in N-formyl morpholine was measured at five temperatures over a partial pressure range from 0.8 kPa to about 7000 kPa using apparatus and procedure described earlier (1). Where necessary nitrogen was added to maintain a total pressure above 200 kPa. The gas phase was analysed by gas chromatography. The liquid phase was analysed by absorption of dissolved gas in sodium hydroxide solution and subsequent estimation of carbonate by precipitation as barium carbonate. The data were correlated by the Peng-Robinson equation of state as described earlier (2). Relationships described by Bender et al.(3) were used to obtain parameters of the Krichevky-Il'inskaya equation (4) which are given above.

### SOURCE AND PURITY OF MATERIALS:

No information

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ 

- Jou, F-Y.; Mather, A.E.;
   Otto, F.D.
   Ind. Eng. Process Des. Dev.
- 1982, 21, 539.

  2. Jou, F-Y.; Deshmukh, R.D.;
  Mather, A.E.; Otto, F.D.
  Fluid Phase Equilibria 1987, 36,
  121.
- Bender, E.; Klein, U.; Schmitt, W.P.; Prausnitz, J.M. Fluid Phase Equilibria 1984, 15, 241.
- Krichevsky, I.R.;
   Il'inskaya, A.A.
   Acta Physicochim. URSS 1945, 20, 327.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. 3-Methyl-1H-pyrazole; C<sub>4</sub>H<sub>6</sub>N<sub>2</sub>; [1453-58-3] VARIABLES: P/kPa = 60-2533; T/K = 273-313 ORIGINAL MEASUREMENTS: Egorova, V.I.; Grishko, N.I.; Neokladnova, L.N.; Furmanov, A.S. Podvigailova, I.G. Deposited Document 1976, VINITI 2907-76 PREPARED BY: P.G.T. Fogg

EXPERIMENTAL.	WAT HEC.

T/K	P/mmHg	P/kPa	Solubility* vol/vol	H/mmHg**	*CO <sub>2</sub>
273.15	760	101.33		83500	0.0091
283.15	760	101.33		87600	0.0087
298.15	450	60.00	1.02 _		0.0041
	760	101.33	1.56 ¶	120600	0.0063
313.15	760	101.33		158300	0.0048

<sup>\*</sup> Solubility of carbon dioxide was given as the volume of gas, reduced to 273.15 K and 101.325 kPa absorbed by unit volume of the solvent.

760 mmHg

It is not constant over the pressure range at which measurements were made.

- † calculated by the compiler
- ¶ extrapolated value

Measurements were also given for 100 and 200 mmHg at 298.15 K. These appear to have been subject to typing errors. Solubilities at 273.15 and 313.15 K in the range 10 to 25 atm (1013-2533 kPa) are given in graphical form.

# METHOD/APPARATUS/PROCEDURE: The volume of gas absorbed by the solvent held in a thermostatted cell was measured at various pressures. The temperature was controlled to ±0.1 K. ESTIMATED ERROR: $\delta T/K = \pm 0.1$ REFERENCES:

<sup>\*\*</sup> Henry's law constant, H, was defined by the authors as mole fraction solubility at a pressure of 760 mmHg

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. 1,3-Dimethyl-1H-pyrazole; C<sub>5</sub>H<sub>8</sub>N<sub>2</sub>; [694-48-4] VARIABLES: P/kPa = 29-2533; T/K = 273-313 ORIGINAL MEASUREMENTS: Egorova, V.I.; Grishko, N.I.; Neokladnova, L.N.; Furmanov, A.S. Podvigailova, I.G. Deposited Document 1976, VINITI 2907-76 PREPARED BY: P.G.T. Fogg

EXPERIMENTAL V	VALUES:				
T/K	P/mmHg	P/kPa	Solubility* vol/vol	H/mmHg**	× <sub>CO₂</sub> †
273.15	760	101.33		36310 38090	0.0209
283.15 298.15	760 216 258	101.33 28.80 34.40	0.96 1.06	36090	0.0200
	321 491	42.80 65.46	1.43 2.12		0.0062 0.0092
313.15	760 760	101.33 101.33	3.40 ¶	51350 65240	0.0148 0.0116

<sup>\*</sup> Solubility of carbon dioxide was given as the volume of gas, reduced to 273.15 K and 101.325 kPa absorbed by unit volume of the solvent.

mole fraction solubility at a pressure of 760 mmHg

760 mmHg

Solubilities in the range 10 to 25 atm (1013-2533 kPa) at 273.15 and 313.15 K were given in graphical form.

AUXILIARY INFORMATION				
METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
The volume of gas absorbed by the solvent held in a thermostatted cell was measured at various pressures. The temperature was controlled to ±0.1 K.	2. b.pt 131-145°C.			
	ESTIMATED ERROR:			
	$\delta T/K = \pm 0.1$			
	REFERENCES:			
	1. Weast, R.C.; Astle, M.J.  Handbook of Data on Organic  Cmpds, 1985, CRC Press,  Boca Raton, Florida, USA.			

<sup>\*\*</sup> Henry's law constant, H, was defined by the authors as

 $<sup>^\</sup>dagger$  calculated by the compiler. The density was taken to be equal to 0.936, the value for 1-ethyl-3-methyl-1 $^H$ -pyrazole at 293.15 K (1).

<sup>¶</sup> extrapolated value

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Ethyl-3-methyl-1H-pyrazole; C<sub>6</sub>H<sub>10</sub>N<sub>2</sub>; [30433-57-9]

### ORIGINAL MEASUREMENTS:

Egorova, V.I.; Grishko, N.I.; Neokladnova, L.N.; Furmanov, A.S. Podvigailova, I.G.

Deposited Document 1976, VINITI 2907-76

### VARIABLES:

P/kPa = 25-101; T/K = 298

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	P/mmHg	P/kPa	Solubility* vol/vol	** CO <sub>2</sub>
298.15	189	25.20	0.82	0.0043
	257	34.26	1.09	0.0057
	392	52.26	1.68	0.0088
	447	59.60	1.93	0.0101
	760	101.33	3.20†	0.0166

<sup>\*</sup> Solubility of carbon dioxide was given as the volume of gas, reduced to 273.15 K and 101.325 kPa absorbed by unit volume of the solvent.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The volume of gas absorbed by the solvent held in a thermostatted cell was measured at various pressures. The temperature was controlled to ±0.1 K.

### SOURCE AND PURITY OF MATERIALS:

No information

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ 

### REFERENCES:

 Weast, R.C.; Astle, M.J. Handbook of Data on Organic Compounds CRC Press, Boca Raton, Florida 1985.

<sup>\*\*</sup> calculated by the compiler from the density of solvent given in ref.(1).

<sup>†</sup> extrapolated value

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Methyl(1-methylethyl)-1Hpyrazole; C<sub>7</sub>H<sub>12</sub>N<sub>2</sub>; [67759-35-7]

### ORIGINAL MEASUREMENTS:

Egorova, V.I.; Grishko, N.I.; Neokladnova, L.N.; Furmanov, A.S. Podvigailova, I.G.

Deposited Document 1976, VINITI 2907-76

### VARIABLES:

P/kPa = 24-101; T/K = 298

PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	P/mmHg	P/kPa	Solubility* vol/vol	**CO <sub>2</sub>
298.15	183	24.40	0.65	0.00386
	286	38.13	0.91	0.0054
	431	57.46	1.57	0.0093
	495	65,99	1.87	0.0110
	760	101.33	2.83 †	0.0166

<sup>\*</sup> Solubility of carbon dioxide was given as the volume of gas, reduced to 273.15 K and 101.325 kPa absorbed by unit volume of the solvent.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The volume of gas absorbed by the solvent held in a thermostatted cell was measured at various pressures. The temperature was controlled to  $\pm 0.1$  K.

SOURCE AND PURITY OF MATERIALS:

No information

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ 

### REFERENCES:

 Weast, R.C.; Astle, M.J. Handbook of Data on Organic Cmpds, 1985, CRC Press, Boca Raton, Florida, USA.

<sup>\*\*</sup> calculated by the compiler. The density was taken to be equal to 0.936, the value for 1-ethyl-3-methyl-1H-pyrazole at 293.15 K (1).

<sup>†</sup> extrapolated value

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Methyl(3-methylbutyl)-1Hpyrazole;  $C_9H_{16}N_2$ ;
  [67759-37-9]

### ORIGINAL MEASUREMENTS:

Egorova, V.I.; Grishko, N.I.; Neokladnova, L.N.; Furmanov, A.S. Podvigailova, I.G.

Deposited Document 1976, VINITI 2907-76

### VARIABLES:

P/kPa = 30-101; T/K = 298

### PREPARED BY:

P.G.T. Fogg

### **EXPERIMENTAL VALUES:**

T/K	P/mmHg	P/kPa	Solubility* vol/vol	** CO <sub>2</sub>
298.15	223	29.73	0.52	0.0038
	342	45.60	0.84	0.0061
	503	67.06	1.26	0.0091
	560	74.66	1.44	0.0104
	760	101.33	1.88†	0.0136

- \* Solubility of carbon dioxide was given as the volume of gas, reduced to 273.15 K and 101.325 kPa absorbed by unit volume of the solvent.
- \*\* calculated by the compiler. The density of the solvent was assumed to be the same as that of 1-ethyl-3-methyl-1H-pyrazole, 0.936 g cm<sup>-3</sup> at 293 K (1).
- t extrapolated value

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The volume of gas absorbed by the solvent held in a thermostatted cell was measured at various pressures. The temperature was controlled to  $\pm 0.1$  K.

### SOURCE AND PURITY OF MATERIALS:

No information

### ESTIMATED ERROR:

 $\delta T/\mathrm{K} = \pm 0.1$   $\delta x_{\mathrm{CO}_2} = \pm 3\%$  due to uncertainty in the value of the density of solvent.

### REFERENCES:

1. Weast, R.C.; Astle, M.J.
Handbook of Data on Organic
Compounds, 1985, CRC Press,
Boca Raton, Florida, USA.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Diazene, bis(4-ethoxyphenyl)l-oxide or p-azoxyphenetole;
  C16H18N2O3; [4792-83-0]

### ORIGINAL MEASUREMENTS:

Homfray, I. F.

J. Chem. Soc. 1910, 97, 1669 - 1676.

VARIABLES:

T/K = 407.2 - 442.2 $p_1/kPa = 118$  (88.5 cmHg) PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Temperature		Physical	, ,		Volume Absorbed	Volume	
t/°C	<i>T</i> /K	State of Solvent	Obs.	Calc.	Diff.	v/cm <sup>3</sup>	Absorbed in 100 cm <sup>3</sup> Solvent (293 K,88.5 cmHg
134.0	407.2	Solid	31.0	31.0	0.0	0	0
139.5	412.7		34.8	33.4	-1.4	_	-
145.5	418.7	Nematic	17.7	35.8	18.1	0.543	29.3
149.0	422.2	Liquid	19.6	37.2	17.6	0.528	28.5
156.5	429.7	11 - 11	22.5	40.1	17.6	0.528	28.5
160.0	433.2	11 11	23.0	41.4	18.4	0.552	29.8
164.5	437.7	11 11	24.2	43.0	18.8	0.564	30.4
166.5	439.7	11 11	24.3	43.8	19.5	0.585	31.6
166.5	439.7	Isotropic	17.4	43.8	26.4	0.792	42.4
167.5	440.7	Liquid	18.0	44.2	26.2	0.786	42.1
169.0	442.2	11 11	18.6	44.7	26.1	0.783	42.0

The calculated manometer reading is the value expected if there is no gas absorption.

The difference between the calculated and the observed manometer reading is a measure of the gas absorbed. The manometer tube had a volume of 0.03 cm<sup>3</sup> per cm of length.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A 2 g sample is enclosed in a bulb and manometer system of known volume. The bulb and contents are in a refluxing aniline bath. The temperature is controlled by the pressure over the aniline.

At each temperature the gas volume is compared with a gas volume calculated assuming ideal gas behavior and no gas absorption by the solvent. The difference in the volumes is the gas volume absorbed by the sample at a temperature of 293 K and a pressure of 118 kPa (88.5 cmHg).

The solvent volume is stated to be 1.824 cm³ at 145.5 °C and 1.866 cm³ at 166.5 °C. The compiler calculated the CO<sub>2</sub> absorption in the sample and in 100 cm³ of solvent assuming the sample volumes above.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Dry gas.
- (2) p-Azoxyphenetole. Commercial sample of unknown purity.

  Prepared from purified p-nitrophenetole by heating with sodium in absolute alcohol. Product recrystallised 20 times from alcohol. Solid to nematic liquid transition 138.5 °C, nematic to isotropic liquid transition 168 °C.

### ESTIMATED ERROR:

5 - 10 per cent (Compiler)

### COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Shenderei, E.R.; Ivanovsky, F.P. [124-38-9] Khim. Prom. 1963, (2), 91-97. 1-Methyl-2-pyrrolidinone, (N-methylpyrrolidone); C<sub>5</sub>H<sub>9</sub>NO; [872-50-4] VARIABLES: PREPARED BY: P/kPa = 13-101P.G.T. Fogg T/K = 273.15-318.15

### EXPERIMENTAL VALUES:

т/к	Henry's o	constant, H /kPa*	*CO <sub>2</sub> at 101.3 kPa*
273.15	26650	3553	0.0285
283.15	32200	4293	0.0236
288.15	36600	4880	0.0208
298.15	42800	5706	0.0178
308.15	54550	7273	0.0139
318.15	61900	8253	0.0123

Henry's constant, H, is defined by the equation:

$$H = \frac{P_{\text{CO}_2}}{x_{\text{CO}_2}}$$

The authors published a graph which showed that the variation of mole fraction solubility with partial pressure of carbon dioxide was linear in the experimental pressure range (13-101 kPa).

 $^{st}$  calculated by the compiler.

AUXILIARY II	NFO	RMA	TI	ON
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AUXIL	IARY INFORMATION
METHOD /APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experimental method given in ref. (1).	2. b.pt. = 206°C (760 mmHg)  ρ = 1.0220 g cm <sup>-3</sup> n <sup>20</sup> = 1.4700  η (20°C) = 1.84 × 10 <sup>-4</sup> Pa s
	REFERENCES:  1. Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovsky, F.P. Gaz. Prom. 1958, (12), 36.

COMPONENTS:		ORIGINAL MEASUREMENTS:	
2.	Carbon dioxide; CO <sub>2</sub> ; [124-38-9]  1-Methyl-2-pyrrolidinone (N-methylpyrrolidone); C <sub>5</sub> H <sub>9</sub> NO; [872-50-4]	Usyukin, I.P.; Shleynikov, V.M.  Neftepererab. Neftekhim. 1963, (1), 39-43	
VARIABLES: T/K = 253.2-293.2 P/kPa = 101.3		PREPARED BY: P.G.T. Fogg	

### EXPERIMENTAL VALUES:

т/к	P/kPa	Mole fraction solubility <sup>†</sup> *CO <sub>2</sub>	Volume of gas* /vol. of solvent
253.2	101.3	0.0719	17.20
263.2	101.3	0.0506	12.00
273.2	101.3	0.0353	8.30
283.2	101.3	0.0261	6.10
293.2	101.3	0.0175	4.05

<sup>\*</sup> volume of gas reduced to 273.15 K and 101.3 kPa

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No information	No information
	ESTIMATED ERROR:
	REFERENCES:

<sup>†</sup> calculated by the compiler

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO2; Demidova, Yu.A.; Usyukin, I.P.; Shleynikov, V.M. [124-38-9] 1-Methyl-2-pyrrolidinone Neftepererab. Neftekhim. 1966, (N-methylpyrrolidone); C<sub>5</sub>H<sub>9</sub>NO; [872-50-4] (12), 36-39. VARIABLES: PREPARED BY: T/K = 253.2-293.2P.G.T. Fogg P/kPa = 101.3 - 1026.25

EXPERIMENTAL T/K	VALUES: P/kPa	Mole fraction solubility	Volume of gas** /vol. of	Henry	's law	Coeff. β
		<sup>X</sup> CO₂	solvent	/acm	/kPa	
253.2	101.3	0.0404 *		22.4	2270	-0.159
253.2	202.6	0.091	22.6			
263.2	101.3	0.0306 *		32.4	3280	-0.148
263.2	202.6	0.064	15.6			
273.2	101.3	0.0235 *		42.6	4320	0.029
273.2	202.6	0.051	12.10			
283.2	101.3	0.0154 *		65.4	6630	0.189
283.2	202.6	0.0313	7.34	-		
293.2	101.3	0.0099 *		101.4	10270	0.20
293.2	202.6	0.019	4.38			

<sup>\*\*</sup> volume of gas reduced to 273.15 K and 101.3 kPa

Measurements made over the pressure range 202.6 kPa to 2026 kPa were fitted to the Krichevsky-Il'inskaya equation in the form :

$$RT \ln \frac{f_1}{x_1} = RT \ln H - \beta (1-x_2^2)$$

where  $f_1$  is the fugacity of carbon dioxide in the gas phase;

 $x_2$  is the mole fraction of solvent in the liquid phase;

 $x_1$  is the mole fraction of gas in the liquid phase; H is the limiting value of Henry's law constant at zero pressure;

 $\beta$  is a coefficient.

\* values at 101.3 kPa calculated by the compiler from the above equation

### AUXILIARY INFORMATION

<b></b>	
METHOD /APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method is described in ref. (1).	No information
	ESTIMATED ERROR:
	REFERENCES:
	1. Usyukin, I.P.; Shleynikov, V.M. Timofeev, A.I.; Shekina, G.I.
	Neftepererab. Neftekhim. 1963, (11), 35.
l .	

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Methyl-2-pyrrolidinone, (N-methylpyrrolidone); C<sub>5</sub>H<sub>9</sub>NO [872-50-4]

ORIGINAL MEASUREMENTS:

Shakhova, S.F.; Bondareva, T.I.; Sergeeva, L.E.

Khim. Prom. 1966, (7), 516-518.

VARIABLES: T/K = 283-393 P/kPa = 12-98 PREPARED BY: P.G.T. Fogg

EXPERIMENTAL VALUES:

т/к	P <sub>CO<sub>2</sub></sub> /mmHg	P <sub>CO2</sub> /kPa*	Solubility <sup>†</sup> vol./vol.	Mole fraction of CO <sub>2</sub> in liquid, *CO <sub>2</sub>
283.15	130.0	17.33	0.843	0.00359
283.15	201.0	26.80	1.31	0.00556
283.15	262.5	35.00	1.71	0.00725
283.15	311.5	41.53	1.98	0.00839
283.15	384.5	51.26	2.47	0.01040
283.15	452.5	60.33	2.91	0.01230
283.15	467.5	62.33	3.10	0.01310
283.15	497.0	66.26	3.20	0.01350
283.15	580.5	77.39	3.76	0.01580
283.15	611.0	81.46	3.95	0.01660
283.15	644.5	85.93	4.28	0.01790
283.15	710.0	94.66	4.62	0.01930
288.15	131.0	17.47	0.782	0.00334
288.15	153.5	20.46	0.885	0.00378
288.15	177.0	23.60	1.01	0.00431
288.15	288.0	38.40	1.70	0.00724
288.15	295.5	39.40	1.76	0.00748
288.15	379.0	50.53	2.19	0.00931
288.15	418.0	55.73 57.33	2.47	0.01050
288.15	430.0		2.54	0.01070
288.15 288.15	505.5 615.5	67.39 82.06	2.96 3.68	0.01260 0.01550
288.15	672.0	89.59	4.00	0.01690
288.15	695.5	92.73	4.15	0.01750
298.15	90.0	12.00	0.418	0.00180
298.15	156.5	20.86	0.693	0.00299
298.15	160.0	21.33	0.74	0.00319
298.15	192.0	25.60	0.893	0.00383
298.15	290.0	38.66	1.37	0.00589
298.15	305.0	40.66	1.43	0.00615
298.15	352.0	46.93	1.62	0.00696
298.15	392.5	52.33	1.86	0.00797
298.15	465.5	62.06	2.17	0.00930
298.15	496.0	66.13	2.37	0.01010
298.15	600.0	79.99	2.87	0.01230
298.15	738.5	98.46	3.45	0.01470

<sup>\*</sup> calculated by the compiler

### AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A static method was used as described in ref. (1).	<ol> <li>99.98% pure by chromatographic analysis.</li> <li>99.7% pure by chromatographic analysis.</li> </ol>
REFERENCES: 1. Braude, G.E.; Leites, I.L.; Dedova, I.V. Khim. Prom. 1963, (7), 510.	ESTIMATED ERROR:

<sup>†</sup> volume of gas, reduced to 101.3 kPa and 273.15 K, absorbed by one volume of solvent.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Methyl-2-pyrrolidinone, (N-methylpyrrolidone); C<sub>5</sub>H<sub>9</sub>NO [872-50-4]

### ORIGINAL MEASUREMENTS:

Shakhova, S.F.; Bondareva, T.I.; Sergeeva, L.E.

Khim. Prom. 1966, (7), 516-518.

### EXPERIMENTAL VALUES:

	P <sub>CO<sub>2</sub></sub> /mmHg	P <sub>CO2</sub> /kPa*	Solubility <sup>†</sup> vol./vol.	Mole fraction of CO <sub>2</sub> in liquid, *CO
308.15	131.0	17.47	0.488	0.00212
308.15	280.5	37.40	1.04	0.00452
308.15	395.0	52.66	1.51	0.00653
308.15	454.5	60.60	1.69	0.00731
308.15	527.0	70.26	2.04	0.00883
308.15	547.0	72.93	2.05	0.00885
308.15	628.0	83.73	2.41	0.01040
308.15	645.5	86.06	2.45	0.01050
308.15	689.5	91.93	2.60	0.01120
308.15	709.0	94.53	2.68	0.01150
363.15	148.0	19.73	0.258	0.00118
363.15	153.0	20.40	0.264	0.00121
363.15	300.5	40.06	0.525	0.00240
363.15 363.15	329.0 472.5	43.86 62.99	0.561 0.811	0.00256
	472.5	63.13	0.817	0.00370
363.15 363.15	568.0	75.73	0.827	0.00377 0.00447
363.15	602.0	80.26	1.05	0.00447
363.15	669.0	89.19	1.16	0.00528
363.15	713.0	95.06	1.24	0.00564
373.15	162.0	21.60	0.248	0.00115
373.15	168.0	22.40	0.262	0.00121
373.15	291.5	38.86	0.442	0.00204
373.15	355.0	47.33	0.548	0.00253
373.15	455.5	60.73	0.703	0.00324
373.15	496.0	66.13	0.777	0.00358
373.15	566.0	75.46	0.87	0.00401
373.15	607.0	80.93	0.929	0.00428
373.15	673.0	89.73	1.03	0.00474
373.15	714.0	95.19	1.09	0.00500
393.15	143.5	19.13	0.177	0.00083
393.15	166.0	22.13	0.216	0.00102
393.15	279.0	37.20	0.348	0.00164
393.15	331.0	44.13	0.438	0.00206
393.15	419.5	55.93	0.535	0.00251
393.15	452.0	60.26	0.598	0.00281
393.15 393.15	528.5 535.5	70.46 71.39	0.694	0.00326
393.15	613.5	81.79	0.683 0.763	0.00321 0.00358
393.15	657.0	87.59	0.763	0.00392

T/K	Henry's co /mmHg	onstant, H, /kPa*
283.15	36700	4890
288.15	40000	5330
298.15	49700	6630
308.15	61500	8200
363.15	126000	16800
373.15	141000	18800
393.15	166000	22100

<sup>\*</sup> calculated by the compiler

 $<sup>^{\</sup>dagger}$  volume of gas, reduced to 101.3 kPa and 273.15 K, absorbed by one volume of solvent.

### 334 COMPONENTS: ORIGINAL MEASUREMENTS: Lenoir, J-Y.; Renault, P.; Renon, H. Carbon dioxide; CO<sub>2</sub>; [124-38-9] J. Chem. Eng. Data 1971, 16, 340-2 1-Methyl-2-pyrrolidinone 2. $C_5H_9NO; [872-50-4]$ VARIABLES: PREPARED BY: T/K = 298.15C.L. Young EXPERIMENTAL VALUES: T/KHenry's Constant Mole fraction at 101.3 kPa $H_{\rm CO_2}/{\rm atm}$ <sup>x</sup>CO₂ (1 atm) 0.0169 298.15 59.1 Calculated by compiler assuming a linear function of $p_{\text{CO}_2}$ vs $x_{\text{CO}_2}$ , ie. $x_{CO_2}$ (1 atm) = 1/ $H_{CO_2}$ AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A conventional gas-liquid chromato-(1) L'Air Liquide sample, minimum graphic unit fitted with a thermal purity 99.9 mole per cent. conductivity detector was used. The (2) Touzart and Matignon or carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value Serlabo sample, purity 99 per cent cent. applies to very low partial pressures of gas and there may be a substantial difference from that measured at l atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for ESTIMATED ERROR: although its possible existence was $\delta T/K = \pm 0.1$ ; $\delta H/atm = \pm 6$ % noted.

(estimated by compiler).

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Methyl-2-pyrrolidinone; C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]

### ORIGINAL MEASUREMENTS:

Rivas, O.R.; Prausnitz, J.M.

Am. Inst. Chem. Engnrs. J. 1979, 25, 975-984.

### VARIABLES:

T/K = 263.2-373.2P/kPa < 101.3

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Henry's o	constant, H /kPa *	$x_{\text{CO}_2}$ at $P_{\text{CO}_2}$ = 101.3 kPa*
263.15	2.80	2800	0.0362
298.15	6.69	6690	0.01515
323.15	10.00	10000	0.01013
348.15	13.90	13900	0.00729
373.15	18.26	18260	0.00555

\* calculated by the compiler

### AUXILIARY INFORMATION

### METHOD APPARATUS/PROCEDURE:

The apparatus is described in ref. (1). The volume of gas absorbed was measured. Pressures were measured with a high precision bourdon pressure gauge. Temperatures were controlled to 0.05 K by a thermostat bath.

### SOURCE AND PURITY OF MATERIALS:

Supplied by standard laboratory reagent suppliers; purities at least 99%

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ 

### REFERENCES:

1. Rivas, O.R.; Prausnitz, J.M.

Ind. Eng. Chem. Fundam. 1979, 18, 289-292.

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Rivas, O.R.; Prausnitz, J.M. [124-38-9] Ind. Eng. Chem. Fundam. 1979, 18, 1-Methyl-2-pyrrolidinone; 289-292. C<sub>5</sub>H<sub>9</sub>NO; [872-50-4] VARIABLES: PREPARED BY: T/K = 293.15, 308.15C.L. Young. EXPERIMENTAL VALUES: T/KHenry's constant Mole fraction at 101.3 kPa / atm (1 atm) partial pressure\* 0.0166 293.15 60.1 77.8 0.0129 308.15 Calculated by compiler assuming mole fraction solubility linear with pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus with a fused quartz precision bourdon pressure gauge. Solubility apparatus care-No details given. fully thermostatted. Solvent degassed in situ. Apparatus described in ref (1) and modifications given in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05$ ; $\delta x_{CO_2} = \pm 1$ %. REFERENCES: 1. Cukor, P.M.; Prausnitz, J.M. Ind. Eng. Chem. Fundam. 1971, 10, 638.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> </ol>	Zubchenko, Yu.P.; Shakhova, C.F.; Ladigina, O.P.
<pre>2. 1-Methyl-2-pyrrolidinone,   (N-methyl pyrrolidone);   C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]</pre>	Khim. Prom-st. (Noscow) <u>1985</u> , (9), 535-6.
VARIABLES:	PREPARED BY:
T/K = 258.2-313.2 P/kPa = 380-55600	P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	<i>H</i> /kPa	<sup>x</sup> co₂*
		at P <sub>CO<sub>2</sub></sub> = 101.3 kPa
258.2	2840	0.0357
273.2	4050	0.0250
288.2	5470	0.0185
298.2	6790	0.0149
313.2	8440	0.0120

The authors measured solubilities at pressures from 380 kPa to 55600 kPa. Solubilities in this pressure range were given in the paper. At each temperature Henry's constant was found from the slope of the linear part of a plot of mole fraction solubility against partial pressure of carbon dioxide.

\* calculated by the compiler

AUXILIARY INFORMATION			
METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A static method was used as described in ref. (1)	-		
	ESTIMATED ERROR:		
	REFERENCES:		
	1. Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P. Khim. Prom. 1960, (5), 370.		

## 338 COMPONENTS: ORIGINAL MEASUREMENTS: Byeseda, J.J.; Deetz, J.A.; Manning, W.P. Carbon dioxide; CO2; [124-38-9] 2. 1-Methyl-2-pyrrolidinone, Proc.Laurance Reid Gas Cond.Conf. (N-methyl pyrrolidone); C<sub>5</sub>H<sub>9</sub>NO; [872-50-4] 1985. VARIABLES: PREPARED BY: T/K = 297.1P/kPa = 101.6P.G.T. Fogg EXPERIMENTAL VALUES: $P_{\text{CO}_2}/\text{psia}$ $P_{\text{CO}_2}/\text{kPa}^*$ Ostwald coeff. T/KMole fraction in liquid\* <sup>X</sup>CO₂ 3.80 297.1 14.73 101.6 0.0150 \* calculated by compiler using the density give in ref.(1). AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 2. Sample referred to as ®MPYROL. The CO2 was contained in a thermostatted metal cylinder connected to a pressure gage, vacuum

The CO2 was contained in a thermostatted metal cylinder connected to a pressure gage, vacuum pump and supply of gas. A tight fitting internal piston sealed with an O-ring fitted into the cylinder so that the volume of gas could be changed by controlled movement of the piston. A measured volume of solvent was injected into the cylinder by a syringe. The absorption of gas was found from the movement of the piston which was necessary to maintain constant pressure.

ESTIMATED ERROR:

### REFERENCES:

 Riddick, J.A.; Bunger, W.B.; Sakano, T.K.

Organic Solvents 1986, Wiley, New York.

Carbon dioxide; CO<sub>2</sub>; [124-38-9]

2. 1-Methyl-2-pyrrolidinone
 (N-methylpyrrolidone);
 C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]

### ORIGINAL MEASUREMENTS:

Wu, Z.; Zeck, S.; Knapp, H.

Ber. Bunsenges. Phys. Chem. 1985, 89, 1009-1013.

### VARIABLES:

T/K = 298.15P/kPa = 101.3

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	P/kPa	Henry's /bar	constant, H /kPa*	Oswald coeff. L/cm <sup>3</sup> cm <sup>-3</sup>	Mole fraction* <sup>×</sup> CO₂
208 15	101 3	650	6500	1 - 885	0.01559

<sup>\*</sup> calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

The volume of gas which was absorbed by a weighed quantity of solute was measured with a gas buret to  $\pm 0.02~\rm cm^3$ . The solute was weighed to an accuracy of  $\pm 5 \times 10^{-4}\rm g$ . The cell containing the solvent was magnetically stirred and the temperature of the apparatus was controlled to  $\pm 0.01~\rm K$  by a thermostat. The apparatus and procedure have been described in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity better than 99.9 vol.%
- 2. A sample provided by Merck of minimum purity of 99%. was treated with molecular sieve 4% to reduce the water content to less than 0.01 wt.% as indicated by Karl-Fischer titration. Chromatographic analysis indicated a purity of 99.9% The material was also degassed before use.

### ESTIMATED ERROR:

 $\delta L/L \le \pm 0.01$  $\delta T/K = \pm 0.01$ 

### REFERENCES:

 Zeck, S. Dissertation, TU Berlin, 1985.

Coupouruma	ODTOTALL AGREEMENTS
COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Kassim, D.M.; Zainel, H.A.; Al-Asof, S.A.; Talib, E.K.
2. 1-Methyl-2-pyrrolidinone; C <sub>5</sub> H <sub>9</sub> NO; [872-50-4]	Fluid Phase Equilibria
	<u>1988</u> , <i>41</i> , 287-294.
VARIABLES:	PREPARED BY:
Temperature	C. L. Young
EXPERIMENTAL VALUES:	
T/K Mole frac	tion of carbon dioxide in liquid, <sup>x</sup> CO <sub>2</sub>
303.15	0.0138
313.15 323.15	0.0126 0.0106
333.15	0.0097
AUXILIARY	INFORMATION
METHOD APPARATUS PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Falling film flow apparatus similar	1. Purity 99.99 mole per cent.
to that of Morrison and Billet (1). Apparatus consisted of (i) degassing	2. Fluka AG puriss grade sample,
section in which solvent could be degassed by freezing and thawing	purity better than 99 mole per cent.
under vacuum and (ii) absorption	,
section. The latter consisted of a gas buret and absorption spiral.	
Mole fraction solubility corrected to 1 atm partial pressure by	
assuming Henry's law was valid.	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1;  \delta x/x = \pm 0.02$
	(estimated by compiler).
	REFERENCES:
	1. Morrison, T.J.; Billet, F.J.
	J. Chem. Soc. 1948, 2033.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Methyl-2-pyrrolidinone, (N-methylpyrrolidone); C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]

### ORIGINAL MEASUREMENTS:

Murrieta-Guevara, F.; Romero-Martinez, A.; Trejo, A.

Fluid Phase Equilibria, 1988, 44, 105-115.

### VARIABLES:

T/K = 298.15-373.15P/kPa = 184.8-1438.5

### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Henry's la H/MPa	aw constant H/kPa	<sup>x</sup> <sub>CO<sub>2</sub></sub> (101.3 kPa)*
298.15	6.38	6380	0.01588
323.15	10.13	10130	0.01000
373.15	23.91	23910	0.00424

<sup>\*</sup> estimated by the compiler as  $P_{\rm CO_2}/H$ 

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus and method of calculation have been described in previous publications (refs. 1 and 2). The limiting values of Henry's law constant which are given above were found by fitting the experimental data to the Krichevsky-Kasarnovsky equation (3).

### SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Infra S.A.; reported purity 99.7 mol%.
- 2. Purity better than 99.5 mol%.

### ESTIMATED ERROR

 $\delta T/K = \pm 0.02$  to 343 K;  $\pm 0.5$  at 373 K. (authors)  $\delta P/kPa = \pm 3.5$ 

- Murrieta-Guevara, F.; Trejo, A., J. Chem. Eng. Data, 1984, 29, 456.
- 2. Gonzalez, R.;
  Murrieta-Guevara, F.; Parra, O.;
  Trejo, A., Fluid Phase
  Equilibria, 1987, 34, 69.
- Prausnitz, J.M.; Lichtenthaler, R.N.; Gomes de Azevedo, E. Molecular Thermodynamics of Fluid-Phase Equilibria, Prentice-Hall, Englewood Cliffs, 1986, Chap.7

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]

### ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès, fac. sci. Univ. Strasbourg (France) 1954.

### VARIABLES:

T/K = 293.15p/kPa = 101.325

### PREPARED BY:

H. L. Clever

### **EXPERIMENTAL VALUES:**

<i>T</i> /K	Ostwald Coefficient <sup>a</sup> L/cm <sup>3</sup> cm <sup>-3</sup>	Bunsen b Coefficient /cm³(STP) cm⁻³atm⁻¹	Mole Fraction $x_1$
293.15	5.10	4.75	0.0164

a Original data.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Dimethylformamide. S.E.P.P.I.C. of Paris. Purity not given. Exposure to air avoided. Distilled prior to use.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$  $\delta p/kPa = \pm 0.1$ 

 $\delta L/L = \pm 0.02$  (compiler)

### REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Comp rend. <u>1952</u>, 234, 2546-8.

b Calculated by compiler using real gas molar volumes.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]</li> </ol>	Du Pont de Nemours and Co., (Inc.)  Chem. Eng. News 1955, 33, 2366.
VARIABLES:	PREPARED BY:
T/K = 298.2 P/kPa = 101.3	P.G.T. Fogg
EXPERIMENTAL VALUES:	
T/K P <sub>CO2</sub> /kPa Bunsen	coefficient x <sub>CO2</sub> *
298.2 101.3	4.4 0.0142
* calculated by the compiler	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Not stated.	Not stated.
	ESTIMATED ERROR:  REFERENCES:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) N,N-Dimethylformamide;  $C_3H_7NO$ ; [68-12-2]

### ORIGINAL MEASUREMENTS:

Haidegger, E.; Szebenyi, I.;
Szekely, A.

Magy. Kem. Foly. 1958, 64, 365-71.

### VARIABLES:

$$T/K = 278.15 - 313.15$$
  
 $p_1/kPa = 26.66 - 119.99$ 

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	erature	Pressure	Absorption Coefficient	Bunsen Coefficient
t/°C	<i>T</i> /K	$\frac{p_1}{mmHg}$	/cm <sup>3</sup> (STP) cm <sup>-3</sup>	α/cm³ (STP) cm <sup>-3</sup> atm <sup>-1</sup>
5	278.15	200	1.51	5.74
		400	3.15	5.99
		600	4.72	5.98
		760	5.96	5.96
		900	7.25	6.12
20	293.15	200	1.15	4.37
	400	2.38	4.52	
		600	3.61	4.57
		760	4.60	4.60
		900	5.49	4.64
40	313.15	200	0.49	1.86
		400	1.30	2.47
		600	2.15	2.72
		760	2.75	2.75
		900	3.30	2.79

The compiler calculated the Bunsen coefficients.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of an absorption flask in a thermostated bath and a water-jacketed buret.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information.
- (2) N,N-Dimethylformamide. Distilled, dried. Refractive index  $n_{\perp}^{25} = 1.4265$ , density  $\rho_{\perp}^{25} = 0.9451$  g cm<sup>-3</sup>. The water content was 0.2 wt percent.

### ESTIMATED ERROR:

 $\delta\alpha/\alpha = \pm 0.03$  (compiler)

At pressures 600 mmHg and above.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2] VARIABLES: T/K = 298-353 P/kPa = 13.3-53.3 PRIGINAL MEASUREMENTS: Braude, G.E.; Leites, I,L.; Dedova, I.V. Khim. Prom. 1961, (4), 232-235. PREPARED BY: PREPARED BY:

### EXPERIMENTAL VALUES:

T/K	Henry's la /mmHg	w constant /kPa*	$x_{\text{CO}_2}$ at $P_{\text{CO}_2} = 101.3 \text{ kPa}^*$
298.15	47000	6270	0.0162
313.15	58500	7800	0.0130
333.15	86000	11470	0.0088
353.15	107000	14270	0.0071

The Henry's law constant is the limiting value of  $P_{\rm CO_2}/x_{\rm CO_2}$  at zero partial pressure,  $P_{\rm CO_2}$ , of carbon dioxide.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A static method was used with the partial pressure of the carbon dioxide from 100 mmHg to 400 mmHg. The absorption vessel was magnetically stirred and held in a thermostat bath. Details of the apparatus are given in the paper.

SOURCE AND PURITY OF MATERIALS:

2. Contained 0.03 wt% of water.

ESTIMATED ERROR:

<sup>\*</sup> calculated by the compiler.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]</li> </ol>	Usyukin, I.P.; Shleynikov, V.M.  Neftepererab. Neftekhim. 1963, (1), 39-43
VARIABLES:	PREPARED BY:
T/K = 213.2-293.2 P/kPa = 101.3	P.G.T. Fogg

T/K	P/kPa	Volume of gas* /vol. of solvent	Mole fraction solubility <sup>†</sup> *CO <sub>2</sub>
213.15	101.3	83.0	0.2241
223.15		53.4	0.1567
233.15		35.0	0.1086
243.15		23.5	0.0756
253.15		16.0	0.0527
263.15		11.5	0.0385
273.15		8.0	0.0271
283.15		6.0	0.0205
293.15		4.0	0.0137

 $<sup>^{*}</sup>$  volume of gas reduced to 273.15 K and 101.3 kPa

AUXILIARY INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
No information	No information		
	ESTIMATED ERROR:		
	REFERENCES:		

 $<sup>^{\</sup>dagger}$  calculated by the compiler

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Byeseda, J.J.; Deetz, J.A.; [124-38-9] Manning, W.P. N, N-Dimethylformamide; C3H7NO; Proc.Laurance Reid Gas Cond.Conf. [68-12-2] 1985. VARIABLES: PREPARED BY: P/kPa = 101.6T/K = 297.1P.G.T. Fogg EXPERIMENTAL VALUES:

T/K	<sup>P</sup> CO₂/psia	P <sub>CO₂</sub> /kPa*	Ostwald coeff. $\it L$	Mole fraction in liquid* *CO2
297.1	14.73	101.6	4.91	0.0155

<sup>\*</sup> calculated by compiler

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The CO2 was contained in a thermostatted metal cylinder connected to a pressure gage, vacuum No information. pump and supply of gas. A tight fitting internal piston sealed with an O-ring fitted into the cylinder so that the volume of gas could be changed by controlled movement of the piston. A measured volume of ESTIMATED ERROR: solvent was injected into the cylinder by a syringe. The absorption of gas was found from the movement of the piston which was REFERENCES: necessary to maintain constant pressure.

- Carbon dioxide; CO2;
  - [124-38-9]
- 2. N, N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]
- 3. Ethyne;  $C_2H_2$ ; [74-86-2]

# ORIGINAL MEASUREMENTS:

Shenderei, E.R.

Khim. Prom. 1966, (7), 514-516.

# VARIABLES:

 $P_{\text{CO}_2}/\text{kPa} = 13.3-101.3$ T/K = 218.15 $x_{C_2H_2} = 0.085 - 0.444$ 

PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K Conc of e /cm <sup>3</sup>	n. *C2H2 thyne g-1**	* Po	CO <sub>2</sub> /kPa*	<sup>x</sup> CO₂	Solubility of CO <sub>2</sub> /cm <sup>3</sup> g <sup>-1</sup> **
1 1 1 1 1 1 1 1 2 2 2	33.8	100 300 500 760 100 300	13.33 40.00 66.66 101.32 13.33 40.00 66.66 101.32 13.33 40.00 66.66 101.32	0.02023 0.06054 0.10090 0.15340 0.01746 0.05237 0.08729 0.13270 0.01618 0.04853 0.08089 0.12290 0.01524 0.04572 0.07619 0.11580	6.94 21.74 37.87 61.14 7.19 22.38 38.72 61.95 7.70 23.86 41.17 65.65 8.55 26.45 45.49 72.32

- \* calculated by the compiler.
  \*\* concentrations were expressed as volume of gas, corrected to 273.15 K and 101.325 kPa, dissolved by one gram of dimethylformamide.

#### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

Method described in ref. (1).

No information

ESTIMATED ERROR:

# REFERENCES:

Shenderei, E.R.; Zel'venskii, F.P.; Ivanovskii, F.P.

Gaz. Prom. 1958, (2), 36.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Nitrobenzene; C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>; [98-95-3]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

#### VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm)

# PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

ANTOES:			
T/K	Mol Fraction	Bunsen	Ostwald
	10 <sup>2</sup> x <sub>1</sub>	Coefficient \alpha/cm3 (STP) cm-3 atm-1	Coefficient L/cm³cm <sup>-3</sup>
88.15	1.21	2.70	2.845
93.15	1.12	2.47	2.655
98.15	1.03	2.25	2.456
	88.15 93.15	T/K Mol Fraction 10 <sup>2</sup> x <sub>1</sub> 88.15 1.21 93.15 1.12	T/K     Mol Fraction     Bunsen $10^2 x_1$ Coefficient $\alpha/\text{cm}^3 (\text{STP}) \text{ cm}^{-3} \text{ atm}^{-1}$ 88.15     1.21     2.70       93.15     1.12     2.47

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an 'absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Nitrobenzene. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- Timofejew, W.
   Phys. Chem. <u>1890</u>, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Nitrobenzene; C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>; [98-95-3]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

J. Chr. Gjaldbaek

EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2x_4$	Bunsen Coefficient c/cm <sup>3</sup> (STP) cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm³cm-3
298.15	1.02	2.23	2.43
	1.01	2.17	2.37

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Carbon dioxide from a cylinder (99.61% CO<sub>2</sub>) was bubbled through the solvent until saturation. A portion of the saturated solution was titrated as described in the paper.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Commercial cylinder, source not given. 99.61 per cent carbon dioxide.
- (2) Nitrobenzene. Purified by fractional freezing and by fractional distillation in vacuum. M.p./°C = 5.75, b.p. (760 mmHg)/°C = 211.94 - 211.95, refractive index, n<sub>D</sub>(20°C) = 1.5524 - 1.5527.

ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- 1. Carbon dioxide; CO,; [124-38-9]
- 2. Nitrobenzene; [98-95-3]

C<sub>6</sub>H<sub>5</sub>NO<sub>2</sub>;

# ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data, 1971, 16, 340-2.

#### VARIABLES:

T/K = 298.2

PREPARED BY:

C. L. Young

#### EXPERIMENTAL VALUES:

298.2

76.7

0.0130

\* Calculated by compiler assuming a linear function of

$$p_{\text{CO}_2}$$
 vs  $x_{\text{CO}_2}$ , ie,  $x_{\text{CO}_2}(1 \text{ atm}) = 1/H_{\text{CO}_2}$ 

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

# SOURCE AND PURITY OF MATERIALS:

- (1) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6\%$  (estimated by compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Quinchon, J.; Gerber, A.; Molinet, G
2. Hydrocyanic acid; HCN; [74-90-8]	Мет. Poudres, <u>1961</u> , 43, 331-342.
VARIABLES:	PREPARED BY:
T/K = 268.15-283.15 P/kPa = 101.3	P.G.T. Fogg

#### EXPERIMENTAL VALUES:

<i>T</i> /K	Absorption vol.of gas/vol.of solvent*
268.15 273.15	6.8 5.9
278.15	2.5
283.15	0.9

 $<sup>^{</sup>st}$  volumes of gas were reduced to 273.15 K and 101.3 kPa

The compiler assumes that the absorption corresponds to a total pressure equal to barometric pressure rather than a partial pressure equal to barometric pressure. The vapor pressure of pure hydrocyanic acid is about 28 kPa at 268.15 K and about 54.5 kPa at 283.15 K.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Solubilities were measured by a static method. Liquid hydrocyanic acid was introduced into a calibrated buret. A second calibrated buret contained carbon dioxide over mercury. Burets were maintained at the required temperature by circulation of a coolant through outer jackets. The reduction in volume of carbon dioxide at a total pressure equal to barometric pressure was measured when taps connecting the burets were opened. The volumes of gas were corrected to 273.15 K.

# SOURCE AND PURITY OF MATERIALS:

- Commercial sample dried with Actige1 before use.
- Refluxed for 2.5 h to remove dissolved gases and then sealed in ampoules.

ESTIMATED ERROR:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Propanenitrile; C<sub>3</sub>H<sub>5</sub>N; [107-12-0] Acta Chem. Scand. <u>1954</u>, 8,

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

1398 - 1413.

**VARIABLES:** 

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

PREPARED BY:

J. Chr. Gjaldbaek

**EXPERIMENTAL VALUES:** 

<i>T</i> /K	Mol Fraction	Bunsen Coefficient	Ostwald Coefficient
	$\frac{10^2 x}{1}$	$\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	1.69 1.69	5.39 5.38	5.88 5.87
			3.0.

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a calibrated all-glass manometer and bulb enclosed in an air thermostat. solvent is addéd and degassed in the apparatus. The gas is added. The apparatus and contents are shaken until equilibrium is attained. Mercury is used for calibration and as the confining liquid.

The absorbed volume of gas is calculated from the initial and final amounts of gas, both saturated with solvent vapor. The amount of solvent is determined by the weight of dis-Placed mercury. Further details are in the references (1, 2).

The mole fraction values are at one atm pressure assuming Henry's law is obeyed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate and sulfuric acid. 99.8 - 99.9% CO2.
- (2) Propanenitrile. Rubber Industries and Sherman Chemicals. Fractionated by distillation. B.p. (760 mmHg)/°C = 97.31 - 97.35, refractive index n<sub>D</sub>(20°C) = 1.3664 - 1.3665.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- 1. Lannung, A. J. Am. Chem. Soc. 1930, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Hexanedinitrile, (adiponitile);  $C_6H_8N_2$ ; [111-69-3]

#### ORIGINAL MEASUREMENTS:

Sadilenko, A.S.; Bondareva, T.I.;
Furmer, I.E.

Tr. Mosk. Khim. Technol. Inst. 1973, 72, 167-170.

# VARIABLES:

T/K = 288.2-373.2P/kPa = 12-103 kPa

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

A small scale graph showed that the mole ratio solubility of carbon dioxide varied linearly with pressure, within experimental error, at 15, 25, 40, 55, 70 and  $100\,^{\circ}\text{C}$  over the pressure range of 12-103 kPa. The mole fraction solubility may be considered to vary linearly with pressure over this pressure range, within the experimental error of the measurements.

The authors also gave the following equation for Henry's law constant over the pressure and temperature range

$$log_{10}(H/mmHg) = 7.83 - 920/(T/K)$$

Henry's law constant, H, was defined by the equation

$$H = \frac{P_{\text{CO}_2}}{x_{\text{CO}_2}}$$

T/K	H	$_{H}^{*}$	
	/mmHg	/kPa	<sup>x</sup> CO₂
288.2	43400	5790	0.01750
298.2	55600	7410	0.01368
313.2	78100	10400	0.00973
328.2	106400	14200	0.00714
343.2	141000	18800	0.00539
373.2	232000	30900	0.00328

<sup>\*</sup> calculated by the compiler from the equation above.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The authors used a static method. Details have been published in earlier papers (1-3).

# SOURCE AND PURITY OF MATERIALS:

No information

#### ESTIMATED ERROR:

- Braude, G.E.; Shakhova. S.F. Khim. Prom. 1961, (3), 177.
- Braude, G.E.; Leites, I.L.; Dedova, I.V. Khim. Prom. 1961, (4), 232.
- Tsiklis, G.M.; Svetlova, G.M. Zh. Fiz. Khim. 1958, 32, 1476.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzeneacetonitrile or benzyl cyanide; C<sub>8</sub>H<sub>7</sub>N; [140-29-4]

# ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.; Andersen, E. K.

Acta Chem. Scand. 1954, 8, 1398 - 1413.

# VARIABLES:

$$T/K = 298.15$$
  
 $p_1/kPa = 101.325$  (1 atm)

# PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

т/к	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm-³atm-1	Ostwald Coefficient L/cm³cm-3
298.15	1.06	2.07	2.26
	1.04	2.03	2.22

The mole fraction and Ostwald coefficient values were claculated by the compiler.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Carbon dioxide from a cylinder (99.61% CO<sub>2</sub>) was bubbled through the solvent until saturation. A portion of the saturated solution was titrated as described in the paper.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Commercial cylinder, source not given. 99.61 per cent carbon dioxide.
- (2) Benzeneacetonitrile. Fractional
   distillation in vacuum. B.p.
   (760 mmHg)/°C = 233.49 233.55,
   refractive index n<sub>D</sub>(20°C) =
   1.5233.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:	
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>3-(Dimethylamino)propanenitrile; C<sub>5</sub>H<sub>1</sub> <sub>0</sub>N<sub>2</sub>; [1738-25-6]</li> </ol>	Bryukhanova, L.A.; Nikitina A.K.  Zh. Prikl. Khim. (Leningrad) 1986, 59(2), 432-4.	
VARIABLES: T/K = 303.15-333.15	PREPARED BY: P.G.T. Fogg	

# EXPERIMENTAL VALUES:

Solubilities were measured at various pressures to a maximum of about 60 atm (6080 kPa) and interpreted by the Krichevskii-Il'inskaya equation in the form

$$\log_{10}(P_2/x_2) = \log_{10}H - \beta(1-x_1^2)$$

 $P_2$  is the partial pressure of carbon dioxide,  $x_2$  the mole fraction of carbon dioxide in the liquid phase, H the limiting value of the Henry's law constant,  $\beta$  a constant and  $x_1$  the mole fraction of 3-(dimethylamino)-propionitrile in the liquid phase. Henry's law constant is taken to be the ratio of the pressure of the partial pressure of carbon dioxide to the mole fraction of carbon dioxide in the liquid phase.

T/K	Henry's law constant, H/atm	β**	H/kPa*	$x_2$ at $P_2 = 101.3 \text{ kPa}^*$
303.15	32.43	-0.49801	3286	0.02889
313.15 323.15	51.52 79.43	-0.3333 -0.1739	5220 8048	0.01886 0.01247
333.15	122.2	-0.01555	12382	0.00818

<sup>\*</sup> calculated by the compiler

# AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A static method was used as described in ref. (1).	2. Pure sample, distilled in vacuum.
	ESTIMATED ERROR:
	REFERENCES:
	1. Freudlin, G.N.; Vyshinskiy, V.I.  Zh. Prik1. Khim. 1970, 43(2), 385.

<sup>\*\*</sup> given as a positive quantity in the original paper. This appears to be a mistake.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO <sub>2</sub> ;	Wehner, K.; Burk, W.; Kisan, W.
[124-38-9]  2. Hexahydro-1-methyl-2 <i>H</i> -azepin-2-one, ( <i>N</i> -methyl-\varepin-caprolactam); C <sub>7</sub> H <sub>13</sub> NO; [2556-73-2]	Chem. Tech. (Leipzig) 1977, 29(8), 445-448.
VARIABLES:	PREPARED BY:
T/K = 293.2	P.G.T. Fogg
EXPERIMENTAL VALUES:	S,* Mole fraction (101.3kPa)**
T/K Kuenen coefficient, c/cm³g <sup>-1</sup> atm <sup>-1</sup>	x <sub>CO<sub>2</sub></sub>
293.2 2.90	0.0166
The authors also gave a small scale groefficient with temperature from about * This is the volume of gas, reduced dissolved by one gram of solvent, divigas in atmospheres.  ** Calculated by the compiler on the applicable to a partial pressure of 1	at 280 K to about 400 K.  to 273.15 and 1 atm, which is ided by the partial pressure of the assumption that the value of S is
AUXILIARY	INFORMATION
METHOD APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made by staff at VEB Leuna-Werke 'Walter Ulbricht'. No other details were given.	No information given.
	ESTIMATED ERROR:
	REFERENCES:

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- Compounds of Phosphorus, Silicon or Sulfur

#### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

Solubility of carbon dioxide in solvents containing phosphorus, silicon or sulfur.

# Solubility in solvents containing phosphorus

Mole fraction solubility in hexamethylphosphoric triamide at a partial pressure of 101.3 kPa may be estimated from data published by Bryukhanova and Nikitina (1), Schay et al.(2), Lenoir et al.(3) and Bratzler et al.(4). There is poor agreement between the sets of data. A selection of values of mole fraction solubility at 101.3 kPa are given below.

	293.2 K	298.2 K	333.2 K
Bryukhanova and Nikitina	0.0338*	0.0313*	0.01942
Schay et al.	0.0303	0.0282	0.0144
Lenoir et al.		0.0329	
Bratzler et al.	0.037		

# \* extrapolated

The following equation based upon data from the four sources can be used as an approximate guide to solubility at 101.3 kPa in this solvent. Further measurements are needed to resolve discrepancies between the solubility data.

 $\ln x_{CO_2} = -9.074 + 1667.6/(T/K)$ 

temperature range = 273.2-363.2 K standard deviation in values of  $x_{CO_2}$  = 0.0030

Solubility in tributyl phosphate at 223.2 K to 313.2 K from 13.6 kPa to 101.0 kPa has been published by Kosyakov et a1.(5). Henry's constant at various temperatures from 243.2 K to 383.2 K have been published by Lenoir et a1.(3), Gudasheva and Furmer (6), Sweeney (7), and Vei et a1.(8) There is satisfactory agreement between mole fraction solubilities at a partial pressure of 101.3 kPa calculated from data from the five sources. The recommended smoothing equation is given below.

$$\ln x_{CO_2} = 17.505 + 591.57/(T/K) \sim 4.0173 \ln(T/K)$$

temperature range = 223.2-383.2 K standard deviation in values of  $x_{CO_2} = 0.0055$ 

Solubility in triethyl phosphate was measured at 298.15 K; 101.3 kPa by Schay et al.(2). Lenoir et al.(3) reported a limiting value of Henry's constant at 325.7 K measured by gas-liquid chromatography. The corresponding values of mole fraction solubility at a partial pressure of 101.3 kPa are compatible with each other.

Lenoir et al.(3) also reported values of Henry's constant for the trimethyl, tripropyl and tris(2-methylpropyl) esters of phosphoric acid. No other measurements on these systems are available for comparison.

# Solubility in solvents containing silicon

Wilcock et al.(9) measured solubility in octamethylcyclotetrasiloxane at 292.2 K to 313.1 K; 101.3 kPa. The data are likely to be reliable but no other measurements on this system are available for comparison. Mole fraction solubility is high compared with a reference line based upon Raoult's law.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Compounds of Phosphorus, Silicon or Sulfur

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

Solubility in tetramethyl silane at 291.5 K has been reported by Horsman-van den Dool and Warman (10). The solubility measurement needs to be confirmed by other workers before it can be recommended.

Solubility in solvents containing sulfur

Kassim et al.(11) measured solubility in tetrahydrothiophene, 1,1-dioxide at 303.2 K to 333.2 K; 101.3 kPa. Xu et al.(12) reported solubility measured at about 100 kPa from 303.2 K to 359.9 K. Roberts and Mather (13) measured solubility to high pressures at 313.2 K and 373.2 K. Rivas and Prausnitz (14) published Henry's constants for 303.2 K to 373.2 K. Murrieta-Guevara et al.(15) reported limiting values of Henry's constants from 303.2 K to 373.2 K.

The evaluator recommends the following equation based upon data from references (11-14) for the mole fraction solubility at a partial pressure of 101.3 kPa.

 $\ln x_{CO_2} = -67.177 + 4443.1/(T/K) + 8.4001\ln(T/K)$ 

temperature range = 303.2-373.2 K standard deviation in  $x_{CO_2}$  = 1.9 × 10<sup>-4</sup>

Values estimated from Henry's constants published by Murrieta-Guevara  $et\ al.$  (15) differ from values from this equation by 8%, 2% and 12% at 303.2 K, 323.2 K and 373.2 K respectively.

Solubility in carbon disulfide at or close to 101.3 kPa has been reported by Just (16) from 288.2 K to 298.2 K and Kobatake and Hildebrand (17) from 281.7 K to 306.4 K. Solubility at lower pressures has been reported by Woukoloff (18) from 280.2 K to 293.7 K and Gjaldbaek (19) from 298.1 to 298.5 K. There is good agreement between values of mole fraction solubility corrected to a partial pressure of 101.3 kPa from data given by Kobatake and Hildebrand, Woukoloff, and by Gjaldbaek. A smoothing equation for these values are given below. Data published by Just are very low when compared with that from the other sources.

 $lnx_{CO_2} = 65.328 - 2496.8/(T/K) - 11.0008ln(T/K)$ 

temperature range = 280.2-306.4 K standard deviation in  $x_{CO}$  =  $3.8 \times 10^{-5}$ 

The value mole fraction solubility in sulfinylbismethane at 101.3 kPa and 298.2 K published by Dymond (20) is 0.00908. Lenoir et al.(3) reported a limiting value of Henry's law constant measured by gas-liquid chromatography at this temperature. This corresponds to a mole fraction solubility at 101.3 kPa of about 0.00943. Solubilities measured by gas chromatography are always subject to uncertainty because of the possibility of surface effects affecting the result. Dymond's value may therefore be the more reliable one but confirmation by other measurements is needed.

Selected values of solubilities in solvents containing phosphorus or silicon are given in Table 1 and shown in Fig 1.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Compounds of Phosphorus, Silicon or Sulfur

# **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

- Bryukhanova, P.A.; Nikitina, A.K. Zh. Prikl. Khim. (Leningrad) 1985, 58(3), 667-669.
- Schay, G.; Szekely, Gy.; Racz, Gy.; Traply, G. Periodica Polytech. 1958, 2, 1-24.
- Lenoir, J-Y.; Renault, P.; Renon, H. J. Chem. Eng. Data 1971, 16, 340-342.
- Bratzler, K.D.; Doerges, A.; Herbert, W. German Patent No. 1 769 197 to Metallgesellschaft AG. 1971.
- Kosyakov, N.Ya.; Yushko, V.L.; Sergienko, I.D.; Khokhlov, S.F.; Taraba, R.F. Khim. Prom. (Moscow) 1972, 48(6), 432-433.
- Gudasheva, V.M.; Furmer, I.E. Tr. Mosk. Khim. i Tekh. Inst. 1970, 2, 15-17.
- 7. Sweeney, C.W. Chromatographia, 1984, 18, 663-667.
- Vei, D.; Furmer, I.E.; Sadilenko, A.S.; Efimova, N.M.; Stepanova, Z.G.; Gracheva, N.V. Gaz. Prom. 1975, 7, 47-49.
- 9. Wilcock, R.J.; McHale, J.L.; Battino, R.; Wilhelm, E. Fluid Phase Equilibria 1978, 2, 225-230.
- 10. Horsman-van den Dool, L.E.W.; Warman, J.W. Interuniversity Reactor Institute (IRI)-Report 134-81-01.
- 11. Kassim, D.M.; Zainel, H.A.; Al-Asof, S.A.; Talib, E.K. Fluid Phase Equilibria 1988, 41, 287-294.
- Xu, S.; Wang, Y-w.; Otto, F.D.; Mather, A.E. J. Chem. Tech. Biotechnol. 1991, 51, 197-208.
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- 14. Rivas, O.R.; Prausnitz, J.M. Am. Inst. Chem. Engnrs. 1979, 25, 975-984.
- 15. Murrieta-Guevara, F.; Romero-Martinez, A.; Trejo, A. Fluid Phase Equilibria 1988, 44, 105-115.
- 16. Just, G. Z. Phys. Chem. 1901, 37, 342-367.
- 17. Kobatake, Y.; Hildebrand, J.H. J. Phys. Chem. 1961, 65, 331-335.
- 18. Woukoloff, Comptes Rendus 1889, 108, 674-675.
- 19. Gjaldbaek, J.C. Acta Chem. Scand. 1953, 7, 537-544.
- 20. Dymond, J. J. Phys. Chem. 1967, 71, 1829-1831.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Compounds of Phosphorus, Silicon or Sulfur

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

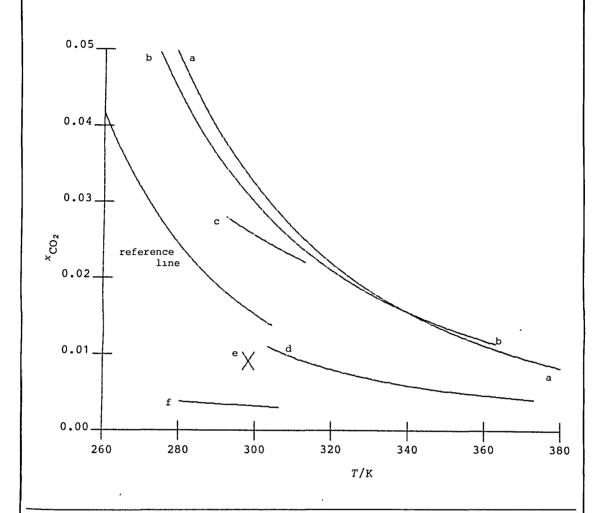


Fig. 1 Mole fraction solubility of carbon dioxide in various solvents containing phosphorus, silicon or sulfur at a partial pressure of gas of 101.3 kPa.

- a tributyl phosphate
- b hexamethylphosphoric triamide
- c octamethylcyclotetrasiloxane
- d tetrahydrothiophene, 1,1-dioxide (sulfolane)
- e sulfinylbismethane (dimethylsulfoxide) (20)
- f carbon disulfide

The curves showing the variation of solubility with temperature correspond to equations derived by the evaluator.

A reference line corresponding to values from the Raoult's law equation is also shown.

COMPONENTS:		EVALUATOR:	
1.	Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London,	
2.	Compounds of Phosphorus, Silicon or Sulfur	Holloway Road, London, N7 8DB, U.K.  July 1991	

CRITICAL EVALUATION:

Table 1. Solubility of carbon dioxide at a partial pressure of 101.3 kPa in solvents containing sulfur, phosphorus or silicon .

Solvent	T/K	<sup>X</sup> CO₂	Reference
Hexamethylphosphoric	triamide 298.15	0.0308 ±0.0030	*
Tributyl phosphate	298.15	0.0334 ±0.0055	*
Triethyl phosphate	298.15	0.0275	2
Octamethylcyclotetras	siloxane 298.04	0.02633	9
Tetrahydrothiophene,	1,1-dioxi 298.15	de 0.01223 ±0.000	08 *
Carbon disulfide	298.15	0.00327 ±0.000	04 *
Sulfinylbismethane	298.15	0.00908	20

<sup>\*</sup> from the equation given by the evaluator on a previous page

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Phosphoric acid, triethyl ester, (triethylphosphate);
   C<sub>6</sub>H<sub>1</sub>SO<sub>4</sub>P; [78-40-0]

Phosphoric triamide, hexamethyl; (hexamethylphosphorictriamide); C<sub>6</sub>H<sub>18</sub>N<sub>3</sub>OP; [680-31-9]

# ORIGINAL MEASUREMENTS:

Schay, G.; Szekely, Gy.; Racz, Gy.; Traply, G.

Periodica Polytech. 1958, 2, 1-24.

# VARIABLES:

T/K = 273.2-363.2P/kPa = 27-108 kPa

# PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

Solvent	P <sub>CO₂</sub> /kPa	T/K	Volume of gas absorbed <sup>†</sup> /cm <sup>3</sup> g <sup>-1</sup>	Mole fraction solubility*  *CO2
TEP	101.3	298.15	3.45	0.0275
HMP	101.3	273.15	6.06 ¶	0.0465
	101.3	298.15	3.60	0.0282
	101.3	333.15	1.82 ¶	0.0144
	101.3	363.15	1.18 ¶	0.0094

TEP = triethylphosphate

HMP = hexamethylphosphorictriamide

- t volumes of gas have been reduced to 273.2 K and 101.3 kPa
- $\P$  values were given for 298.15 K in a table. Small scale graphs (4cm  $\times$  4cm) showing a linear variation of absorption of gas in HMP with change in partial pressure were also published. The values which have been estimated by the compiler from the graphs are marked with  $\P$ .
- \* calculated by the compiler.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static methods were used. For measurements above room temperature condensation of solvent vapor in the cooler parts of the system was reduced by use of capillary tubes to connect parts of the apparatus and by measuring the pressure by a null method. A magnetic stirrer was used to stir the solvent in the absorption cell.

# SOURCE AND PURITY OF MATERIALS:

No information

# ESTIMATED ERROR:

Error of about 0.15 cm<sup>3</sup>g<sup>-1</sup> in reading data from the graphs (compiler).

# ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Lenoir, J-Y.; Renault, P.; Renon, H. 2. Phosphoric triamide, hexamethyl-; C<sub>6</sub>H<sub>18</sub>N<sub>3</sub>OP; [680-31-9] VARIABLES: PREPARED BY:

EXPERIMENTAL VALUES:

T/K = 298.2

\* Calculated by compiler assuming a linear function of  ${}^{P}_{CO_{2}}$  vs  ${}^{x}_{CO_{2}}$ , i.e.,  ${}^{x}_{CO_{2}}$  (1 atm) =  $1/H_{CO_{2}}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retnetion time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

# SOURCE AND PURITY OF MATERIALS:

(]) L'Air Liquide sample, minimum purity 99.9 mole per cent.

C. L. Young

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

	369
COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Carbon dioxide; CO<sub>2</sub>; [124-38-9]</li> <li>Hexamethylphosphoric triamide,         (hexametapol); C<sub>6</sub>H<sub>18</sub>N<sub>3</sub>OP; [680-31-9]</li> </ol>	Bryukhanova, P.A.; Nikitina A.K.  Zh. Prikl. Khim. (Leningrad) 1985, 58(3), 667-9.
VARIABLES:	PREPARED BY:
T/K = 313.15-348.15	P.G.T. Fogg
EXPERIMENTAL VALUES:	
Solubilities were measured at various (4053 kPa) and interpreted by the Krithe form $\log(P_2/x_2) = \log H - \beta$	icĥevskii-Il'inskaya equation in
$P_2$ is the partial pressure of carbon carbon dioxide in the liquid phase, $R$	H the limiting value of the Henry's

law constant,  $\beta$  a constant and  $x_1$  the mole fraction of hexametapol in the liquid phase. Henry's law constant is taken to be the ratio of the partial pressure of carbon dioxide to the mole fraction of carbon dioxide in the liquid phase.

T/K	Henry's law constant, H/atm	β**	H/kPa*	$x_2$ at $P_2 = 101.3 \text{ kPa*}$
313.15	37.93	-0.33085	3843	0.02538
333.15	50.12	-0.30709	5078	0.01942
348.15	59.02	-0.28876	5980	0.01658

calculated by the compiler

# AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A static method was used as described in ref.(1).	2. Pure sample, distilled in vacuum.
	ESTIMATED ERROR:
	REFERENCES:
	1.Freidlin, G.N.; Bushinskii, V.I.  Zh. Prikl. Khim. 1970, 43(2), 385
	Zh. Prikl. Khim. <u>1970</u> , 43(2), 38

given as a positive quantity in the original paper. This appears to be a mistake.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Phosphoric acid, tributyl ester, (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>PO<sub>4</sub>; [126-73-8]

# ORIGINAL MEASUREMENTS:

Kosyakov, N. Ya.; Yushko, V.L. Sergienko, I.D.; Khokhlov, S.F.; Taraba, R.F.

Khim. Prom. (Moscow) 1972, 48, (6), 432-3.

# VARIABLES:

T/K 223.15 - 313.15 P/kPa 13.6 - 101.0

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

	DRIPHHIND V	and deb.			
	T/K	P/Torr	P/kPa	<sup>x</sup> CO₂	Henry's law constant, H /kPa*
	223.15	102	13.6	0.0316	
	223.15	344	45.9	0.1068	
l	223.15	449	59.8	0.1358	
	223.15	569	75.8	0.1684	
l	223.15	682	91.0	0.1960	
l					
ľ	223.15	760	101.3	0.2201 *	
	223.15				418
ì	233.15	124	16.6	0.0264	
l	233.15	316	42.1	0.0681	
	233.15	491	65.5	0.1055	
	233.15	502	67.0	0.1099	
i	233.15	544	72.6	0.1165	
ļ.	233.15	602	80.3	0.1279	
	233.15	631	84.1	0.1323	
ļ					
I	233.15	760	101.3	0.1623 *	
	233.15				622
ı					

<sup>\*</sup> estimated by the compiler by fitting the experimental data to the Krichevsky-Il'inskaya equation in the form

$$\log_{10} \frac{P/\text{kPa}}{x_{\text{CO}_2}} = \log_{10} (H/\text{kPa}) - \beta(1 - x_{\text{tbp}}^2)$$

where  ${\it H}$  is the Henry's law constant,  ${\it \beta}$  is a constant and  ${\it x}_{\rm tbp}$  is the mole fraction of tributyl phosphate.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Solubility measured by a static method described in the literature (1).

# SOURCE AND PURITY OF MATERIALS:

- Purified by freezing. Chromatographic analysis indicated that impurities did not exceed 0.1 vol.%
- 2. Pure grade material used.

ESTIMATED ERROR:

# REFERENCES:

 Braude, G. E.; Shakhova, S.F. Khim. Prom. <u>1961</u>, (3), 177.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Phosphoric acid, tributyl ester, (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>PO<sub>4</sub>; [126-73-8]

# ORIGINAL MEASUREMENTS:

Kosyakov, N. Ya.; Yushko, V.L. Sergienko, I.D.; Khokhlov, S.F.; Taraba, R.F.

Khim. Prom. (Moscow) 1972, 48, (6), 432-3.

# EXPERIMENTAL VALUES:

T/K	P/Torr	P/kPa	<sup>×</sup> CO₂	Henry's law constant, H /kPa*
253.15 253.15 253.15 253.15 253.15 253.15 253.15	124 369 433 500 660 698 760	16.6 49.2 57.8 66.7 88.0 93.0 101.3	0.0145 0.0422 0.0527 0.0593 0.0791 0.0774 0.0887 *	
273.15	156	20.7	0.0110	1137
273.15 273.15 273.15 273.15 273.15	440 462 600 644 718	58.7 61.6 80.0 85.9 95.7	0.0308 0.0352 0.0440 0.0444 0.0510	
273.15	760	101.3	0.0546 *	1866
293.15 293.15 293.15 293.15 293.15 293.15	398 562 620 676 758 760	53.0 75.0 82.7 90.1 101.0 101.3	0.0207 0.0295 0.0303 0.0360 0.0396	
313.15 313.15 313.15 313.15 313.15	191 176 378 520 653	25.5 23.4 50.4 69.3 87.1	0.0066 0.0084 0.0132 0.0185 0.0220	2650
313.15 313.15 313.15 313.15	658 756 760	87.7 100.7 101.3	0.0264 0.0273 0.0275	× 3384

<sup>\*</sup> estimated by the compiler by fitting the experimental data to the Krichevsky-Il'inskaya equation in the form

$$\log_{10} \frac{P/kPa}{x_{CO_2}} = \log_{10} (H/kPa) - \beta(1 - x_{tbp}^2)$$

where  ${\it H}$  is the Henry's law constant,  $\beta$  is a constant and  $x_{\rm tbp}$  is the mole fraction of tributyl phosphate.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Phosphoric acid, tributyl ester (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8] VARIABLES: T/K = 243.15-358.15 P/kPa = 0-101.3 PRIGINAL MEASUREMENTS: Gudasheva, V.M.; Furmer, I.E. Tr. Mosk. Khim. i Tekh. Inst. 1970, 2, 15-17. PREPARED BY: P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K	Henry's com	nstant, <i>H</i> , /kPa <sup>*</sup>	$^{x}_{\text{CO}_{2}}$ at $P_{\text{CO}_{2}}$ = 101.3 kPa,
243.15	7300	973	0.1041
263.15	11900	1587	0.0639
273.15	15500	2066	0.0490
298.15	21400	2853	0.0355
313.15	28200	3760	0.0270
328.15	35400	4720	0.0215
343.15	50000	6666	0.0152
358.15	69100	9213	0.0110

<sup>\*</sup>Calculated by the compiler. Mole fraction solubility was proportional to pressure, within experimental error, in the pressure range from 0 to 101.3 kPa.

Solubilities at pressures to 5066 kPa in the temperature range  $288-313\ \mathrm{K}$  were also measured

# AUXILIARY INFORMATION

AUXILIARY INFORMATION			
METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
A static method was used as described in refs. (1) and (2).	2. 'Pure' grade tributyl phosphate was vacuum distilled.		
	LSTIMATED ERROR:		
	REFERENCES:		
	1. Braude, E.R.; Shakhova, S.F. Khim. Prom. 1961, (3), 177		
	2. Shenderei, E.P.; Zel'venskii, Ya.D.; Ivanovskii, F.P. Khim. Prom. 1960, (5), 370.		

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Phosphoric acid, tributyl ester (tributyl phosphate); C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8]

# ORIGINAL MEASUREMENTS:

Vei, D.; Furmer, I.E.;
Sadilenko, A.S.; Efimova, N.M.;
Stepanova, Z.G.; Gracheva, N.V.

Gaz. Prom. <u>1975</u>, 7, 47-49.

# VARIABLES:

T/K = 343.15-383.15P/kPa = 0-101.3 PREPARED BY:

P.G.T. Fogg

#### **EXPERIMENTAL VALUES:**

T/K	Henry's co	nstant, H,	Mole fraction $x_{CO_2}$	
	/mmHg	/kPa*	at P <sub>CO2</sub> = 101.3 kPa,	
343.15	50300	6706	0.0151	
363.15	80400	10719	0.0095	
383.15	119800	15972	0.0063	

\* calculated by the compiler on the assumption that  $x_{\text{CO}_2} = P_{\text{CO}_2}/H$ 

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

A static method was used. The compiler was not able to consult the original Russian paper. Literature references could not be included in the English translation from which the compilation was prepared (1).

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

# REFERENCES:

 British Gas Corporation Translations, T5408/BG/LRS/LRST492/80

# 370 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Lenoir, J-Y.; Renault, P.; Renon, H. 2. Esters of phosphoric acid. J. Chem. Eng. Data, 1971, 16, 340-2. **VARIABLES:** PREPARED BY: T/K = 298.2-343.2C. L. Young EXPERIMENTAL VALUES: Mole fraction at 1 atm\* Henry's constant T/K $^{H}$ co<sub>2</sub>/atm xco, Phosphoric acid, trimethyl ester; C3H3OLP; [512-56-1] 325.2 Phosphoric acid, triethyl ester; C<sub>6</sub>H<sub>15</sub>O<sub>4</sub>P; [78-40-0] 325.7 Phosphoric acid, tripropyl ester; C,H2,O,P; [513-08-6] 298.2 28.1 0.0356 42.4 323.2 0.0236 59.5 343.2 0.0168 Phosphoric acid, tributyl ester; C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-73-8] 0.0233 325.2 Phosphoric acid, tris(2-methylpropyl)ester; C<sub>12</sub>H<sub>27</sub>O<sub>4</sub>P; [126-71-6] 325.2 28.4 Calculated by compiler assuming a linear function of $P_{CO_2}$ vs $x_{CO_2}$ , i.e., $x_{CO_2}(1 \text{ atm}) = 1/H_{CO_2}$ . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at latm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

- (1) L'Air Liquide sample, minimum purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Octamethylcyclotetrasiloxane;  $C_8H_{24}O_4Si_4$ ; [556-67-2]

# ORIGINAL MEASUREMENTS:

Wilcock, R. J.; McHale, J. L.; Battino, R.; Wilhelm, E.

Fluid Phase Equilib. 1978, 2, 225-230.

VARIABLES:

T/K: 292.15 - 313.05 p/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^2 x_1$	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient _L/cm³cm-3
292.15	2.794	2.068	2.212
298.04	2.633	1.933	2.109
313.05	2.209	1.586	1.818

The solubility values were adjusted to a gas partial pressure of 101.325 kPa by Henry's law.

The Bunsen coefficients were calculated by the compiler.

Smoothed Data: For use between 292.15 and 313.05 K.

 $\ln x_{\tau} = -7.1315 + 10.3956/(T/100K)$ 

The standard error about the regression line 2.15 x  $10^{-4}$ .

T/K	Mol Fraction 10 <sup>2</sup> x <sub>1</sub>
298.15	2.613
308.15	2.333

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus is based on the design of Morrison and Billett (1), and the version used îs described by Battino, Evans, and Danforth (2). The degassing apparatus and procedure are described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm³ of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is applied intermittently through a liquid N2 trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass spiral tube containing the solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Stated to be 99.8 mole percent minimum purity.
- (2) Octamethylcyclotetrasiloxane. General Electric Co. Distilled, density at 298.15 K was 0.9500 g cm<sup>-3</sup>.

#### ESTIMATED ERROR:

 $\delta T/K = 0.03$   $\delta p/mmHg = 0.5$  $\delta x_1/x_1 = 0.1$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1</u>948, 2033.
- Battino, R.; Evans, F.D.; Danforth, W.F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Tetramethyl silane; C<sub>4</sub>H<sub>12</sub>Si; [75-76-3]

# ORIGINAL MEASUREMENTS:

Horsman-van den Dool, L. E. W.; Warman, J. W.

Interuniversity Reactor Institute (IRI)-Report 134-81-01

# VARIABLES:

$$T/K = 291.5$$
  
 $p_1/kPa = not given$ 

#### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

Temperature		Ostwald Coefficient	Number
t/°C	<i>T</i> /K	L/cm³ cm <sup>-3</sup>	of Runs
18.3	291.5	3.59	3

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A cylindrical glass container of approximately 15 cm³ volume is partly filled with solvent and closed with a half-hole septum. An amount of the gaseous solute is added to the container. The closed container is shaken for 30 minutes. Samples of both the vapor and liquid phases are taken in a calibrated syringes. The samples are injected into a gas chromatograph. The Ostwald coefficient is calculated from the known sample size and the measured peak areas.

The chromatograph is a Hewlett-Packard model 5750 equipped with a thermal conductivity cell detector. The carrier gas is helium. A 200 cm Porapak Q column is used for the separation.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Baker Chemical Co. Instrument grade, 99.99 percent. Used as received.
- (2) Tetramethyl silane. Merck. Uvasol grade. Impurities which give the same retention time as the gas are removed before the experiment by adsorption or distillation.

ESTIMATED ERROR:

 $\delta L/L = \pm 0.05$ 

# 373 COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Rivas, O.R.; Prausnitz, J.M. 1. [124-38-9] Am. Inst. Chem. Engnrs. J. 1979, 25, 975-984. Tetrahydrothiophene, 1,1-2. dioxide (Sulfolane); C4H8O2S; [126-33-0] VARIABLES: PREPARED BY: T/K = 303.15-373.15C.L. Young EXPERIMENTAL VALUES: Mole fraction of + T/KHenry's constant, H carbon dioxide in /MPa liquid, x<sub>CO2</sub> 9.26 0.01094 303.15 323.15 13.30 0.007618 0.005364 18.89 348.15 25.07 0.004042 373.15 + at a partial pressure of 101.3 kPa calculated by compiler assuming Henry's law applies at that pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. and 2. Purity at least Volumetric apparatus with a fused 99 mole per cent. quartz precision bourdon pressure gauge. Solubility apparatus carefully thermostatted. Solvent degassed in situ. Apparatus described in ref. (1) and modifications given in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05; \ \delta x_{CO_2} = \pm 1\%.$

REFERENCES:

10, 638.

1. Cukor, P.M.; Prausnitz, J.M.

Ind. Eng. Chem. Fundam. 1971,

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- Tetrahydrothiophene, 1,1dioxide, (Sulfolane); C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S; [126-33-0]

# ORIGINAL MEASUREMENTS:

Murrieta-Guevara, F.; Romero-Martinez, A.; Trejo, A.

Fluid Phase Equilibria, 1988, 44, 105-115.

#### VARIABLES:

T/K = 303.15-373.15P/kPa = 81.2-2263.4

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/K	Henry's la H/MPa	aw constant H/kPa	x <sub>CO₂</sub> (101.3 kPa)*
303.15	8.61	8610	0.01177
323.15	13.17	13170	0.00769
373.15	22.39	22390	0.00453

<sup>\*</sup> estimated by the compiler as  $P_{\rm CO_2}/H$ 

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus and method of calculation have been described in previous publications (refs. 1 and 2). The limiting values of Henry's law constant which are given above were found by fitting the experimental data to the Krichevsky-Kasarnovsky equation (3).

# SOURCE AND PURITY OF MATERIALS:

- Supplied by Infra S.A.; reported purity 99.7 mol%.
- 2. Purity better than 99.5 mol%.

# ESTIMATED ERROR

 $\delta T/K = \pm 0.02$  to 343 K;  $\pm 0.5$  at 373 K. (authors)  $\delta P/kPa = \pm 3.5$ 

- Murrieta-Guevara, F.; Trejo, A., J. Chem. Eng. Data, 1984, 29, 456.
- 2. Gonzalez, R.;
   Murrieta-Guevara, F.; Parra, O.;
   Trejo, A., Fluid Phase
   Equilibria, 1987, 34, 69.
- Prausnitz, J.M.; Lichtenthaler, R.N.; Gomes de Azevedo, E. Molecular Thermodynamics of Fluid-Phase Equilibria, 1986 Prentice-Hall, Englewood Cliffs, NJ, USA; Chap. 7.

# 375 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Kassim, D.M.; Zainel, H.A.; Al-Asof, S.A.; Talib, E.K. 2. Tetrahydrothiophene, 1,1-dioxide Fluid Phase Equilibria (Sulfolane); C4H8SO2; [126-33-0] 1988, 41, 287-294. VARIABLES: PREPARED BY: C. L. Young T/K = 303.15-333.15EXPERIMENTAL VALUES: Mole fraction of carbon dioxide in liquid at a partial pressure of 101.3 kPa T/K(1 atm) <sup>x</sup>CO₂ 0.0111 303.15 0.0089 313.15 0.0075 323.15 0.0064 333.15 AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Falling film flow apparatus similar 1. Purity 99.99 mole per cent.

Falling film flow apparatus similar to that of Morrison and Billet (1). Apparatus consisted of (i) degassing section in which solvent could be degassed by freezing and thawing under vacuum and (ii) absorption section. The latter consisted of a gas buret and absorption spiral. Mole fraction solubility corrected to 1 atm partial pressure by assuming Henry's law was valid.

Fluka AG puriss grade sample, purity better than 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta x/x = \pm 0.02$  (estimated by compiler).

# REFERENCES:

Morrison, T.J.; Billet, F.J.
 J. Chem. Soc. <u>1948</u>, 2033.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Tetrahydrothiophene, 1,1dioxide, (Sulfolane); C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S; [126-33-0]

# ORIGINAL MEASUREMENTS:

Roberts, B.E.; Mather, A.E.

Can. J. Chem. Eng. 1988, 67, 519-520.

# VARIABLES:

T/K = 313.15, 373.15P/kPa = 105-5900

# PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

T/K	P/kPa <sup>*</sup>	Mole fraction of CO <sub>2</sub> in solution	Henry's constant, /MPa	H,†
313.15	105 101.3 <sup>¶</sup> 103 185 278	0.00971 0.0094 0.00985 0.01770 0.02610	10.4	-
373.15	249 101.3 <sup>¶</sup>	0.01040 0.0040	25.8	

<sup>\*</sup>The partial pressure of carbon dioxide was approximately equal to the total pressure under the conditions of the measurements.

Measurements were also carried out at higher pressures to a maximum of  $5900\ \mathrm{kPa}$ .

$$H = \lim_{x_1 \to 0} \left[ f_1/x_1 \right]$$

where  $f_1$  = fugacity of  $CO_2$ 

 $x_1$  = mole fraction of  $CO_2$  in solution.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus was similar to that described by Jou et al.(1). sulfolane was introduced into a windowed equilibrium cell in a constant temperature bath. Gas was added until sufficient pressure was reached. The gas was circulated by a magnetic pump and bubbled through the liquid until the pressure remained constant for several hours. The vapor phase was then analysed by gas chromatography. Samples of the liquid phase were withdrawn, added to a solution of sodium hydroxide and the amount of carbon dioxide in the samples found by titration.

# SOURCE AND PURITY OF MATERIALS:

 Sulfolane supplied by Aldrich Chemical Company; purity 99%

ESTIMATED ERROR:  $\delta x_1/x_1 = \pm 2-3\%$  (authors)

# REFERENCES:

Jou, F.-Y.; Mather, A.E.;
 Otto, F.D.
 Ind. Eng. Chem. Process Des. Dev.
 1982, 21, 539.

<sup>¶</sup>Estimated by the compiler on the assumption that the variation of mole fraction solubility with partial pressure of carbon dioxide was approximately linear to a mole fraction solubility of 0.01.

<sup>&</sup>lt;sup>†</sup>Limiting values of Henry's constant estimated by the authors as

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Tetrahydrothiophene, 1,1dioxide (Sulfolane);
  C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>S; [126-33-0]

# ORIGINAL MEASUREMENTS:

Xu, S.; Wang, Y-w.; Otto, F.D.;
Mather, A.E.

J. Chem. Tech. Biotechnol. 1991, 51, 197-208.

# VARIABLES:

T/K = 303.2-359.9 $P/kPa \simeq 100$ 

# PREPARED BY:

P.G.T. Fogg

# **EXPERIMENTAL VALUES:**

t/°C	T/K	Solubility /kPa m³ kmol-1	$x_{\text{CO}_2}$ at $P_{\text{CO}_2}$ = 101.3 kPa *
30.0	303.2	911.9	0.01050
40.2	313.4	1116.1	0.00866
55.4	328.6	1429.3	0.00684
70.5	343.7	1806.9	0.00548
86.7	359.9	2276.7	0.00442

<sup>\*</sup> estimated by the compiler.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus was similar to that described by Haimour and Sandall (1) which consisted essentially of a glass flask maintained at constant temperature connected to a gas buret. The flask was first purged with gas under test. A measured volume of solvent was then injected into the flask. The flask was mechanically shaken and the reduction of volume of gas in the gas buret recorded.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide supplied by Union Carbide Canada Ltd.; purity at least 99.9%
- Sulfolane supplied by Aldrich Chemical Company; purity 99%

# ESTIMATED ERROR:

 $\delta(\text{solubility}) = \pm 2\%$  (authors)

#### REFERENCES:

 Haimour, N.; Sandall, O.C. Chem. Eng. Sci. 1984, 33, 29.

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] Woukoloff, (No initial given) (2) Carbon disulfide; CS<sub>2</sub>; [75-15-0] Comptes rendus 1889, 108, 674 - 675. VARIABLES: T/K = 280.23 - 293.74 P<sub>1</sub>/kPa = 13.48 - 63.73 (101.11 - 478.25 mmHq)

EXPERIMENTAL VALUES:

Temp	erature	Carbon Dioxide	Carbon Dioxide	Pungon
t/ºC	T/K	Pressure p <sub>1</sub> /mmHg	Absorption A/cm³(STP) cm <sup>-3</sup>	Bunsen Coefficient α/cm³(STP)cm <sup>-1</sup> atm <sup>-1</sup>
7.08	280.23	452.93	0.84818	1.423
7.1	280.25	185.5	0.33395	1.368
13.04	286.19	478.05	0.84427	1.342
13.04	286.19	195.8 ¹	0.33244	1.290
20.53	293.68	410.25	0.67281	1.246
20.59	293.74	101.11	0.16723	1.257

 $<sup>^{\</sup>rm 1}$  The pressure in the paper is given as 918.5 mmHg, however, other values in the paper indicate it should be 195.8 mmHg.

The Bunsen coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No information.	(1) Carbon dioxide. No information.
Although the author does not describe the method, he does clearly state that the volume of gas absorbed is reduced to the standard conditions of 0 $^{\circ}$ C and 760 mmHg.	(2) Carbon disulfide. Specified as 880 <sup>gr</sup> .
	ESTIMATED ERROR:
	REFERENCES:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Carbon disulfide; CS<sub>2</sub>; [75-15-0]

# ORIGINAL MEASUREMENTS:

Just, G.

Z. Phys. Chem. 1901, 37, 342 - 367.

# VARIABLES:

T/K = 288.15 - 298.15 $p_1/kPa = 101.325$  (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

#### EXPERIMENTAL VALUES:

<i>T/</i> K	Mol Fraction $10^3 x_1$	Bunsen Coefficient a/cm³(STP)cm⁻³atm⁻¹	Ostwald Coefficient L/cm³cm-3
288.15	2.39	0.895	0.9446
293.15	2.22	0.828	0.8888
298.15	2.15	0.797	0.8699

The author measured the Ostwald coefficient at a pressure of about 746 mmHg. The compiler assumed the Ostwald coefficient to be independent of pressure, and calculated the mole fraction and Bunsen coefficient values at 101.325 kPa (1 atm) partial pressure of the gas.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

An Ostwald apparatus as modified by Timofejew (1), and Steiner (2) is used. The apparatus consists of a gas buret, an absorption flask, and a mercury manometer. The system is thermostated with a water jacket.

The gas is introduced into the degassed liquid. The gas volume absorbed is determined by the gas buret. The solvent volume is determined at the end of the experiment by pouring the solvent into a graduated flask.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Generated in a Kipp apparatus using marble and hydrochloric acid.
- (2) Carbon disulfide. No information.

# ESTIMATED ERROR:

 $\delta L/L = 0.03$  (compiler)

- 1. Timofejew, W. Z. Phys. Chem. 1890, 6, 141.
- Steiner, P.
   Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Carbon disulfide; CS<sub>2</sub>; [75-15-0]

### ORIGINAL MEASUREMENTS:

Gjaldbaek, J. C.

Acta Chem. Scand. 1953, 7, 537 - 544.

# VARIABLES:

$$T/K = 298.05 - 298.45$$
  
 $p_1/kPa = 101.325$  (1 atm)

#### PREPARED BY:

J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

T/K	Carbon Dioxide Pressure p <sub>1</sub> /mmHg	Mol Fraction <sup>1</sup> 10 <sup>3</sup> x <sub>1</sub>	Bunsen Coefficient α/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald- Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.05	433.0	3.30	1.21	1.32
298.35	394.8	3.30	1.21	1.32
298.45	479.2	3.33	1.22	1.33

The mole fraction solubility values were adjusted to a gas partial pressure of 101.325 kPa by the compiler assuming that Henry's law is obeyed.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as confining liquid. The solvent was degassed in the apparatus.

The absorbed volume of gas is calculated from the initial and final amounts, both saturated with solvent vapor. The amount of solvent is determined by the weight of displaced mercury.

The mole fraction solubility values are at 1 atm assuming Henry's law is obeyed.

Details of the apparatus and procedure are given in ref. 1 and 2.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Prepared from potassium bicarbonate (analytical reagent) and concentrated sulfuric acid. 99.9 per cent CO<sub>2</sub>.
- (2) Carbon disulfide. Merck and Co. Analytical reagent. B.p. (760 mmHg)/°C = 46.21 - 46.26.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.05$$
  
 $\delta x_1/x_1 = \pm 0.015$ 

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. <u>1952</u>, 6, 623.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Carbon disulfide; CS<sub>2</sub>; [75-15-0]

# ORIGINAL MEASUREMENTS:

Kobatake, Y.; Hildebrand, J. H.

J. Phys. Chem. 1961, 65, 331 - 335.

VARIABLES:

T/K: 281.65 - 306.36 P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick

H. L. Clever

#### **EXPERIMENTAL VALUES:**

Tempe	rature	Mol Fraction	Bunsen Coefficient	Ostwald Coefficient
t/°C	T/K	10 <sup>3</sup> x <sub>1</sub>	$\alpha/\text{cm}^3$ (STP) cm <sup>-3</sup> atm <sup>-1</sup>	$L/\text{cm}^3$ cm $^{-3}$
8.50	281.65	3.785	1.431	1.476
16.55	289.70	3.538	1.325	1.405
25.00	298.15	3.280	1.22	1.33
33.21	306.36	3.020	1.11	1.24

The Bunsen and Ostwald coefficients were calculated by the compiler. Smoothed Data: For use between 281.65 and 306.36 K.

$$\ln x_7 = -8.3618 + 7.8588/(T/100K)$$

The standard error about the regression line is  $2.64 \times 10^{-5}$ .

T/K	Mol Fraction	
	10 <sup>3</sup> x <sub>1</sub>	
283.15	3.749	
288.15	3.573	
293.15	3.410	
298.15	3.260	
303.15	3.122	

# AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: consists of a gas measuring buret, an absorption pipet, and a reservoir for the solvent. The buret is thermostated at 25°C, the pipet at any temperature from 5 to 30°C. The pipet contains an iron bar in glass for magnetic stirring. The pure solvent is degassed by freezing with liquid nitrogen, evacuating, then boiling with a heat lamp. The degassing process is repeated three times. The solvent is flowed into the pipet where it is again boiled for final degassing. Manipulation of the apparatus is such that the solvent never comes in contact with The liquid in the stopcock grease. pipet is sealed off by mercury. Its volume is the difference between the capacity of the pipet and the volume of mercury that confines it. Gas is admitted into the pipet. Its exact amount is determined by P-V measurements in the buret before and after

- The apparatus SOURCE AND PURITY OF MATERIALS:
  - (1) Carbon dioxide. California Dry Ice Co. Standard grade. Dried by passing through a trap at dry ice-acetone temperature, and tubes containing CaCl2 then P2O5. The dried gas was distilled at liquid N2 temperature several times.
  - (2) Carbon disulfide. Mallinckrodt Chemical Works. Analytical Reagent grade. Shaken successively with Hg and HgCl2, filtered, distilled, and stored over Hg more than 5 days before use.

ESTIMATED ERROR:

$$\delta T/K = 0.02$$
  
 $\delta x_1/x_1 = 0.003$ 

The stirrer is set in motion. introduction of the gas into the pipet. Equilibrium is attained within 24 hours.

# 382 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] Dymond, J. H. (2) Sulfinylbismethane or dimethyl J. Phys. Chem. 1967, 71, 1829-1831. sulfoxide; C<sub>2</sub>H<sub>6</sub>OS (CH<sub>3</sub>SOCH<sub>3</sub>); [67-68-5] **VARIABLES:** PREPARED BY: T/K: 298.15 M. E. Derrick p/kPa: 101.325 (1 atm) H. L. Clever EXPERIMENTAL VALUES: T/K Mol Fraction Bunsen Ostwald $10^{\overline{3}}x_1$ Coefficient $\alpha/cm^3$ (STP) $cm^{-3}$ atm<sup>-1</sup> Coefficient $L/\text{cm}^3\text{cm}^{-3}$ 298.15 9.08 3.14 The Bunsen and Ostwald coefficients were calculated by the compiler.

#### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The liquid is saturated with the gas at a gas partial pressure of 1 atm.

The apparatus is that described by Dymond and Hildebrand (1). The apparatus uses an all-glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressure.

## SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Western Gas, Inc. Dried.
- (2) Dimethylsulfoxide. Matheson, Coleman and Bell Co. Spectroquality. Dried and fractionally frozen. m.p. 18.37°C.

ESTIMATED ERROR:

### REFERENCES:

Dymond, J.; Hildebrand, J. H.
 *Ind. Eng. Chem. Fundam.* 1967,
 6, 130.

# 383 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Lenoir, J-Y.; Renault, P.; Renon, H. Sulfinylbismethane; J. Chem. Eng. Data, 1971, 16, 340-2. (Dimethylsulfoxide); C,H,SO; 167-68-51 VARIABLES: PREPARED BY: T/K = 298.2C. L. Young EXPERIMENTAL VALUES: Mole fraction at 101.3 kPa (1 atm)\* Henry's constant T/KH<sub>co,</sub>/atm xco, 298.2 106 0.00943 Calculated by compiler assuming a linear function of $p_{CO_2}$ vs $x_{CO_2}$ , ie, $x_{CO_2}$ (1 atm) = 1/ $H_{CO_2}$ AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: A conventional gas-liquid chromato-L'Air Liquide sample, minimum

graphic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

- purity 99.9 mole per cent.
- (2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta H/atm = \pm 6$ % (estimated by compiler).

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. Mixed Solvents

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

Solubility of carbon dioxide in mixed solvents

Sichkova and co-workers (1,2) have measured the solubility of carbon dioxide in solutions of 2-aminoethanol in various organic solvents. Measurements on solutions in methanol were made at partial pressures of carbon dioxide from 6.7 kPa to 101.3 kPa, temperatures from 223.2 K to 293.2 K and concentrations of 2-aminoethanol of 5, 15 and 18 wt%. At a fixed temperature and a fixed concentration of 2-aminoethanol there is relatively little change in the mole fraction solubility of carbon dioxide with change in pressure over the pressure range studied. At 293.2 K and 15 wt% of 2-aminoethanol the mole fraction solubility at 6.7 kPa is 0.0391 and at 101.3 kPa is 0.0629. This behaviour is similar to that of aqueous solution of aminoalkanols. At a fixed partial pressure of carbon dioxide and a fixed temperature, extrapolation of mole fraction solubility of carbon dioxide to zero concentration of 2-amimoethanol gives a solubility close to that predicted from the smoothing equation recommended for solubility in methanol (see page 128). Solutions of 2-aminoethanol in other solvents were studied at one concentration of 2-aminoethanol (2.5 mol  $dm^{-3}$ ) and, in most cases, at one temperature, 293.2 K, only. The nature of the solvent affects the absorption of carbon dioxide to some extent. At 293 K, 99.1 kPa the solubility in benzenemethanol solution is 30.7 cm $^3$  gas (corrected to 101.3 kPa and 273.2 K)/cm $^3$  of solvent. The corresponding solubility in N, N-dimethylformamide solution at 98 kPa is 40.6 cm<sup>3</sup>/cm<sup>3</sup>. There is no reason to doubt the reliability of the measurements on 2-aminoethanol solutions reported by Sichkova and co-workers. The data may be accepted on a provisional basis.

Rivas and Prausnitz (3) measured solubility in solutions of 2-aminoethanol in 1-methyl-2-pyrrolidinone. This system was also studied by Sichkova et al. Data are presented in the form of small scale graphs. The graph for solutions containing 3 and 5 wt% of 2-aminoethanol shows the variation of mole fraction of carbon dioxide with partial pressure of carbon dioxide for each solution. A second graph for a solution of 15 wt% of aminoethanol shows the variation of moles of  $\mathrm{CO}_2/\mathrm{dm}^3$  with partial pressure of carbon dioxide. The first graph indicates that absorption of carbon dioxide per unit volume of solvent increases with concentration of 2-aminoethanol whereas the second graph indicates that the absorption in the 15 wt% solution is less than in the 5% solution for the same partial pressure of carbon dioxide. In the opinion of the evaluator the second graph should also be labelled to show the variation of mole fraction solubility of carbon dioxide with partial pressure of gas. The variation is then in accord with the variation in solubility in a solution of approximately 13 wt% reported by Sichkova et al.

Rivas and Prausnitz (4) also measured the solubility of carbon dioxide in a solution of 2-(2-aminoethoxy)-ethanol at 263.1 K and 298.3 K and pressures from 7.9 kPa to 35.0 kPa. These data are consistent with data for solutions of 2-aminoethanol.

Takahashi et al.(5) measured solubility of carbon dioxide in benzene, tetrachloromethane, 1-propanol, 1-octanol, 2-methyl-1-propanol and formamide and mixtures of pairs of these solvents. They used an indirect method in which the rate of absorption of gas was measured. The solubility data for the pure solvents are low compared with values found by other workers using conventional methods. The mole fraction solubility in ethanol at 298.2 K; 101.3 kPa from this work is 0.00624 compared with a smoothed value from other sources of 0.00727. The value for benzene is 0.00824 compared with a smoothed value of 0.00927. Viscosity of mixtures was also measured. The authors found a correlation between the variation of their solubility values and variation of viscosity as composition of a mixture was varied.

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. Mixed Solvents

#### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

Koudelka (6) measured solubilities in pure samples of methanol, 2-propanone, trichloromethane, and benzene and in mixtures of pairs of these solvents. Measurements were carried out at 293.15 K and data given for a partial pressure of gas of 101.3 kPa. Solubility data on the pure solvents are in good accord with data obtained by other workers. It is therefore likely that data for the mixtures are reliable. In all cases the variation of mole fraction solubility of carbon dioxide with molar composition of the mixed solvent lay on smooth curves. In one case, that of mixtures of methanol and trichloromethane, the mole fraction solubility of carbon dioxide passes through a minimum.

Byrne et al.(7) measured Ostwald coefficients for dissolution of carbon dioxide in solutions of cephalin, lecithin or cholesterol in benzene. In each case the Ostwald coefficient was lower than the value for pure benzene. Similar measurements were made of the solubility of cholesterol in 2-methyl-1-propanol but, in this case, the added solid did not affect the value of the Bunsen coefficient. There is no reason to doubt the reliability of this work but no other measurements on these systems are available for comparison.

Rosenthal (8) measured the effects on the solubility of carbon dioxide of adding polymeric material to various solvents. Cellulose acetate lowered the Ostwald coefficient for dissolution in N,N-dimethylformamide and for dissolution in 2-propanone. Polystyrene and polyisobutylene both lowered the coefficient for dissolution in benzene. Polyacrylonitrile raised the coefficient for dissolution in N,N-dimethylformamide. In all cases the effects were small. The addition of 0.0987 g of polystyrene of relative molecular mass 180 000 lowered the Ostwald coefficient for dissolution in benzene from 2.66 to 2.44 at 293.15 K. No similar measurements are available to confirm these results. However the measurements of solubility in the pure liquids, in the absence of polymeric material, which was carried out as part of the same research, are in good agreement with measurements by other workers.

Rosenthal (8) measured the solubility of carbon dioxide in solutions of sodium iodide in 2-propanone. The molal concentration of sodium iodide varied from 0.55 to 2.07. Ostwald coefficients decreased with addition of sodium iodide with the Sechenov constant ranging from 0.119 to 0.129. Addition of sodium iodide to N,N-dimethylformamide also reduced the Ostwald coefficient of carbon dioxide. The Sechenov constant for a solution saturated with sodium iodide, calculated from the solubility measurements, is 0.199. These measurements appear to be reliable but need confirmation.

Rosenthal (8) also investigated the effect of adding octadecanoic acid to 2-propanone and to N,N-dimethylformamide. The Ostwald coefficient for solutions in N,N-dimethylformamide passed through a maximum with increasing concentration of octadecanoic acid. Perhaps this behaviour was due to an increasing formation of micelles as the concentration of octadecanoic acid was increased. Addition of octadecanoic acid caused a decrease in the Ostwald coefficient for dissolution in 2-propanone at the two concentrations of acid which were studied. Addition of a mole fraction of 0.00506 of acid to 2-propanone caused the Ostwald coefficient to fall from 6.88 to 5.01. Further addition to give a mole fraction of acid of 0.00805 caused a much smaller fall in the Ostwald coefficient to 4.93. These systems would bear re-investigation.

Kosakewitsch (9) measured solubility at 288.15 K and a partial pressure of 101.3 kPa in methanol containing various proportions of lithium chloride, bromide or iodide or sodium iodide. Maximum mole ratios of salt to

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Mixed Solvents

#### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

methanol were LiCl:0.0917, LiBr:0.1031, LiI:0.0241, NaI:0.0835. The solubility in solutions of these salts in ethanol at 293.15 K and 101.3 kPa was also measured. Maximum mole ratios in this case were LiCl:0.1511, LiBr:0.0642, LiI:0.1040, NaI:0.0844. The evaluator has found that plots of ln(mole ratio solubility) against the mole ratio concentration of salt in methanol are close to straight lines. Under these conditions solubility in methanol approximates to a Sechenov type relationship i.e.

 $ln(mole ratio CO_2/CH_3OH) = A - B(mole ratio MX/CH_3OH)$ 

(MX = salt; A & B are constants) Addition of salt decreases the solubility of the gas in each case and there is negligible differences between the effects of the different salts. The value of A is -4.798. The average value of B is 7.368.

Solubility in ethanol follows similar relationships to a maximum mole ratio of salt to ethanol of about 0.06. The value of A is -4.869. The value of B is about 6.173 for LiCl, LiBr and NaI but is about 8.193 for LiI. The values of B decrease at higher concentrations of salt.

No other measurements of the solubility of carbon dioxide in solutions of salts in methanol or ethanol are available to the evaluator for a direct comparison. However there is good agreement between the author's values of solubility in pure methanol and in pure ethanol and values reported by other workers. The mole fraction solubility in methanol at 288.15 K from Kosakewitsch's work is 0.00818. The value from the smoothing equation given by the evaluator on page 128 is  $0.0080 \pm 0.0014$ . The mole fraction solubility in ethanol at 293.15 K from the work is 0.00762 compared with a value of  $0.00789 \pm 0.00002$  from the equation for solubility in ethanol on page 128.

- Sichkova, O.P.; Shinelis, A.F.; Leites, I.L. Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin. 1972, No.17, 125-135.
- Sichkova, O.P.; Shinelis, A.F.; Voskresenskaya, N.S.; Leites, I.L. Khim. Prom. (Moscow) 1984, (4), 207-209.
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- 9. Kosakewitsch, P.P. Zeit. Phys. Chem. (A) 1929, 143, 216-224.

- Carbon dioxide; CO2; [124-38-9]
- 2. 2-Aminoethanol, (monoethanolamine); C2H7NO; [141-43-5]
- Methanol; CH<sub>4</sub>O; [67-56-1] З.

#### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Voskresenskaya, N.S.; Leites, I.L.

Khim. Prom. (Moscow) 1984, (4), 207-209.

## VARIABLES:

T/K = 223.2-293.2P/kPa = 0-103 kPawt% MEA = 5-18

#### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

Wt% ME	ea <sup>§</sup> T/K	density of solvent /g cm <sup>-3</sup>	P CO <sub>2</sub> /mmHg	PCO <sub>2</sub> /kPa	Solubility <sup>†</sup> S	<sup>x</sup> CO₂*
5	223.2	0.8650 0.8650	50 100	6.7 13.3	16.9 19.2	0.0280
		0.8650	300	40.0	27.7	0.0451
		0.8650	600	80.0	40.4	0.0644
		0.8650	760	101.3	47.2	0.0746
	243.2	0.8465	50	6.7	15.0	0.0255
		0.8465	100	13.3	16.1	0.0272
		0.8465	300	40.0	19.8	0.0334
		0.8465	600	80.0	25.8	0.0431
		0.8465	760	101.3	28.7	0.0477
	263.2	0.8264	50	6.7	11.8	0.0207
		0.8264	100 300	13.3 40.0	13.6 16.4	0.0237 0.0285
		0.8264 0.8264	600	80.0	20.1	0.0265
		0.8264	760	101.3	22.0	0.0377
	273.2	0.8181	50	6.7	10.7	0.0189
	2:3.2	0.8181	100	13.3	12.0	0.0212
		0.8181	300	40.0	14.6	0.0256
		0.8181	600	80.0	17.8	0.0312
		0.8181	760	101.3	19.6	0.0342

 $<sup>\</sup>S$  wt% of monoethanolamine (MEA) in the solvent before addition of CO<sub>2</sub>

#### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The authors used a static method described in ref. (1). Two small scale graphs (7.5 cm  $\times$  7 cm;  $8 \text{ cm} \times 5 \text{ cm}$ ) showing experimental values of S at closely spaced pressures for the temperatures and solvent mixtures under investigation. Smooth curves were drawn through the experimental points. The compiler has measured the positions of these lines at five arbitrary pressures to Obtained the values of S given above.

### SOURCE AND PURITY OF MATERIALS:

- Purity at least 99.93%
   Vacuum distilled; no impurities detected by chromatography.
- Fractionally distilled;
   b.pt. (101.3 kPa) = 64.4-64.5°C
   ρ (20°C) = 0.7925 g cm<sup>-3</sup> refractive index within 0.1% of the value in the literature.

### ESTIMATED ERROR:

 $\delta S \simeq \pm 1.5\%$  (authors)

 $\delta S = \pm 0.3$  (compiler - error in measurements from the graphs)

### REFERENCES:

 Sichkova, O.P.; Shinelis; A.F. Leites, I.L. Trudy GIAP, 1972, 17, 125.

volume of gas (reduced to 273.2 K and 101.3 kPa) absorbed by one volume of solvent; taken from graphs given in the paper.

calculated by the compiler

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Aminoethanol,
   (monoethanolamine); C<sub>2</sub>H<sub>7</sub>NO;
   [141-43-5]
- 3. Methanol; CH<sub>4</sub>O; [67-56-1]

### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Voskresenskaya, N.S.; Leites, I.L.

Khim. Prom. (Moscow) 1984, (4), 207-209.

### EXPERIMENTAL VALUES:

Wt% ME	A <sup>§</sup> T/K	density of solvent /g cm <sup>-3</sup>	<sup>P</sup> CO₂ /mmHg	<sup>P</sup> CO₂ /kPa	Solubility <sup>†</sup> S	X <sub>CO2</sub> *
5	283.2	0.8109 0.8109 0.8109 0.8109 0.8109	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	9.0 10.4 13.6 16.4 17.8	0.0161 0.0186 0.0242 0.0290 0.0314
	293.2	0.7990 0.7990 0.7990 0.7990 0.7990	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	7.5 9.1 12.1 14.7 16.0	0.0137 0.0165 0.0219 0.0265 0.0286
15	223.2	0.8872 0.8872 0.8872 0.8872 0.8872	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	46.3 49.9 58.1 68.0 71.2	0.0749 0.0803 0.0927 0.1063 0.1107
	243.2	0.8700 0.8700 0.8700 0.8700 0.8700	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	40.2 43.4 49.5 55.2 58.1	0.0668 0.0718 0.0817 0.0897 0.0938
	263.2	0.8528 0.8528 0.8528 0.8528 0.8528	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	29.6 34.0 39.5 45.3 48.2	0.051 0.058 0.067 0.076 0.080
	273.2	0.8443 0.8443 0.8443 0.8443 0.8443	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	13.0 28.5 36.7 35.8 43.7	0.023 0.049 0.063 0.061 0.074
	283.2	0.8357 0.8357 0.8357 0.8357 0.8357	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	22.5 27.7 33.6 37.9 39.7	0.0400 0.0489 0.0588 0.0657
	293.2	0.8273 0.8273 0.8273 0.8273 0.8273	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	21.7 25.7 30.5 34.2 35.8	0.039 0.046 0.054 0.0602 0.0629
18	293.2	0.8337 0.8337 0.8337 0.8337 0.8337	50 100 300 600 760	6.7 13.3 40.0 80.0 101.3	27.6 31.4 36.0 39.7 41.8	0.0495 0.0555 0.0637 0.0698 0.0732

 $<sup>\</sup>S$  wt% of monoethanolamine (MEA) in the solvent before addition of  $CO_2$ 

<sup>&</sup>lt;sup>†</sup> volume of gas (reduced to 273.2 K and 101.3 kPa) absorbed by one volume of solvent; taken from graphs given in the paper.

<sup>\*</sup> calculated by the compiler

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2-Aminoethanol, (monoethanolamine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]
- Various organic compounds

#### VARIABLES:

T/K = 293.2-323.2P/kPa = 1.2-102.7

### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Leites, I.L.

Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin. 1972, No 17, 125-135.

### PREPARED BY:

P.G.T. Fogg

#### EXPERIMENTAL VALUES:

The solvent, in each case, consisted of ethanolamine (concentration  $2.5~\text{mol}~\text{dm}^{-3}$ ) plus component 3.

Measurements were given as points on small scale graphs (approx.

6 cm × 8 cm) Component 3	T/K	P/mmHg	P/kPa	Solubility*
1,2-Ethanediol, (ethylene glycol); C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> ; [107-21-1]	293.15	56 130 380 390 500 672	7.5 17.3 50.7 52.0 66.7 89.6	30.6 32.7 36.2 35.8 36.8 37.9
2,2'[1,2-Ethanediylbis- (oxy)]bisethanol, (triethylene glycol); C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> ; [112-27-6]	293.15	80 355 379 541 735	10.7 47.3 50.5 72.1 98.0	29.1 32.0 32.2 33.5 34.7

<sup>\*</sup> solubilities were reported as volumes of gas (corrected to 273.15 K and 101.325 kPa) absorbed by one volume of the mixed solvent under the stated conditions.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A sample of the mixture under test was placed in an absorbtion bulb fitted with a magnetic stirrer. mixture was frozen and degassed under vacuum. The bulb was then maintained at the required temperature by thermostatic control. The vapor pressure of the solvent mixture was measured. Appropriate taps were then opened to allow carbon dioxide from one or more bulbs of known volume to come into contact with the sample. The pressure of gas before and after coming into Contact with the liquid was measured With mercury manometers. Allowance was made for the volumes of various connecting tubes in the calculation of the quantity of carbon dioxide absorbed by the liquid.

## SOURCE AND PURITY OF MATERIALS:

- 2. distilled; purity checked by measurement of the refrective index which differed by less than 0.1% from the value quoted in the literature.
- 3. fractionally distilled under vacuum; refractive indices differed by less than 0.1% from literature values.

### ESTIMATED ERROR:

 $\delta$ (solubility) = ±0.3 (compiler's estimated error in reading values from the graphs supplied)

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Aminoethanol, (monoethanol-amine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]
- 3. Various organic compounds

#### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Leites, I.L.

Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin. 1972, No 17, 125-135.

### EXPERIMENTAL VALUES:

The solvent, in each case, consisted of ethanolamine (concentration 2.5 mol  $\mbox{dm}^{-3}$  ) plus component 3.

Component 3	T/K	P/mmHg	P/kPa	Solubility*
2,2'-[Oxylbis(2,1-ethane-diyloxy)]bisethanol, (tetraethylene glycol): C <sub>8</sub> H <sub>18</sub> O <sub>5</sub> ; [112-60-7]	293.15	131 215 335 485 755	17.5 28.7 44.7 64.7 100.7	29.9 31.0 31.9 32.8 34.2
2,2'-Oxybisethanol, (diethylene glycol); C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> ; [111-46-6]	293.15	81 175 366 543 708	10.8 23.3 48.8 72.4 94.4	28.1 29.9 31.2 32.7 33.5
Oxybispropanol, (dipropylene glycol); C <sub>6</sub> H <sub>1</sub> 4O <sub>3</sub> ; [25265-71-8]	293.15	30 186 335 525 669	4.0 24.8 44.7 70.0 89.2	26.1 29.1 30.2 30.9 31.6
1,3-Propanediol, (propylene glycol), C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> ; [26264-14-2]	293.15	32 51 165 223 365 475 566	4.3 6.8 22.0 29.7 48.7 63.3 75.5 89.3	28.4 28.5 30.7 30.7 32.1 32.6 32.9 33.3
2,3-Butanediol; C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> ; [513-85-9]	293.15	9 131 255 415 509 615 770	1.2 17.5 34.0 55.3 67.9 82.0	25.8 28.7 29.8 30.6 31.0 31.4 32.2
1,3-Butanediol; C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> ; [107-88-0]	293.15	16 45 70 81 155 161 300 349 500 530 650 720	2.1 6.0 9.3 10.8 20.7 21.5 40.0 46.5 66.7 70.7 86.7 96.0	25.3 26.7 26.9 27.3 28.5 28.1 29.5 29.8 30.5 30.8 31.3 31.6

 $<sup>^{*}</sup>$  solubilities were reported as volumes of gas (corrected to 273.15 K and 101.325 kPa) absorbed by one volume of the mixed solvent under the stated conditions.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Aminoethanol, (monoethanolamine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]
- 3. Various organic compounds

### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Leites, I.L.

Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin. 1972, No 17, 125-135.

### EXPERIMENTAL VALUES:

The solvent, in each case, consisted of ethanolamine (concentration 2.5 mol  $\mbox{dm}^{-3}$  ) plus component 3.

Component 3	T/K	P/mmHg	P/kPa	Solubility*
Methanol; CH4O; [67-56-1]	293.15	28 80 300 496 499 589	3.7 10.7 40.0 66.1 66.5 78.5	24.5 30.4 36.0 38.8 39.1 40.1
Tetrahydro-2-furanmethanol, (tetrahydrofurfuryl alcohol) C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> ; [97-99-4]	293.15 ;	10 50 135 222 260 373 431 623 741	1.3 6.7 18.0 29.6 34.7 49.7 57.5 83.1 98.8	24.9 26.4 27.6 29.2 29.3 29.7 30.3 31.7 32.4
Benzenemethanol, (benzyl alcohol); C <sub>7</sub> H <sub>8</sub> O; [100-51-6]	293.15	25 65 89 214 239 353 400 575 743	3.3 8.7 11.9 28.5 31.9 47.1 53.3 76.7 99.1	23.4 25.4 26.3 27.7 27.7 28.7 28.8 30.0 30.7
2-Methoxyethanol, (ethylene glycol monomethyl ether); C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> ; [109-86-4]	293.15	14 25 45 85 200 353 406 512 631 651	1.9 3.3 6.0 11.3 26.7 47.1 54.1 68.2 84.1 86.8 92.1	26.4 26.3 28.3 29.3 30.9 32.1 32.4 33.1 33.7 34.3

 $<sup>^{*}</sup>$  solubilities were reported as volumes of gas (corrected to 273.15 K and 101.325 kPa) absorbed by one volume of the mixed solvent under the stated conditions.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Aminoethanol, (monoethanol-amine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]
- 3. Various organic compounds

### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Leites, I.L.

Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin. 1972, No 17, 125-135.

### EXPERIMENTAL VALUES:

The solvent, in each case, consisted of ethanolamine (concentration 2.5 mol  $\mbox{dm}^{-3}\,)$  plus component 3.

Component 3	T/K	P/mmHg	P/kPa	Solubility*
1-Methyl-2-pyrrolidinone, (N-Methylpyrrolidone); C <sub>5</sub> H <sub>9</sub> NO; [872-50-4]	303.15	22 55 115 235 344 400 556 700	2.9 7.3 15.3 31.3 45.9 53.3 74.1 93.3	27.3 29.3 30.8 33.1 34.1 34.7 35.9 37.1
	323.15	29 63 110 200 451 612	3.9 8.4 14.7 26.7 60.1 81.6	23.4 27.5 26.6 28.7 31.5 32.8
N,N-Dimethylacetamide; C4H9NO; [127-19-5]	293.15	15 32 119 180 287 350 383 414 509 528 663	2.0 4.2 15.9 24.0 38.2 46.7 51.1 55.2 67.9 70.4 88.4	27.2 30.4 33.5 34.9 36.4 37.1 37.9 38.4 38.7 38.9
N,N-Dimethylformamide; C <sub>3</sub> H <sub>7</sub> NO; [68-12-2]	293.15	7 119 170 214 233 254 272 394 413 552 565 669 735	0.9 15.9 22.7 28.5 31.0 33.8 36.2 52.5 55.1 73.6 75.4 89.1 98.0	26.6 32.4 33.5 34.7 34.8 34.7 35.4 36.9 37.0 39.3 38.8 39.2 40.6

 $<sup>^{*}</sup>$  solubilities were reported as volumes of gas (corrected to 273.15 K and 101.325 kPa) absorbed by one volume of the mixed solvent under the stated conditions.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 2-Aminoethanol, (monoethanolamine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]
- 3. Various organic compounds

### ORIGINAL MEASUREMENTS:

Sichkova, O.P.; Shinelis, A.F.; Leites, I.L.

Tr. Nauch.-Issled. Proekt. Inst. Azotn. Prom. Prod. Org. Sin. 1972, No 17, 125-135.

#### EXPERIMENTAL VALUES:

The solvent, in each case, consisted of ethanolamine (concentration 2.5 mol  $\mbox{dm}^{-3}$  ) plus component 3.

Component 3	T/K	P/mmHg	P/kPa	Solubility*
2-(2-Methoxyethoxy)ethanol, (diethylene glycol monomethy ether); C <sub>5</sub> H <sub>12</sub> O <sub>3</sub> ; [111-77-3]	293.15 1	31 65 135 160 244 332 451 546 677	4.1 8.7 18.0 21.4 32.6 44.3 60.1 72.8 90.2 99.4	27.6 28.2 29.6 30.1 30.9 31.6 32.2 32.8 33.6 34.2
2-Phenoxyethanol, (ethylene glycol monophenyl ether); C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> ; [122-99-6]	293.15	29 40 80 159 216 314 346 522 661	3.9 5.3 10.7 21.2 28.8 41.9 46.2 69.5 88.1	22.3 25.5 26.7 27.5 -28.1 28.7 29.0 29.7 30.4
2-Pyrrolidinone; C <sub>4</sub> H <sub>7</sub> NO; [616-45-5]	293.15	11 32 74 110 165 374 506 541 660	1.5 4.3 9.9 14.7 22.0 49.9 67.5 72.1 88.0	29.1 30.5 31.8 32.8 33.9 35.7 36.7 37.1
1-Methyl-2-pyrrolidinone, (N-Methylpyrrolidone); C <sub>5</sub> H <sub>9</sub> NO; [872-50-4]	293.15	16 55 140 185 237 315 455 555	2.1 7.3 18.7 24.7 31.6 42.0 60.7 74.0 91.9	23.8 31.8 34.4 35.2 36.1 37.1 38.6 39.7 40.8

<sup>\*</sup> solubilities were reported as volumes of gas (corrected to 273.15 K and 101.325 kPa) absorbed by one volume of the mixed solvent under the stated conditions.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Methyl-2-pyrrolidinone; C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]
- 2-Aminoethanol, (monoethanolamine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]

#### ORIGINAL MEASUREMENTS:

Rivas, O.R.; Prausnitz, J.M.

Am. Inst. Chem. Engnrs. J. <u>1979</u>, 25, 975-984.

### VARIABLES:

T/K = 298.15-373.15P/kPa < 101.3

### PREPARED BY:

P.G.T. Fogg

## EXPERIMENTAL VALUES:

EXPERIMENTAL  T/K	VALUES: Wt% MEA <sup>†</sup>	P <sub>CO2</sub> /kPa	Solubility of CO <sub>2</sub> * /mol dm <sup>-3</sup>
298.15	3	0 25 50 75 100 125 150 175 200	0.0200 0.0328 0.0420 0.0480 0.0530 0.0580 0.0610 0.0640 0.0680
298.15	5	0 25 50 75 100 125 150 175 200	0.0400 0.0532 0.0608 0.0666 0.0726 0.0770 0.0810 0.0850 0.0886

<sup>\*</sup> data were presented in the form of smooth curves on a small scale graph (5.5 cm  $\times$  8.0 cm). The compiler has measured the co-ordinates at arbitrary points on the curves.

### AUXILIARY INFORMATION:

### METHOD/APPARATUS/PROCEDURE:

The apparatus is described in ref. (1). The volume of gas absorbed was measured. Pressures were measured with a high precision bourdon pressure gauge. Temperatures were controlled to 0.05 K by a thermostat bath.

## SOURCE AND PURITY OF MATERIALS:

Supplied by standard laboratory reagent suppliers; purities at least 99%

## ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ 

### REFERENCES:

1. Rivas, O.R.; Prausnitz, J.M.

Ind. Eng. Chem. Fundam. 1979, 18, 289-292.

<sup>†</sup> MEA = 2-aminoethanol (monoethanolamine)

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. 1-Methyl-2-pyrrolidinone; C<sub>5</sub>H<sub>9</sub>NO; [872-50-4]
- 3. 2-Aminoethanol, (monoethanol-amine); C<sub>2</sub>H<sub>7</sub>NO; [141-43-5]

### ORIGINAL MEASUREMENTS:

Rivas, O.R.; Prausnitz, J.M.

Am. Inst. Chem. Engnrs. J. 1979, 25, 975-984.

### EXPERIMENTAL VALUES:

T/K	Wt% MEA <sup>†</sup>	P <sub>CO2</sub> /kPa	Solubility of CO <sub>2</sub> * /mol dm <sup>-3</sup>
298.15	15	0 25 50 75 100 125 150	0.0637 0.1168 0.1430 0.1600 0.1735 0.1848 0.1958 0.2053
373.15	15	0 25 50 75 100 125 150	0.0000 0.0127 0.0230 0.0304 0.0368 0.0425 0.0467

<sup>\*</sup> data were presented in the form of smooth curves on a small scale graph (5.5 cm  $\times$  8.0 cm). The compiler has measured the co-ordinates at arbitrary points on the curves.

<sup>†</sup> MEA = 2-aminoethanol (monoethanolamine)

#### COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO<sub>2</sub>; [124-38-9] 1. Rivas, O.R.; Prausnitz, J.M. 1-Methyl-2-pyrrolidinone; C<sub>5</sub>H<sub>9</sub>NO; [872-50-4] 2-(2- aminoethoxy)-ethanol, Ind. Eng. Chem. Fundam. 1979, 18, 289-292. (Diglycolamine); C4H11NO2; [929-06-6] VARIABLES: PREPARED BY: Temperature, liquid composition C.L. Young. **EXPERIMENTAL VALUES:** Mole fraction T/Kp/mmHg p/kPa Component in liquid, x in gas, y 0.9964 263.08 6.113 1 0.0157 8.150 0.9550 0.00364 2 ~ 0.00001 3 0.0293 26.28 35.04 1 0.0216 0.9992 2 0.9493 0.0008 3 0.0291 7.883 1 0.938 298.25 5.913 0.00874 0.9618 2 0.0618 3 0.0295 0.0002 13.42 17.89 1 0.0130 0.9728 0.9577 2 0.0271 0.0294 0.0001 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus with a fused quartz precision bourdon pressure gauge. Solubility apparatus carefully thermostatted. Solvent No details given. degassed in situ. Apparatus described in ref. (1) and modifications given in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05$ ; $\delta x_{\text{CO}_2} = \pm 1$ %. REFERENCES: 1. Cukor, P.M., Prausnitz, J.M. Ind. Eng. Chem. Fundam. 1971, 10, 638.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]
- (3) Tetrachloromethane or carbon tetrachloride; CCl<sub>4</sub>; [56-23-5]

## ORIGINAL MEASUREMENTS:

Takahashi, M.; Kobayashi, Y.; Takeuchi, H.

J. Chem. Eng. Data 1982, 27, 328-31.

VARIABLES:

$$T/K = 298$$
  
 $p_1/kPa = 101.3$ 

Composition.

PREPARED BY:

H. L. Clever

## EXPERIMENTAL VALUES:

T/K	Benzene Mol Fraction	Viscositya	Diffusion Coefficient	Solubility
	x <sub>2</sub>	$10^3 \mu_{\rm m}/Pa$ s	109 D <sub>A</sub> /m <sup>2</sup> s <sup>-1</sup>	$e_1/\text{mol m}^{-3}$
298	0.00	0.88	3.17	91.2
	0.20	0.82	3.25	72.0
	0.40	0.76	3.35	82.2
	0.60	0.70	3.60	84.1
	0.80	0.64	3.65	86.7
	1.00	0.60	3.85	92.9

a Literature values taken from Ishikawa, T. "Kongoeki Nendo no Riron" (Theories of Viscosity for Mixed Solvents); Maruzen, Tokyo, 1968.

#### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An indirect method (1) was used in which the absorption rate of carbon dioxide into the mixed solvent was measured as a function of time.

It was assumed that the film-theory model of the gas absorption process applied. A plot of ln (absorption rate) vs. time is linear. The slope is a function of the diffusion coefficient and the intercept is a function of both the diffusion coefficient and the solubility.

A diaphram cell with interfacial area 5.81 cm² and lower compartment volume for the liquid was 53.5 cm³. The diaphram was Millipore Teflon of mean pore size 10.0  $\mu\text{m}$ , thickness 125  $\pm$  15  $\mu\text{m}$ , and porosity 0.68. The liquid was stirred at a constant rate of 1.33 rotations s $^{-1}$ .

The solutions were prepared and then degassed by refluxing for five hours. Their compositions were determined by density or refractive index. The CO<sub>2</sub> was presat. with solvent vap.

## SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not identified. From cylinder.
- (2, 3) Benzene and tetrachloromethane.

It was stated that the chemicals were of special grade.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.1$$
  
 $\delta c_1/c_1 = \pm 0.05 - 0.10$  (compiler).

### REFERENCES:

 Takeuchi, H.; Fujine, M.; Sato, T.; Onda, K.
 J. Chem. Eng. Jpn. 1975, 8, 25 and 252.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]
- (3) Tetrachloromethane or carbon tetrachloride; CCl<sub>4</sub>; [56-23-5]

### ORIGINAL MEASUREMENTS:

Takahashi, M.; Kobayashi, Y.; Takeuchi, H.

J. Chem. Eng. Data 1982, 27, 328-31.

## VARIABLES:

$$T/K = 298$$
  
 $p_1/kPa = 101.3$   
Composition.

PREPARED BY:

H. L. Clever

## EXPERIMENTAL VALUES:

T/K	1-Octanol Mol Fraction	Viscosity <sup>a</sup>	Diffusion Coefficient	Solubility
	x <sub>2</sub>	$10^3 \mu_{\rm m}/Pa$ s	109 D <sub>A</sub> /m <sup>2</sup> s <sup>-1</sup>	$c_1/\text{mol m}^{-3}$
298	0.00 0.20 0.40 0.60 0.80 1.00	0.88 1.40 2.25 3.55 5.25 7.35	3.17 2.70 2.40 1.96 1.80 1.53	91.2 68.8 71.7 73.7 55.4 49.6

a Literature values taken from Ishikawa, T. "Kongoeki Nendo no Riron" (Theories of Viscosity for Mixed Solvents); Maruzen, Tohyo, 1968.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An indirect method (1) was used in which the absorption rate of carbon dioxide into the mixed solvent was measured as a function of time.

It was assumed that the film-theory model of the gas absorption process applied. A plot of ln (absorption rate) vs. time is linear. The slope is a function of the diffusion coefficient and the intercept is a function of both the diffusion coefficient and the solubility.

A diaphram cell with interfacial area  $5.81~\text{cm}^2$  and lower compartment volume for the liquid was  $53.5~\text{cm}^3$ . The diaphram was Millipore Teflon of mean pore size  $10.0~\mu\text{m}$ , thickness  $125~\pm~15~\mu\text{m}$ , and porosity 0.68. The liquid was stirred at a constant rate of  $1.33~\text{rotations}~\text{s}^{-1}$ .

The solutions were prepared and then degassed by refluxing for five hours. Their compositions were determined by density or refractive index. The CO 2 was presat. With solvent vap.

## SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not identified. From cylinder.
- (2, 3) 1-Octanol and tetrachloromethane.

It was stated that the chemicals were of special grade.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.1$$
  
 $\delta c_1/c_1 = \pm 0.5 - 0.10$  (compiler).

## REFERENCES:

 Takeuchi, H.; Fujine, M.; Sato, T.; Onda, K.
 J. Chem. Eng. Jpn. 1975, 8, 25 and 252.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-methyl-1-propanol or isobutyl alcohol;  $C_AH_{1,0}O$ ; [78-83-1]
- (3) Formamide; CH<sub>3</sub>NO; [75-12-7]

### ORIGINAL MEASUREMENTS:

J. Chem. Eng. Data 1982, 27, 328-31.

### VARIABLES:

$$T/K = 298$$
  
 $p_1/kPa = 101.3$   
Composition.

PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

	/•			
T/K	Isobutyl Alcohol Mol Fraction	Viscosity <sup>a</sup>	Diffusion Coefficient	Solubility
	x <sub>2</sub>	$10^3 \mu_{\rm m}/{\rm Pa}$ s	10° D <sub>A</sub> /m <sup>2</sup> s <sup>-1</sup>	$c_1/\text{mol m}^{-3}$
298	0.00 0.20 0.40 0.60 0.80 1.00	3.30 3.64 3.86 3.68 3.31 3.36	0.946 1.15 1.27 1.49 1.76 2.02	75.6 77.8 86.7 87.8 86.0 68.1

a Literature values taken from Ishikawa, T. "Kongoeki Nendo no Riron" (Theories of Viscosity for Mixed Solvents); Maruzen, Tohyo, 1968.

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

An indirect method (1) was used in which the absorption rate of carbon dioxide into the mixed solvent was measured as a function of time.

It was assumed that the film-theory model of the gas absorption process applied. A plot of ln (absorption rate) vs. time is linear. The slope is a function of the diffusion coefficient and the intercept is a function of both the diffusion coefficient and the solubility.

A diaphram cell with interfacial area  $5.81~{\rm cm}^2$  and lower compartment volume for the liquid was  $53.5~{\rm cm}^3$ . The diaphram was Millipore Teflon of mean pore size  $10.0~{\rm \mu m}$ , thickness  $125~{\rm \pm}~15~{\rm \mu m}$ , and porosity 0.68. The liquid was stirred at a constant rate of  $1.33~{\rm rotations~s}^{-1}$ .

The solutions were prepared and then degassed by refluxing for five hours. Their compositions were determined by density or refractive index. The CO<sub>2</sub> was presat. with solvent vap.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not identified. From cylinder.
- (2, 3) Isobutyl alcohol, formamide.

It was stated that the chemicals were of special grade.

## ESTIMATED ERROR:

$$\delta T/K = \pm 0.1$$
  
 $\delta c_1/c_1 = \pm 0.05 - 0.10$  (compiler).

#### REFERENCES:

 Takeuchi, H.; Fujine, M.; Sato, T.; Onda, K.
 J. Chem. Eng. Jpn. 1975, 8, 25 and 252.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]
- (3) 1-Propanol; C<sub>3</sub>H<sub>8</sub>O; [71-23-8]

### ORIGINAL MEASUREMENTS:

Takahashi, M.; Kobayashi, Y.; Takeuchi, H.

J. Chem. Eng. Data 1982, 27, 328-31.

**VARIABLES:** 

T/K = 298  $p_1/kPa = 101.3$ Composition. PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

<i>T</i> /K	Benzene Mol Fraction	Viscosity <sup>a</sup> 10 <sup>3</sup> µ <sub>m</sub> /Pa s	Diffusion Coefficient 10° D <sub>A</sub> /m <sup>2</sup> s <sup>-1</sup>	Solubility  c <sub>1</sub> /mol m <sup>-3</sup>
298	0.00	1.97	3.06	62.9
	0.20	1.49	3.20	71.0
	0.40	0.67	4.20	59.0
	0.60	0.62	4.18	69.1
	0.80	0.61	3.95	71.4
	1.00	0.60	3.85	92.9

a Literature values taken from Ishikawa, T. "Kongoeki Nendo no Riron" (Theories of Viscosity for Mixed Solvents); Maruzen, Tohyo, 1968.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

An indirect method (1) was used in which the absorption rate of carbon dioxide into the mixed solvent was measured as a function of time.

It was assumed that the film-theory model of the gas absorption process applied. A plot of ln (absorption rate) vs. time is linear. The slope is a function of the diffusion coefficient and the intercept is a function of both the diffusion coefficient and the solubility.

A diaphram cell with interfacial area  $5.81~\text{cm}^2$  and lower compartment volume for the liquid was  $53.5~\text{cm}^3$ . The diaphram was Millipore Teflon of mean pore size  $10.0~\mu\text{m}$ , thickness  $125~\text{t}~15~\mu\text{m}$ , and porosity 0.68. The liquid was stirred at a constant rate of  $1.33~\text{rotations}~\text{s}^{-1}$ .

The solutions were prepared and then degassed by refluxing for five hours. Their compositions were determined by density or refractive index. The  ${\rm CO}_2$  was presat. with solvent vap.

## SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide. Source not identified. From cylinder.
- (2, 3) Benzene and 1-propanol.

It was stated that the chemicals were of special grade.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.1$$
  
 $\delta c_1/c_1 = \pm 0.05 - 0.10$  (compiler).

## REFERENCES:

 Takeuchi, H.; Fujine, M.; Sato, T.; Onda, K. J. Chem. Eng. Jpn. 1975, 8, 25 and 252.

COMPONENTS:  1. Carbon dioxide; CO <sub>2</sub> ; [124-38-9]  2. Mixed solvents	ORIGINAL MEASUREMENTS: Koudelka, L. Chem. Zvesti <u>1964</u> , 18, 178-185.
2. Mixed solvents	
VARIABLES: T/K = 293.15 P/kPa = 101.3	PREPARED BY: P.G.T. Fogg
EXPERIMENTAL VALUES:	
in s	e fraction of A Mole fraction of Golvent mixture CO <sub>2</sub> in solution ore addition of CO <sub>2</sub>
(A) Methanol; CH <sub>4</sub> O; [67-56-1] (B) 2-Propanone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1]	1.000 0.00751 0.908 0.00802 0.670 0.01097 0.436 0.01433 0.282 0.01634 0.000 0.02317
(A) 2-Propanone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1] (B) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	1.000 0.02317 0.878 0.02039 0.701 0.01686 0.578 0.01513 0.000 0.01375
(A) Methanol; CH <sub>4</sub> O; [67-56-1] (B) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3]	1.000 0.00751 0.975 0.00732 0.876 0.00687 0.812 0.00698 0.494 0.00848 0.000 0.01375
(A) Methanol; CH <sub>4</sub> O; [67-56-1] (B) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	1.000 0.00751 0.905 0.00735 0.606 0.00755 0.519 0.00788 0.195 0.00866 0.000 0.00989
(A) 2-Propanone; C <sub>3</sub> H <sub>6</sub> O; [67-64-1] (B) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	1.000 0.02317 0.939 0.02214 0.809 0.02014 0.539 0.01612 0.420 0.01480 0.134 0.01170 0.000 0.00989
(A) Trichloromethane; CHCl <sub>3</sub> ; [67-66-3] (B) Benzene; C <sub>6</sub> H <sub>6</sub> ; [71-43-2]	1.000 0.01375 0.831 0.01282 0.627 0.01196 0.324 0.01080 0.123 0.01027 0.000 0.00989
$P_{\text{CO}_2} = 760 \text{ Torr} = 101.325 \text{ kPa}$	'K = 293.15 K
AUXILIARY 1	NFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An Ostwald type apparatus was used. The absorption vessel could be agitated by an electric motor. This vessel and the gas buret system were maintained at constant temperature by circulation of water from a constant temperature bath.	2 Liquids were fractionally distilled before use.  ESTIMATED ERROR:  δT/K = ±0.1 (authors)
-	REFERENCES:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cephalin
- (3) Benzene;  $C_6H_6$ ; [71-43-2]

#### ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Danforth, W. F.

J. Chem. Thermodyn. 1974, 6, 245-250.

#### VARIABLES:

T/K: 310.65

Total P/kPa: 101.325 (1 atm)

#### PREPARED BY:

H. L. Clever

#### **EXPERIMENTAL VALUES:**

<i>T/</i> K	Mass Fraction Cephalin <sup>W</sup> 2	Ostwald Coefficient L/cm³cm-3	"Salting Out" Parameter $k = (1/W_2) \log(L_0/L_w)$
310.64 310.69	0.0	2.284 2.283	
310.53 310.69	0.1994 0.1994	1.99	0.29 ± 0.05
310.65	1.0	1.17*	

<sup>\*</sup>Extrapolated carbon dioxide solubility in hypothetical liquid cephalin.

 $L_{_{
m O}}$  and  $L_{_{
m W}}$  are the carbon dioxide Ostwald coefficients in benzene and in the benzene + cephalin solution, respectively.

#### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to  $500~\text{cm}^3$  of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid nitrogen trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

## SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum purity 99.8 mole per cent.
- (2) Cephalin. Nutritional Biochemicals Corp. Homostatic phosphatide obtained from bovine brain tissue, used as received.
- J. T. Baker Analyzed (3) Benzene. Reagent Grade. 99.9 mole per cent, thiophene free.

ESTIMATED ERROR:  $\delta T/K = 0.01$  $\delta P/\text{mmHg} = 0.5$ 

 $\delta L_{o}/L_{o} = 0.01$  $\delta L_{w}/L_{w} = 0.02$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F.D.; Danforth, W.F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Lecithin
- (3) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

### ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Danforth, W. F.

J. Chem. Thermodyn. 1974, 6, 245-250.

### VARIABLES:

T/K: 310.65

Total p/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mass Fraction Lecithin	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>	"Salting Out" Parameter $k = (1/W_2) \log(L_0/L_W)$
310.64 310.69	0.0	2.284 2.283	
310.62 310.63	0.1998 0.1998	1.93 1.93	0.37 ± 0.05
310.65	1.0	0.97*	

<sup>\*</sup>Extrapolated carbon dioxide solubility in hypothetical liquid lecithin.

#### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm³ of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid nitrogen trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum purity is 99.8 mole per cent.
- (2) Lecithin. Nutritional Biochemicals Corp. Vegetable source, about 95 per cent, used as received.
- (3) Benzene. J. T. Baker Analyzed Reagent Grade. 99.9 mole per cent, thiophene free.

## ESTIMATED ERROR:

 $\delta T/K = 0.01$ 

 $\delta P/\text{mmHg} = 0.5$ 

 $\delta L_{\rm o}/L_{\rm o}=0.01$ 

 $\delta L_{\rm W}/L_{\rm W} = 0.02$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F.D.; Danforth, W.F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

 $L_{_{
m O}}$  and  $L_{_{
m W}}$  are the carbon dioxide Ostwald coefficients in benzene and in the benzene + lecithin solution, respectively.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cholest-5-en-3 $\beta$ -ol or Cholesterol;  $C_{27}H_{46}O$ ; [57-88-5]
- (3) Benzene; C<sub>6</sub>H<sub>6</sub>; [71-43-2]

### ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Danforth, W. F.

J. Chem. Thermodyn. 1974, 6, 245-250.

### VARIABLES:

T/K: 310.65

P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mass Fraction Cholesterol	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>	"Salting Out" Parameter $k = (1/W_3) \log(L_0/L_W)$
310.64 310.69	0.0	2.284 2.283	
310.63 310.63	0.0524 0.0524	2.21 2.18	0.33 ± 0.17
310.64 310.65	0.1049 0.1049	2.12 2.13	0.30 ± 0.08
310.65	1.0	1.15*	

<sup>\*</sup>Extrapolated carbon dioxide solubility in hypothetical liquid cholesterol.

## AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm³ of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid nitrogen trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum purity 99.8 mole per cent.
- (2) Cholesterol. Source not given. Recrystalized from benzene.
- (3) Benzene. J. T. Baker Analyzed Reagent Grade. 99.9 mole per cent, thiophene free.

ESTIMATED ERROR:  $\delta T/K = 0.01$   $\delta P/\text{mmHg} = 0.5$   $\delta L_{\text{O}}/L_{\text{O}} = 0.01$  $\delta L_{\text{W}}/L_{\text{W}} = 0.02$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.
- Battino, R.; Evans, F.D.; Danforth, W.F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.;
   Bogan, M.; Wilhelm, E.
   Anal. Chem. 1971, 43, 806.

 $L_{_{\hbox{\scriptsize O}}}$  and  $L_{_{\hbox{\scriptsize W}}}$  are the carbon dioxide Ostwald coefficients in benzene and in the benzene + cholesterol solution, respectively.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cholest-5-en-3 $\beta$ -ol or cholesterol;  $C_{27}H_{46}O$ ; [57-88-5]
- (3) 2-Methyl-1-propanol or isobutanol; C<sub>4</sub>H<sub>10</sub>O; [78-83-1]

#### ORIGINAL MEASUREMENTS:

Byrne, J. E.; Battino, R.; Danforth, W. F.

J. Chem. Thermodyn. 1974, 6, 245-50.

## VARIABLES:

T/K: 310.65

Total p/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mass Fraction Cholesterol	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>	"Salting Out" Parameter $k = (1/W_2) \log(L_0/L_w)$
310.65	0	1.611	
310.63 310.63	0.0521 0.0521	1.60 1.62	0

Battino, R.; Evans, F. D.; Danforth, W. F. J. Chem. Thermodyn. <u>1971</u>, 3, 743.

 $L_{\rm O}$  and  $L_{\rm W}$  are the carbon dioxide Ostwald coefficients in isobutanol and in the isobutanol + cholesterol solution, respectively.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is based on the design of Morrison and Billett (1) and the version used is described by Battino, Evans and Danforth (2). The degassing apparatus is that described by Battino, Banzhof, Bogan, and Wilhelm (3).

Degassing. Up to 500 cm<sup>3</sup> of solvent is placed in a flask of such size that the liquid is about 4 cm deep. The liquid is rapidly stirred, and vacuum is intermittently applied through a liquid nitrogen trap until the permanent gas residual pressure drops to 5 microns.

Solubility Determination. The degassed solvent is passed in a thin film down a glass helical tube containing solute gas plus the solvent vapor at a total pressure of one atm. The volume of gas absorbed is found by difference between the initial and final volumes in the buret system. The solvent is collected in a tared flask and weighed.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Air Products and Chemicals, Inc. Minimum purity 99+ mole per cent.
- (2) Cholesterol. Source not given. Recrystalized from benzene.
- (3) 2-methyl-1-propanol or isobutanol. Fisher Scientific Certified. 99 mol per cent.

ESTIMATED ERROR:  $\delta T/K = 0.01$   $\delta P/\text{mmHg} = 0.5$   $\delta L_{\text{O}}/L_{\text{O}} = 0.01$  $\delta L_{\text{W}}/L_{\text{W}} = 0.02$ 

- 1. Morrison, T. J.; Billett, F.
- Chem. Soc. 1948, 2033.
   Battino, R.; Evans, F. D.; Danforth, W. F. J. Am. Oil Chem. Soc. 1968, 45, 830.
- Battino, R.; Banzhof, M.;
   Bogan, M.; Wilhelm, E.
   Anal. Chem. 1971, 43, 806.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cellulose, acetate; [9004-35-7]
- (3) N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]

### ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. Univ. Strasbourg (France) 1954.

### VARIABLES:

$$T/K = 293.15$$
  
 $w_2/g g^{-1} = 0, 0.0710$ 

#### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Cellulose Acetate w <sub>2</sub> /g g <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
293.15	0 0.0710	5.10 4.81

The author also determined that 1 g of solid cellulose acetate absorbs 4.65 cm $^3$  CO $_2$  at 293.15 K and 101.325 kPa.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The prepared solvent and solution were charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring buret in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and the volume of gas absorbed. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Cellulose acetate. Rhône-Poulenc. Purity not given.
- (3) Dimethylformamide. S.E.P.P.I.C. of Paris. Purity not given. Exposure to air avoided, distilled prior to use.

## ESTIMATED ERROR:

$$\delta T/K = \pm 0.2$$
  
 
$$\delta p/kPa = \pm 0.1$$
  
 
$$\delta L/L = \pm 0.02 \text{ (compiler)}$$

## REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Compt. rend. <u>1952</u>, 234, 2546-8.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cellulose, acetate; [9004-35-7]
- (3) 2-Propanone (Acetone); C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

## ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès, fac. sci. I niv. Strasbourg (France) 1954.

## VARIABLES:

$$w_2/g g^{-1} = 0, 0.0641$$

### PREPARED BY:

H. L. Clever

### **EXPERIMENTAL VALUES:**

<i>T</i> /K	Cellulose Acetate w <sub>2</sub> /g g <sup>-1</sup>	Ostwald Coefficient L/cm³ cm-3
293.15	0 0.0641	6.88 6.58

The author also determined that 1 g of solid cellulose acetate absorbs 4.65 cm $^3$  CO $_2$  at 293.15 K and 101.325 kPa.

## AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The prepared solvent and solution were charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring buret in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and the volume of gas absorbed. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Cellulose acetate. Rhône-Poulenc. Purity not given.
- (3) Acetone. Research grade. Source not given.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.2$$
  

$$\delta p/kPa = \pm 0.1$$
  

$$\delta L/L = \pm 0.02 \text{ (compiler)}$$

### REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Compt. rend. <u>1952</u>, 234, 2546-8.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Ethenyl benzene, homopolymer (polystyrene); (CoHg); [9003-53-6]
- (3) Benzene;  $C_6H_6$ ; [71-43-2]

## ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. U niv. Strasbourg France) 1954.

# VARIABLES: T/K = 293.15

$$w_2/g g^{-1} = 0 - 0.0884$$

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

<i>T/</i> K	Polystyrene	Viscosity <sup>a</sup> 10 <sup>2</sup> n/g cm <sup>-1</sup> s <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
293.15	0 0.0489b 0.0996b 0.0987c 0.0884d	- 19.59 55.35 411.14	2.66 2.54 2.43 2.44 2.43

a Viscosity for solution 0.099 g g<sup>-1</sup> and temperatures at 19.81, 19.84 and 20.06 C, respectively.

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The prepared solvent and solution were charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring buret in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and the volume of gas absorbed. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

(1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.2$$
  

$$\delta p/kPa = \pm 0.1$$
  

$$\delta L/L = \pm 0.02 \text{ (compiler)}$$

### REFERENCES:

Some data in the thesis have been published. See:

1. Maillard, A.; Rosenthal, W. Compt. rend. 1952, 234, 2546-8.

b Molecular weight 96,000.

<sup>&</sup>lt;sup>C</sup> Molecular weight 180,000.

<sup>&</sup>lt;sup>d</sup> Molecular weight 385,000.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-methyl-1-propene, homopolymer
   (polyisobutylene); (C<sub>4</sub>H<sub>8</sub>)<sub>x</sub>;
   [9003-27-4]
- (3) Benzene;  $C_6^{H}_6$ ; [71-43-2]

## ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thes. fac. sci. Univ. Strasbourg (France) 1954.

## VARIABLES:

$$T/K = 293.15$$
  
 $w_{9}/g g^{-1} = 0 - 0.00798$ 

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Polyiso- butylene w <sub>2</sub> /g g <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
293.15	0 0.0482 <sup>a</sup> 0.00682 <sup>b</sup> 0.00798 <sup>b</sup>	2.66 2.60 2.63 2.60

a Designated low molecular weight.

## AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The prepared solvent and solution were charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring buret in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and the volume of gas absorbed. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Polyisobutylene. BASF Ludwigshafen. Purity not given.
- (3) Benzene. Source and purity not given.

## ESTIMATED ERROR:

$$\delta T/K = \pm 0.2$$
  

$$\delta p/kPa = \pm 0.1$$
  

$$\delta L/L = \pm 0.02 \text{ (compiler)}$$

#### REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Compt. rend. <u>1952</u>, 234, 2546-8.

b Designated high molecular weight.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) 2-Propenenitrile, homopolymer (Polyacrylonitrile);  $(C_3^H_3^N)_x$ ; [25014-41-9]
- (3) N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]

### ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. y niv. Strasbourg (France) 1954.

## VARIABLES:

$$T/K = 293.15$$
  
 $w_2/g g^{-1} = 0 - 0.0666$ 

#### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

<i>T</i> /K	Polyacrylonitrile $w_2/g g^{-1}$	Viscosity <sup>a</sup> $10^2 \eta/g \text{ cm}^{-1} \text{ s}^{-1}$	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
293.15	0 0.0535 <sup>b</sup> 0.0516 <sup>b</sup> 0.0666 <sup>b</sup>	31.55 45.37 58.62	5.10 5.35 5.16 6.66

 $<sup>^{\</sup>rm a}$  Viscosity of 0.049 g g  $^{\rm -1}$  solution at 19.76, 19.84 and 20.00  $^{\rm 0}\text{C},$  respectively.

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The prepared solvent and solution were charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring buret in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and the volume of gas absorbed. Solubilities were measured at pressures above and below atmospheric.

## SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Polyacrylonitrile. BASF of Ludwigshafen. Purity not given.
- (3) Dimethylformamide. S.E.P.P.I.C. of Paris. Purity not given. Exposure to air avoided. Distilled prior to use.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$   $\delta p/kPa = \pm 0.1$  $\delta L/L = \pm 0.02$  (compiler)

#### REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Compt. rend. <u>1952</u>, 234, 2546-8.

 $<sup>^{\</sup>rm b}$  Polymer characterized by solution viscosity and K value of 80, 86 and 90, respectively. The K value is a function of intrinsic viscosity.

VARIABLES:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Sodium iodide; NaI; [7681-82-5]
- (3) 2-Propanone (acetone); C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

### ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. Univ. Strasbourg (France) 1954.

### PREPARED BY:

H. L. Clever

# T/K = 293.15

p/kPa = 101.325 $m_0/\text{mol kg}^{-1} = 0 - 1.582$ 

### EXPERIMENTAL VALUES:

T/K	Salt concentration in solvent:		Ostwald	Sechenov
	Mass fraction <sup>a</sup>	Molal conc. b	Coefficient <sup>a</sup>	Constant <sup>b</sup>
	c <sub>2</sub> /g g <sup>-1</sup>	$m_2/\text{mol kg}^{-1}$	L/cm <sup>3</sup> cm <sup>-3</sup>	$k_{smc}/\text{kg mol}^{-1}$
293.15	0 0.0766 0.1435 0.2371	0 0.553 1.117 2.074	6.88 5.84 5.06 3.83	0.129 0.119 0.122

Original data. The salt concentration was expressed as mass of salt per unit mass of salt solution.

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

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Sodium iodide. Source and purity not given. Recrystallized from water and dried.
- (3) Acetone. Research grade. Purity not given. Dried and distilled.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$  $\delta p/kPa = \pm 0.1$  $\delta L/L = \pm 0.02$  (compiler)

### REFERENCES:

Some data in the thesis have been published. See:

1. Maillard, A.; Rosenthal, W. Compt. rend. 1952, 234, 2546-8.

Molal concentration and Sechenov constant calculated by compiler as follows:

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Octadecanoic (stearic) acid;  $^{\text{C}}_{18}^{\text{H}}_{36}^{\text{O}}_{2}$ ; [57-11-4]
- (3) 2-Propanone (acetone); C<sub>3</sub>H<sub>6</sub>O; [67-64-1]

## ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. Univ. Strasbourg (France) 1954.

VARIABLES: T/K = 293.15

p/kPa = 101.325

 $w_2$ /mass fraction = 0 - 0.0419

PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Stearic acid co	onc.in solvent:	Ostwald	Bunsen	Mole
	Mass fractiona	Mole fractionb	Coefficienta	Coefficienta	Fractionb
	w 2	x_2	L/cm³cm-3	α/cm³(STP)cm <sup>-3</sup>	
293.15	0 0.0243 0.0419	0 0.00506 0.00885	6.88 5.01 4.93	6.40 4.66 4.58	0.0211 0.0154 0.0151

a Original data based on mass fraction stearic acid in gas-free solution.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and below atmospheric.

## SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Stearic acid. Merck. Melting point 69.3 °C. Used without further purification.
- (3) Acetone. Research grade.
  Purity not given. Dried and
  distilled.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$  $\delta p/kPa = \pm 0.1$ 

 $\delta L/L = \pm 0.02$  (compiler)

### REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Compt. rend. <u>1952</u>, 234, 2546-8.

b Calculated by compiler.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Sodium iodide; NaI; [7681-82-5]
- (3) N,N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]

### ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. Univ. Strasbourg (France) 1954.

## VARIABLES:

$$T/K = 293.15$$
  
 $p/kPa = 101.325$   
 $m_2/\text{mol kg}^{-1} = 0, 0.360$ 

#### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Salt concentrat:	ion in solvent:	Ostwald	Sechenov
	Mass fraction <sup>a</sup>	Molal conc.b	Coefficient <sup>a</sup>	Constant <sup>b</sup>
	c <sub>2</sub> /g g <sup>-1</sup>	m <sub>2</sub> /mol kg <sup>-1</sup>	L/cm <sup>3</sup> cm <sup>-3</sup>	$\frac{k_{smc}}{\text{/kg mol}^{-1}}$
293.15	0 0.054 <sup>c</sup>	0 0.3809	5.10 4.28	0.199
_	0.000			

Original data. The salt concentration was expressed as mass of salt per unit mass of salt solution.

b Molal concentration and Sechenov constant calculated by compiler as follows:

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

<sup>C</sup> Solvent saturated with NaI.

## AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and below atmospheric.

### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Sodium iodide. Source and purity not given.
- (3) Dimethylformamide. S.E.P.P.I.C. of Paris. Purity not given. Exposure to air avoided. Distilled prior to use.

## ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$  $\delta p/kPa = \pm 0.1$ 

 $\delta L/L = \pm 0.02$  (compiler)

#### REFERENCES:

Some data in the thesis have been published. See:

 Maillard, A.; Rosenthal, W. Compt. rend. 1952, 234, 2546-8.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Octadecanoic (stearic) acid; C<sub>18</sub>H<sub>36</sub>O<sub>2</sub>; [57-11-4]
- (3) N, N-Dimethylformamide; C<sub>3</sub>H<sub>7</sub>NO; [68-12-2]

### ORIGINAL MEASUREMENTS:

Rosenthal, W.

Thès. fac. sci. Univ. Strasbourg (France) 1954.

### VARIABLES:

VARIABLES: T/K = 293.15 p/kPa = 101.325  $w_2/mass$  fraction = 0 - 0.0347

PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Stearic acid conc.in solvent:		Ostwald	Bunsen	Mole
	Mass fraction <sup>a</sup>	Mole fraction <sup>b</sup>	Coefficienta	Coefficient <sup>b</sup>	Fraction
	w 2	x_2	L/cm <sup>3</sup> cm <sup>-3</sup>	α/cm³(STP)cm <sup>-3</sup>	
293.15	0 0.01515 0.01655 0.0347	0 0.00394 0.00430 0.00915	5.10 7.12 7.10 7.03	4.75 6.62 6.61 6.54	0.0164 0.0229 0.0229 0.0226

a Original data based on mass fraction stearic acid in gas-free solution.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The prepared solvent solution was charged into an evacuated cell after degassing, and the mass of solvent was determined by weight. Gas was introduced into the cell from a measuring burette in which the gas was stored over mercury. The cell was agitated while the gas pressure was maintained by adjusting the gas volume. The Ostwald coefficient was determined from the mass of solvent and volume of gas used. Solubilities were measured at pressures above and below atmospheric.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Source and purity not given. An aqueous "soda" solution absorbed 99.8% of the gas.
- (2) Stearic acid. Merck. Melting point 69.3 C. Used without further purification.
- (3) Dimethylformamide. S.E.P.P.I.C. of Paris. Purity not given. Exposure to air avoided. Distilled prior to use.

## ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ 

 $\delta p/kPa = \pm 0.1$ 

 $\delta L/L = \pm 0.02$  (compiler)

### REFERENCES:

Some data in the thesis have been published. See:

1. Maillard, A.; Rosenthal, W. Compt. rend. 1952, 234, 2546-8.

b Calculated by compiler.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Methanol; CH<sub>4</sub>O; [67-56-1]
- 3. Lithium chloride; LiCl;
  [7447-41-8]
  Lithium bromide; LiBr; [7550-35-8]
  Lithium iodide; LiI; [10377-51-2]
  Sodium iodide; NaI; [7681-82-5]

### ORIGINAL MEASUREMENTS:

Kozakewitsch, P.P

Zeit. Phys. Chem. (A) 1929, 143, 216-224.

### VARIABLES:

T/K = 288.15 P/kPa = 101.3 Conc. of salt = 0-0.103 mole ratio

#### PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Salt	Concentration of salt† 100n(MX) /n(CH <sub>3</sub> OH)	Solubility† 100n(CO <sub>2</sub> ) /n(CH <sub>3</sub> OH)	
Lithium chloride	0.00	0.825 0.629	
	4.92 6.43 9.17	0.585 0.503 0.404	
Lithium bromide	0.00	0.404 0.825 0.655	
	5.74 7.41	0.559 0.490	
Lithium iodide	10.31 0.00	0.402 0.825 0.747	
Sodium iodide	1.17 2.41 0.00	0.747 0.669 0.825	
Dourain Tourac	2.64 2.86	0.675 0.641	
	4.78 8.35	0.553 0.446	

 $<sup>^{\</sup>dagger}$   $n(MX) = \text{no. of moles of salt: } n(CH_3OH) = \text{no. of moles of methanol}$   $n(CO_2) = \text{no. of moles of } CO_2$ .

### AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

Carbon dioxide was bubbled through the alcohol or alcohol and halide for two to four days. A portion of the saturated solution of gas was then added to  $\text{CO}_2$ -free water containing a measured quantity of sodium hydroxide. The mixture of sodium hydroxide and carbonate was then titrated against hydrochloric acid using phenolphthalein as indicator.

Separate portions of the original solution of gas were analysed for halide content by the Volhard method.

Solubilities were corrected to a partial pressure of carbon dioxide of 101.3 kPa.

### SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide was prepared by the action of hydrochloric acid on calcium carbonate. The gas was purified and dried by the usual methods.
- The alcohol was said to be free from water.
- 3. No information.

### ESTIMATED ERROR:

 Carbon dioxide; CO<sub>2</sub>; [124-38-9]

EXPERIMENTAL VALUES:

- 2. Ethanol; C<sub>2</sub>H<sub>6</sub>O; [64-17-5]
- 3. Lithium chloride; LiCl;
   [7447-41-8]
   Lithium bromide; LiBr; [7550-35-8]
   Lithium iodide; LiI; [10377-51-2]
   Sodium iodide; NaI; [7681-82-5]

#### ORIGINAL MEASUREMENTS:

Kozakewitsch, P.P

Zeit. Phys. Chem. (A) 1929, 143, 216-224.

#### VARIABLES:

T/K = 288.15 P/kPa = 101.3 Conc. of salt = 0-0.151 mole ratio

### PREPARED BY:

P.G.T. Fogg

Salt	Concentration of salt† 100n(MX) /n(C <sub>2</sub> H <sub>5</sub> OH)	Solubility† 100n(CO <sub>2</sub> ) /n(C <sub>2</sub> H <sub>5</sub> OH)	
Lithium chloride	0.00	0.768 0.648	
	5.44	0.585	
	8.47	0.498	
	15.11	0.388	
Lithium bromide	0.00	0.768	
	1 56	0 600	

0.680 1.56 2.48 0.662 3.75 0.612 6.42 0.543 0.00 Lithium iodide 0.768 2.18 0.640 5.32 0.498 10.40 0.383 Sodium iodide 0.00 0.768 1.27 0.705 2.97 0.629 3.87 0.612 4.38 0.579

8.44

 $+ n(MX) = \text{no.of moles of salt: } n(C_2H_5OH) = \text{no. of moles of ethanol}$  $n(CO_2) = \text{no.of moles of } CO_2.$ 

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Carbon dioxide was bubbled through the alcohol or alcohol and halide for two to four days. A portion of the saturated solution of gas was then added to  $\text{CO}_2$ -free water containing a measured quantity of sodium hydroxide. The mixture of sodium hydroxide and carbonate was then titrated against hydrochloric acid using phenolphthalein as indicator.

Separate portions of the original solution of gas were analysed for halide content by the Volhard method.

Solubilities were corrected to a partial pressure of carbon dioxide of 101.3 kPa.

#### SOURCE AND PURITY OF MATERIALS:

0.512

- Carbon dioxide was prepared by the action of hydrochloric acid on calcium carbonate. The gas was purified and dried by the usual methods.
- The alcohol was said to be free from water.
- 3. No information.

## ESTIMATED ERROR:

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Mineral Oils

### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

#### CRITICAL EVALUATION:

Solubility of Carbon Dioxide in Mineral Oils

Various groups have measured the solubility of carbon dioxide in petroleum fractions. Precise comparison between different sets of data is not possible because of the differences in chemical nature of the materials under test. A high proportion of cyclic hydrocarbons is likely to lower the solubility of carbon dioxide. In some cases average relative molecular masses have been stated and these enable semi-quantitative comparison of solubility data. Many of the solubility values have been measured at 293.15 K. Bunsen coefficients at this temperature range from 0.76 to 1.54 and mole fraction solubilities from 0.014 to 0.028. At this temperature there is a general tendency for an increase in Bunsen coefficient to be associated with a decrease in the relative molecular mass (see Table 1). Data published by Luther and Hiemenz for a sample of kerosene are contrary to this trend. The Bunsen coefficient is low for an oil of relative molecular mass of 405. This may be due to the large proportion of cyclic hydrocarbons stated to be present. A summary of the available data for mineral oils is shown in Table 1.

- 1. Luther, H.; Hiemenz, W. Chem. Ing. Tech. 1957, 29, 530-535.
- 2. Treshchina, N.I. Trudy Vses. Neft. Nauch.-Issled. Geol.-Razvedoch 1955, No. 83, 566-571.
- 3. Kubie, L.S. J. Biol. Chem. 1927, 72, 545-548.
- Baldwin, R.R.; Daniel, S.G. J. Inst. Petroleum 1953, 39, 105-124.
- Logvinyuk, V.P.; Makarenkov, V.V.; Malyshev, V.V.; Panchenkov, G.M. Khim. Tekhnol. Topl. Masel 1970, 15(5), 27-29.
- Begley, J.W.; Maget, J.R.; Williams, B. J. Chem. Eng. Data 1965, 10, 4-8.
- 7. Rodman, C.J.; Maude, A.H. Trans. Am. Electrochem. Soc. 1925, 47, 71-92.
- 8. Messow, U.; Pape, D. Pol. J. Chem. 1980, 54, 2001-2009.
- Gniewosz, S.; Walfisz, A. Z. Phys. Chem. <u>1887</u>, 1, 70-72.
- Ridenour, W.P.; Weatherford, W.D. Ind. Eng. Chem. <u>1954</u>, 46, 2376-2381.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Mineral Oils

# **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

CRITICAL EVALUATION:

Table 1 Solubilities of carbon dioxide at a partial pressure of 101.3 kPa in mineral oils and wax.

	First author and reference	RMM	T/K	Bunsen coeff.	XCO2	Density* /g cm <sup>-3</sup>
Kerosene Koschagyl Buguruslan Medicinal paraffin Oil B Oil A.1 Oil A.2 Oil A.3 Oil MK-8 Oil A.4 Ramol 350 Oil A.5 Hydrogenated fuel Mineral oil Kulsary Kulsary Diesel fuel Grozny	Treshchina (2) Treshchina Kubie (3) Baldwin (4) Baldwin Baldwin Baldwin Logvinyuk (5) Baldwin (4) Begley (6) Baldwin (4) Logvinyuk (5) Rodman (7) Treshchina (2) Treshchina Messow (8) Treshchina (2)	630 670 610 570 530 400	293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15	0.76 0.81 0.834 0.841 0.85 0.853 0.861 0.91 0.911 0.932 0.966 0.98 0.991 1.01 1.03 1.06	0.0175 0.0269 0.0279 0.026 0.0251 0.0243 0.0193	0.880 0.917 0.913 0.89 1 0.894 1 0.885 1 0.885 1 0.873 1 0.872 0.869 0.832 0.840 0.886 0.832 2
Grozny Grozny Fuel T-1 Petroleum Kerosene Fuel T-6 Fuel TS-1 Kerosene Kerosene Gasoline	Treshchina Logvinyuk (5) Gniewosz (9) Treshchina (2) Logvinyuk (5) Logvinyuk Baldwin (4) Messow (8) Treshchina (2)	165 209	293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15 293.15	1.135 1.14 1.17 1.29 1.29 1.31 1.51 1.542	0.0144 0.0176	0.813 0.816 0.819 0.84 0.775 0.811 <sup>2</sup> 0.746
Paraffin wax	Ridenour (10)	350	345.4	0.548	0.0110	0.772 <sup>3</sup>

RMM = average relative molecular mass (The nature of the average is
 not usually stated; i.e. whether mass average or number average)

<sup>\*</sup> density at 293.15 K except where indicated.

<sup>&</sup>lt;sup>1</sup> 288.15 K

<sup>&</sup>lt;sup>2</sup> 298.15 K

<sup>&</sup>lt;sup>3</sup> 341.45 K

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Paraffin oil Chem. Ing. Tech. 1957, 29, 530-535. VARIABLES: PREPARED BY: T/K = 293.15-355.15 P/kPa = 0-80 kPa

# EXPERIMENTAL VALUES:

T/K	Concentr of CO <sub>2</sub>	T	Ostwald coeff.	Henry's law constant		Mole fraction solubility at 101.3 bar	
	/mol m <sup>-</sup> liquid	gas	L	/atm	/kPa**	101.5 Dar	
293.15	4.67	5.72	0.816	57.2±4.2	5800±430	0.0175	
314.15	3.89	5.30	0.734				
334.65	3.39	5.02	0.675				
355.15	3.05	4.72	0.646				

At 293.15 K the mole fraction solubility was shown to be proportional to the partial pressure of carbon dioxide to a pressure of at least 600 Torr (80 kPa).

- \* concentrations correspond to a partial pressure of carbon dioxide of about 13 kPa.
- \*\* calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A spectroscopic method was used. The gas and solution under test was circulated through cuvettes. The concentration of carbon dioxide in the gas and liquid phases were calculated from the integrated extinction coefficient due to the infra-red band at 2350 cm<sup>-1</sup>.

# SOURCE AND PURITY OF MATERIALS:

- from a cylinder; purified by the usual methods.
- 2. contained about 30% cyclic napthenes and 70% slightly branched alkanes;  $d_4^{20} = 0.8795$ ; relative molecular mass = 405.

ESTIMATED ERROR:

 $\delta L \leq \pm 7.5\%$  (authors)

# 420 COMPONENTS: ORIGINAL MEASUREMENTS: Messow, U.; Pape, D. 1. Carbon dioxide; CO2; [124-38-9] Pol. J. Chem. 1980, 54, 2001-2009. 2. Diesel fuel VARIABLES: PREPARED BY: T/K = 303.15-363.15P.G.T. Fogg P/kPa = 101.3 kPaEXPERIMENTAL VALUES: $x_{\rm CO_2}$ at total pressure of 101.3 kPa T/K303.15 0.01299 333.15 0.00968 363.15 0.00813 The authors stated that the diesel fuel had the following properties: Average molecular weight/g $mol^{-1} = 234$ Average b.p./K Molar volume at 298.2 $K/cm^3 mol^{-1} = 300.12$

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The authors stated that measurements were made in the pressure range 1 atm to 10 atm but no further experimental details or results were given.	No details given
	ESTIMATED ERROR:  REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:			
1. Carbon di [124-38-9		Treshchina, N. I. Trudy Vses. Neft. NauchIssled. GeolRazvedoch 1955, No. 83,			
2. Petroleum		566-571.  Chem. Abstr. 1958, 52, 6771c			
VARIABLES:		PREPARED BY:			
$p_1/kPa =$	101.3	H.L. Clever			
T/K = 29	3, 313				
EXPERIMENTAL VALU	ES:				
Pe	troleum Sample	Temperature Solubility Coefficient <sup>a</sup>			
Location	Specific Gravity	t/°C T/K			
	<del>-</del>				

Petrole	Temper	ature	Solubility Coefficienta		
Location	Specific Gravity	t/°C	<i>T</i> /K		
Koschagyl,	0.917	20	293	0.810	
Emba oilfield		40	313	0.690	
Buguruslan, Volga-Ural oilfield	0.913	20 40	293 313	0.834 0.769	
Kulsary,	0.886	20	293	1.01	
Emba oilfield		40	313	0.805	
Kulsary,	0.887	20	293	1.03	
Emba oilfield		40	313	0.810	
Grozny	0.835	20	293	1.108	
Grozny oilfield		40	313	0.92	
Kulsary,	0.813	20	293	1.135	
Emba oilfield		40	313	0.98	
Kerosene	0.819	20 40	293 313	1.29 1.07	
Gasoline	0.746	20 40	293 313	1.87 1.46	

Solubility coefficient appears to be the Bunsen coefficient,  $\alpha/cm^3$  (STP)  $cm^{-3}$  atm<sup>-1</sup>.

The petroleum viscosities are 47.8, 38.0, 11.4, 6.5, - centistoke at 323 K as one comes down the table above.

Some information on the petroleum compositions are given in the paper.

The solubility of methane (natural gas) in water and mineralized water was given.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A detailed diagram of the apparatus is given in the paper.

# SOURCE AND PURITY OF MATERIALS:

Carbon dioxide. Prepared by the action of hydrochloric acid on marble.
 Petroleum, kerosene, and gasoline. Petroleum from wells in three oil

fields. specific gravity, viscosity, and some information on composition and various fractions was given.

ESTIMATED ERROR: $\delta \alpha / \alpha = \pm 0.05$ (compiler)	REFERENCES:

COMPONENTS:

(1) Carbon dioxide; CO<sub>2</sub>;

[124-38-9]

(2) Mineral oil, white

| ORIGINAL MEASUREMENTS:

| Kubie, L. S.
| J. Biol. Chem. 1927, 72,
| 545 - 548.

VARIABLES: T/K: 297.15 - 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K Bunsen coefficient α/cm³ (STP) cm⁻³ atm⁻¹

297.15 298.15 0.841 ± 0.011

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus was the constant volume Van Slyke and Neill type (1).

Saturation was attained by bubbling the gas through the oil for several hours.

A 1.990  $\pm$  0.007 cm  $^3$  volume of saturated solution was analyzed. The Van Slyke correction factor for unextracted and redissolved gas ranged from 1.07 to 1.09.

# SOURCE AND PURITY OF MATERIALS:

- (1) Oxygen. Commercial cylinder.
- (2) Mineral oil. "Amalie" brand, L. Sonneborn Sons, Inc., NY. A medicinal white oil which meets US Pharmacopeia standards. Prepared by fractional distillation from a naphthalene base, unsaturated hydrocarbons removed. Specific gravity 0.890 -0.895 at 15 °C, viscosity 285 at 100 °F.

# ESTIMATED ERROR:

 $\delta T/K = 1$ 

# REFERENCES:

 Van Slyke, D. D.; Neill, J. M. J. Biol. Chem. 1924, 56, 523.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Petroleum fractions

# ORIGINAL MEASUREMENTS:

Baldwin, R.R.; Daniel, S.G.

J. Inst. Petroleum 1953, 39,

105-124.

# VARIABLES:

T/K = 273.15-373.15; P/kPa = 101.3

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Solvent	Viscosity at 310.93 K /centipoises	Number average R.M.M.	T/K	Bunsen coeff.	Ostwald coeff.	Mole fraction *CO2
Oil <i>A.1</i>	615	670	293.15	0.853	0.915	0.0279
Oil A.2	268	610	273.15	1.115	1.115	
			293.15	0.861	0.924	0.0260
			333.15	0.572	0.697	
			373.15	0.420	0.574	
Oil <i>A.3</i>	181	570	293.15	0.887	0.952	0.0251
Oil A.4	80.3	530	293.15	0.911	0.978	0.0243
Oil A.5	34.9	400	273.15	1.245	1.245	
			293,15	0.966	1.037	0.0193
			333.15	0.640	0.781	
			373.15	0.467	0.638	
Oil B	260	630	293.15	0.850	0.912	0.0269
Kerosene		165	273.15	2.00	2.00	
			293.15	1.51	1.62	

<sup>\*</sup> calculated by the compiler from the density at 15°C given by the authors, assuming that the density at 20°C is approximately that at 15°C.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Most of the dissolved air was removed from a sample of oil by letting it stream into a continuously evacuated vessel. Any traces of air which remained were removed by saturating the oil with carbon dioxide or other gas under test and then subjecting the sample to vacuum treatment again. The oil was then transferred to an evacuated gas buret. The buret was then held in a thermostat bath and gas under test bubbled for 2-5 h until saturation was complete. Sufficient time was allowed for bubbles of gas to disappear and the gas above the oil was then displaced by running mercury into the gas buret. Dissolved gas was then pumped out of solution by a Topler pump, collected and measured.

# SOURCE AND PURITY OF MATERIALS:

- 1. No information.
- 2. Samples A were fractions of the same sample of crude oil. Sample B was from another source. The following properties were given in the paper:

Oil	Density 15°/4°C	Flash point (closed)	Kinem Visco /centip 100°F	sity	V.I.	Pour point °F
A.1 (residual)	0.894	510	615	34.4	95	0
A.2 (residual)†	0.885	460	268	20.3	96	0
A.3 (residual)	0.884	440	181	15.7	97	5
A.4 (distillate)	0.873	445	80.3	9.1	96	Ō
A.5 (distillate)	0.869	350	34.9	5.4	96	0
B+	0.890	460	260	20.0	96	10

<sup>†</sup> conformed to DTD 472B specification

ORIGINAL MEASUREMENTS:
Logvinyuk, V. P.; Makarenkov, V. V.; Malyshev, V. V.; Panchenkov, G. M.
Khim. Tekhnol. Topl. Masel 1970,15, (No. 5), 27 - 29. Chem. Technol. Fuels Oils (Eng. trans) 1970, 15,353 - 355.
PREPARED BY:
S. A. Johnson H. L. Clever
Ostwald t Coefficient 
, density $\rho_{4}^{20} = 0.816$
2.68 1.22
0.90
1, density $\rho_{i_0}^{20} = 0.775$
1.31
, density $\rho_4^{20} = 0.84$
2.25
1.52 1.38
1.38 0.99
0.67
nsity $\rho_{4}^{20}$ 0.832
0.98
° = 0.855
0.98
the Ostwald coefficients.
INFORMATION
SOURCE AND PURITY OF MATERIALS:
No information given.
ESTIMATED ERROR: $\delta \alpha / \alpha \leq 0.06$ (authors)
REFERENCES:  1. Gogitidize, L.D.; Logvinyuk, V.P.; Makarenkov, V.V.; Panchenkov, G.M.; Malyshev, V.V.; Yakovlevskii, V.V. Method of Evaluating the Operating Properties of Jet Fuels and Lubricating Materials (Russ.), Mashinostroenie* 1966.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Ramol 350 (a hydrocarbon oil)

# ORIGINAL MEASUREMENTS:

Begley, J.W.; Maget, J.R.; Williams, B.

J. Chem. Eng. Data 1965, 10, 4-8.

# VARIABLES:

P/kPa = 101.3T/K = 292.65-317.75

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K	Ostwald coefficient L
292.65	0.998
296.25	0.903
300.85	0.800
307.15	0.764
311.25	0.747
315.25	0.717
317.75	0.660

# Ramol 350 was reported to have the following physical properties

T/°C Density/g cm <sup>-3</sup>		T/°C	T/°C Viscosity/cp		Viscosity/cp	
20	0.872	19.4	219.5	37.8	67.9	
38.6	0.861	35.8	77.8	40.5	58.9	
45	0.858	36.6	71.9	44.4	47.9	

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The solvent was boiled to remove any gases in solution and was then introduced into the absorption Vessel without coming into contact with the air. The volume of carbon dioxide absorbed by the liquid from gas buret was then measured. The composition of the solution after equilibrium was attained was measured by chemical analysis. This enabled a check to be made of solubility as calculated from the Volume of gas absorbed. The absorption vessel and the gas buret were kept at constant temperature by circulation of water from a thermostat bath.

# SOURCE AND PURITY OF MATERIALS:

- Carbon dioxide 99.99% pure, from a cylinder supplied by Matheson Chemical Company.
- Ramol 350 supplied by Sherwood Refining Company, Detroit, Mich. USA.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$  Solubility measurements reproducible to about  $\pm 0.5\%$  (authors).

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Mineral oil

# ORIGINAL MEASUREMENTS:

Rodman, C. J.; Maude, A. H.

Trans. Am. Electrochem. Soc. 1925, 47, 71 - 92.

# VARIABLES:

T/K = 298.15 - 353.15 $p_1/kPa = 101.3$  (760 mmHg) PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

Temperature t/°C T/K		Bunsen Coefficient a/cm³(STP)cm <sup>-3</sup> atm <sup>-1</sup>	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>	Solubility g kg <sup>-1</sup>	
25	298.15	0.991	1.083	2,333	
50	323.15	0.774	0.916	1.87	
80	353.15	0.566	0.732	1.396	

These values appear in the International Critical Tables, McGraw-Hill Book Co., New York and London, Vol. III, pp. 261 - 270 where they are credited to an industrial report edited by A. H. Maude.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of an 180 cm<sup>3</sup> absorption bottle connected to a 100 cm<sup>3</sup> gas buret. The absorption bottle sets in a thermostat, which is attached to a shaking machine.

A weighed sample of oil is introduced into the absorption vessel. The sample is degassed by vacuum taking care to avoid excessive foaming. The gas is brought into the system. An initial buret reading taken, and the shaker is started and reading taken every 5 minutes until 2 or 3 constant readings are obtained.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information.
- (2) Mineral oil. A Pennsylvania base oil, 96 per cent saturated hydrocarbons, and distilling between 300 and 400°C. Density at 25°C = 0.840 and at 80°C = 0.800 g cm<sup>-3</sup>. As a commercial product the oil is known as "Wemco A".

ESTIMATED ERROR:

# COMPONENTS: ORIGINAL MEASUREMENTS: Carbon dioxide; CO2; Messow, U.; Pape, D. [124-38-9] Pol. J. Chem. 1980, 54, 2001-2009. 2. Kerosene VARIABLES: PREPARED BY: T/K = 303.15-363.15P.G.T. Fogg P/kPa = 101.3 kPaEXPERIMENTAL VALUES: $x_{\rm CO_2}$ at total pressure of 101.3 kPa T/K 303.15 0.01560 333.15 0.01182 0.00901 363.15 The authors stated that the kerosine had the following properties: Average molecular weight/g mol<sup>-1</sup> = 209 Average b.p./K = 462Molar volume at $298.2 \text{ K/cm}^3 \text{mol}^{-1} = 257.75$ AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: The authors stated that measurements No details given were made in the pressure range 1 atm to 10 atm but no further experimental details or results were given. ESTIMATED ERROR: REFERENCES:

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] (2) Petroleum VARIABLES: T/K = 283.15, 293.15 p/kPa = 101 "atmospheric" ORIGINAL MEASUREMENTS: Gniewosz, S.; Walfisz, A. Z. Phys. Chem. 1887, 1, 70 - 72. M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

Temperature		Bunsen Coefficient	Ostwald Coefficient	
t/°C	<i>T</i> /K	α/cm <sup>3</sup> (STP) cm <sup>-3</sup> atm <sup>-1</sup>	. L/cm <sup>3</sup> cm <sup>-1</sup>	
10	283.15	1.32 1.30 1.32 1.31 Av.	1.36	
20	293.15	1.18 1.15 1.19 1.17 Av.	1.26	

The Ostwald coefficents were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of an absorption flask connected to a gas buret by a flexible lead capillary. The system was thermostated in a large water bath.

The volume of gas absorbed in a known volume of degassed petroleum was measured directly using the gas buret.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. No information
- (2) Petroleum. Russian petroleum. Cleaned by boiling in a large copper flask.

# ESTIMATED ERROR:

 $\delta\alpha/\alpha = \pm 0.05$  (Compiler)

# ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Paraffin wax Ind. Eng. Chem. 1954, 46, 2376-2381. VARIABLES: PREPARED BY: P.G.T. Fogg

# EXPERIMENTAL VALUES:

P/kPa = 34.33 - 100.33

т/к	P/mmHg	P/kPa	Soly./cm3g-1§	Bunsen coe	ff. *CO2
345.4	257.5	34.33	0.208	0.471	0.00325
	379.5	50.60	0.329	0.504	0.00514
1	505.5	67.39	0.457	0.528	0.00714
	613.1	81.74	0.571	0.548	0.00892
	752.5	100.33	0.704	0.548	0.0110
	760	101.3	0.710 *		0.01104

<sup>§</sup> volumes of gas were corrected to 273.15 K and 101.3 kPa

# AUXILIARY INFORMATION

# METHOD / APPARATUS / PROCEDURE:

The apparatus was based upon the equilibrium adsorption apparatus described by Brunauer, Emmett and Teller. Gas was circulated through the vessel containing wax.

Pressures were measured with a mercury manometer. Measured quantities of carbon dioxide were delivered to the system from two calibrated burets. A period of 20-60 minutes was allowed for the system to reach equilibrium after each addition of gas.

# SOURCE AND PURITY OF MATERIALS:

- Obtained by heating NaHCO<sub>3</sub>; contained 0.1% N<sub>2</sub>, 0.1% O<sub>2</sub>, 3.4% CO.
- 2. M.pt 50.7°C (ASTM D 87-22); Density/g cm<sup>-3</sup> 0.7716 (68.3°C) 0.7662 (76.8°C) Relative molecular mass 350

# ESTIMATED ERROR:

 $\delta T/K = \pm 2$   $\delta P/\text{mmHg} = \pm 0.2$  $\delta \alpha = \pm 0.004$ ; high pressure =  $\pm 0.012$ ; low pressure (authors)

# REFERENCES:

 Brunauer, S.; Emmett, P.H.; Teller, E. J. Amer. Chem. Soc. 1938, 60, 309.

<sup>\*</sup> extrapolated value given by the authors

<sup>†</sup> calculated by the compiler

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Animal and Vegetable Oils and Fats

**EVALUATOR:** 

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

Solubility of carbon dioxide in animal and vegetable oils and fats.

There have been several measurements (1-6) of the solubility of carbon dioxide in olive oil at a partial pressure of 101.3 kPa. The most reliable are probably those carried out by Yeh and Petersen (1) from 298.2 K to 318.2 K and by Battino et al.(2) from 298.0 K to 327.9 K. In both cases the oil was carefully degassed before absorption of carbon dioxide. Values of mole fraction solubility from the two sources agree to within 2% The recommended smoothing equation, based on these two sets of data, is given below.

 $\ln x_{CO_2} = -88.009 + 4996.8/(T/K) + 11.9998\ln(T/K)$ 

temperature range = 298.0-327.9 Kstandard deviation in  $x_{CO_2} = 0.00023$ 

The average thermodynamic values for the transfer of one mole of carbon dioxide at a partial pressure of 101.3 kPa to a hypothetical solution of unit mole fraction concentration are

 $\Delta H^{\circ}/J \text{ mol}^{-1} = -10479$  $\Delta S^{\circ}/J \text{ mol}^{-1} \text{ K}^{-1} = -59.1$ 

The equation for the Bunsen coefficient,  $\boldsymbol{\alpha},$  based on data from the two sources is

 $\ln \alpha = -3.0329 + 1328.0/(T/K) - 0.20002\ln(T/K)$ 

temperature range = 298.0-327.9 K standard deviation in  $\alpha = 0.029$ 

Yeh and Petersen (1) measured the solubilities of carbon dioxide in dog fat, rat-pooled fat, and two samples of human fat over the temperature range 298.2-318.2 K. In all cases Bunsen coefficients were within 1.6% of the values which they found for olive oil at the same temperatures. Nichols (7) also measured solubility in dog fat, rat-pooled fat and human fat. Values of Bunsen coefficients from these measurements were close to each other but about 10% lower than Yeh and Peterson's values.

Tomoto and Kusano (5) measured solubility in olive oil, linseed oil and soybean oil. The data which they published are close to those in an earlier paper by Tomoto (4). They found that Bunsen coefficients at 293.2 K and 323.2 K for solution in linseed oil were greater than the coefficients for olive oil. Bunsen coefficients for soybean oil were less than for olive oil. Schmidt-Nielsen's data (3) also indicate that the Bunsen coefficient for carbon dioxide in linseed oil at 293.2 K is greater than that for olive oil at this temperature. However Tomoto's and Schmidt-Nielsen's values of Bunsen coefficients for both linseed oil and olive oil are lower than Bunsen coefficients for olive oil from data published by Yeh and Petersen and by Battino et al. which are recommended above.

Schmidt-Nielsen (3) also found that the solubility of carbon dioxide  $(/cm^3\ g^{-1})$  in cod-liver oil and in herring oil was greater than in olive oil. Further work is needed to establish the relative solubilities in these solvents.

Vibrans (8) measured solubility in cottonseed oil at about 298 and 318 K. Temperature control was poor but averaged values of Bunsen coefficients are close to those for olive oil. The average value for 296-299 K was found to be 1.34  $\pm 0.04$  compared with a value for olive oil at 298.2 K of 1.3565 (Yeh and Petersen). The average value for 318 K was 1.012  $\pm 0.029$  compared with 1.0150 for olive oil (Yeh and Petesen). Vibrans also found

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Animal and Vegetable Oils and Fats

# **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

that the Bunsen coefficient for dissolution in steam rendered lard at 318 K was 1.014 ±0.012, close to the value of 1.012 for cottonseed oil.

Schaffer and Haller (9) measured solubility in cottonseed oil at 313.2 K. Their value for the Bunsen coefficient was 0.876 which is not in accord with values reported by Vibrans. Schaffler and Haller also reported Bunsen coefficients for solubility in lard at 313.2 K and in butter oil at 313.2 K and 333.15 K. The value for lard is, in this case, slightly lower than the value given by Vibrans (Schaffer at 313.2 K: 1.003; Vibrans at about 318 K: 1.014). The Bunsen coefficients for dissolution in butter oil were greater than values for olive oil reported by Yeh and Petersen (1) and by Battino et al.(2).

- 1. Yeh, S.Y.; Peterson, R.E. J. Pharm. Soc. 1963, 52, 453-458.
- Battino, R.; Evans, F.D.; Danforth, W.F. J. Am. Oil Chem. Soc. 1968, 45, 830-833.
- Schmidt-Nielsen, S. Ann. Acad. Sci. Fenn., Ser. A. 1927, 29(No.12), 7pp.
- 4. Tomoto, N. Miyazaki Daigaku Kogakubu Kenkyu Hokoku 1958, No. 4, 39-46. (Bull. Fac. Eng., Miyazaki Univ.)
- Tomoto, N.; Kusano, K. Yukagaku 1967, 16(3), 108-113. (Oil Chemistry)
- 6. Power, G.G.; Stegall, H. J. Appl. Physiology, 1970, 29, 145-149.
- 7. Nichols, G. Science, 1957, 126, 1244-1245.
- 8. Vibrans, F.C. Oil and Soap 1935, 12, 14-15.
- 9. Schaffer, P.S.; Haller, H.S. Oil and Soap 1943, 20, 161-162.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	
(2) Fats	Ann. Acad. Sci. Fenn., Ser. A.
	1927, 29 (No. 12), 7 pp.
	)
VARIABLES:	PREPARED BY:
T/K = 293 $p_1/kPa = 101$ (1 atm)	H. L. Clever
EXPERIMENTAL VALUES:	and the state of t
T/K	Solubility/ cm <sup>3</sup> (STP) per 100 g
Cod-liver oi	1
293	135
Herring oil	
293	134
Linseed oil	
293	160
Olive oil	
293	117
as approximate	values.
AUXILI	ARY INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The oil is degassed for two hours in a vacuum.	No information.
The oil stands for 24 hours with the dry gas.	
The dissolved gas is removed from the oil by a Barcroft gas pum and the gas volume is measured.	p,
	ESTIMATED ERROR:
1	
	REFERENCES:

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] (2) Olive oil VARIABLES: T/K = 303, 323 p<sub>2</sub>/kPa = 28.64 - 111.67 CRIGINAL MEASUREMENTS: Tomoto, N. Miyazaki Daigaku Kogakubu Kenkyu Hokoku 1958, No. 4, 39 - 46. [Bull. Fac. Eng., Miyazaki Univ.] PREPARED BY: H. L. Clever

Temper	cature	Carbon Dioxide	Sc	lubility	Bunsen
t/°C	<i>T</i> /K	Partial Pressure  p <sub>1</sub> /mmHg	mg g <sup>-1</sup>	$cm^3$ (STP) $g^{-1}$	Coefficient
30	303	214.8	0.676	0.342	1.097
		278.7	0.897	0.454	1.123
		366.7	1.133	0.573	1.115
		549.5	1.696	0.858	1.076
		664.2	1.957	0.990	1.028
		765.0	2.307	1.167	1.052
		837.6	2.491	1.260	1.037
					1.063²
50	323	321.5	0.775	0.392	0.828
		426.4	1.036	0.524	0.834
		528.3	1.293	0.654	0.841
		635.8	1.554	0.786	0.840
		757.8	1.864	0.943	0.845
					0.839 <sup>2</sup>

<sup>&</sup>lt;sup>1</sup> Bunsen coefficient α/cm<sup>3</sup> (STP) cm<sup>-3</sup> atm<sup>-1</sup>.

(214.8 - 837.6 mmHg)

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a thermostated absorption flask, a gas reservoir, and a manometer and leveling bulb system.

The oil is placed in the absorption flask and both are weighed, the system is heated to 80°C and evacuated for six hours to degass the solvent. The gas is admitted to the system. The oil is stirred by a magnetic stirrer until equilibrium is attained.

The flask and contents are disconnected from the system and weighed.
The amount of gas absorbed is calculated from the gain in weight. The
loss of oil due to evaporation during
the degassing is considered
negligible.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Commercial cylinder. Passed through the purification train: stannous chloride, NaHCO3, CuSO4, conc. H2SO4, hot copper, and P2O5.
- (2) Olive oil. Iodine value 83, acid value 0.20, density ρ/g cm<sup>-3</sup> = 0.9076, 0.9007, and 0.8940 at 30, 40, and 50°C, respectively.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$   $\delta p_1/mmHg = \pm 0.5$   $\delta w/mg = \pm 0.5$   $\delta \alpha/\alpha = \pm 0.03 \text{ (compiler)}$ 

<sup>&</sup>lt;sup>2</sup> The author's values, probably from their Henry's law diagrams.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Yeh, S. Y.; Peterson, R. E.		
(2) Olive Oil	J. Pharm. Sci. <u>1963</u> , 52, 453 - 458.		
VARIABLES: T/K = 298.15 - 318.15 P/kPa = 101.325 (1 atm)	PREPARED BY: H. L. Clever		

# EXPERIMENTAL VALUES:

T/K		Bunsen Coefficient α/cm³ (STP) cm-³amt-¹ ± Std. Dev.	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15 303.15 310.15	55.96 52.00 47.40	1.3565 ± 0.0013 1.2519 ± 0.0016 1.1306 ± 0.0016	1.4806 1.3893 1.2849
318.15	42.90	1.0150 ± 0.0015	1.1821

The Bunsen coefficients are the average of three measurements. The Ostwald coefficients were fitted by the method of least squares to the equation  $\log L = A/T + B$  by the authors. The same line fitted olive oil and the fats. From the slope and intercept they obtained

 $\Delta H^{\circ}/\text{cal mol}^{-1} = -1217 \pm 30 \text{ and } \Delta S^{\circ}/\text{cal } K^{-1} \text{ mol}^{-1} = -8.5 \pm 0.1.$ 

The thermodynamic values are for the standard state transfer of one mole of carbon dioxide from the gas phase at a concentration of one mole  $dm^{-3}$  to the solution at a concentration of one mole dm-3. See the evaluation of the carbon dioxide + olive oil system for the thermodynamic values of the standard state transfer on one mole of carbon dioxide from the gas phase at a partial pressure of one atm to the hypothetical unit mole fraction solution.

Smoothed Data: For use between 298.15 and 318.15 K.

 $\ln x_1 = -7.1013 + 12.5711/(T/100 \text{ K})$ 

The standard error about the regression line is  $1.15 \times 10^{-4}$ . For more information see the evaluation.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Oil was dried and degassed by stirring (1) Carbon dioxide. Matheson Co., under vacuum at 80°C for about 12 hr. A 50 ml. sample was placed in an absorption flask attached to a Geffken gas buret (1). The oil was constantly stirred and equilibrated with increments of gas until no change was observed in a differential oil manometer for ½ hr. Difference between initial and final buret readings indicated amount of gas absorbed. Absorption at successively lower temperatures was determined. The authors also measured the viscosity and surface tension of the liquid.

# SOURCE AND PURITY OF MATERIALS:

- Inc. Research grade, maximum impurity 0.3 mol per cent N2 or CO.
- (2) Olive Oil. Magnus, Mabee and Raynard Co., U.S.P.

# ESTIMATED ERROR:

 $\delta T/K = 0.05$  $\delta P/\text{nmHg} = 0.5$  $\delta \alpha/\alpha = 0.005$ 

- 1. Geffken, G.
  - Z. Physik Chem. 1904, 49, 257.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbon dioxide; CO <sub>2</sub> ; [124-38-9]	Tomoto, N.; Kusano, K.
(2) Olive oil	Yukagaku <u>1967</u> , 16 (3), 108 - 113.
	[Oil Chemistry]
VARIABLES: T/K = 303, 323 $p_1/kPa = 20.3 - \sim 101$ (0.2 - about 1 atm)	PREPARED BY: H. L. Clever
EXPERIMENTAL VALUES:	
Temperature	Pungon

Temperature t/°C T/K		Bunsen Coefficient α/cm³ (STP) cm-³ atm-¹
30	303	1.076
50	323	0.8376

Five to seven measurements were made at each temperature over the pressure interval of 0.2 to about 1.0 atm. A diagram of solubility (cm $^3$  per g) vs. pressure was linear. Only the values of the Bunsen coefficient above were tabulated in the paper.

# AUXILIARY INFORMATION

١	METHOD/APPARATUS/PROCEDURE:	SOURC	CE AND PURITY OF MATERIALS:
		(1)	Carbon dioxide.
			Olive oil. The oil had a saponification value of 190.2, an acid value of 0.20, and an iodine value of 83.2. Density $\rho^{30}/g$ cm <sup>-3</sup> = 0.9076, mean mol wt = 885, mean molar volume, $V^{\circ}/\text{cm}^{3}$ mol <sup>-1</sup> = 975.1.
		ESTIN	MATED ERROR:
		REFE	RENCES:
1			

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Olive oil

# ORIGINAL MEASUREMENTS:

Battino, R.; Evans, F. D.; Danforth, W. F.

J. Am. Oil Chem. Soc. 1968, 45, 830 - 833.

# VARIABLES:

T/K: 298.00 - 327.94 P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen Coefficient  \alpha/cm^3(STP) cm^{-3} atm^{-1}	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.00	56.5	1.295	1.412
307.91	48.5	1.105	1.246
318.50	42.1	0.9605	1.120
327.94	38.5	0.8688	1.043

The solubility values were adjusted to a partial pressure of carbon dioxide of 101.325 kPa (1 atm) by Henry's law.

The Bunsen coefficients were calculated by the compiler.

Smoothed Data: For 298.15 - 328.15 K.

$$\ln x_7 = -7.1169 + 12.6193/(T/100K)$$

The standard error about the regression line is  $2.34 \times 10^{-4}$ .

See the evaluation of the carbon dioxide + olive oil system for the recommended Gibbs energy equation and smoothed solubility values.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus is based on the design by Morrison and Billett (1) and the version used is a modification of the apparatus of Clever, Battino, Saylor and Gross (2).

The solvent is sprayed into an evacuated chamber of an all glass apparatus; it is stirred and heated until the pressure drops to the vapor pressure of the liquid. Solubility Determination. The degassed liquid passes in a thin film down a glass spiral tube at a total pressure of one atm of solute gas plus solvent vapor. The gas absorbed is measured in the attached buret system, and the solvent is collected in a tared flask and weighed.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. The Matheson Co., Inc. Research grade. Minimum volume % purity is 99.995.
- (2) Olive oil. A. U.S.P. Fisher Scientific Co., 0.58% free fatty acid. B. Nutritional Biochemicals Corp. 0.30% free fatty acid. The density was measured and fitted to the equation ρ/g cm<sup>-3</sup> = 0.9152 - 0.000468t/C. The average mol wt is 884 ± 45.

ESTIMATED ERROR:  $\delta T/K = \pm 0.03$ 

$$\delta T/K = \pm 0.03$$
  
 $\delta P/\text{mmHg} = \pm 0.5$   
 $\delta x_1/x_1 = \pm 0.03$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.
- Clever, H. L.; Battino, R.; Saylor, J. H.; Gross, P. M. J. Phys. Chem. <u>1957</u>, 61, 1078.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] Power, G.G.; Stegall, H. 2. Olive oil. J. Appl. Physiology, 1970, 29, 145-9. VARIABLES: PREPARED BY: C.L. Young T/K = 310.15EXPERIMENTAL VALUES: S.D.\* Bunsen coefficient, T/KNo. of measurements 310.15 1.23 0.02 \* Standard deviation. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Liquid saturated with gas in a stirred cell. 5.0 cm<sup>3</sup> samples of liquid removed in a calibrated Matheson Co. sample, purity better than 99.7 mole per cent. syringe and amount of gas extracted by two extraction in a van Slyke apparatus determined. Details in 2. No details given. source and ref. (1). ESTIMATED ERROR: $\delta T/K = \pm 0.1$ REFERENCES: 1. Power, G.G. J. Appl. Physiology. 1968, 24, 468.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Animal and human fat.

# ORIGINAL MEASUREMENTS:

Nichols, G.

Science, 1957, 126, 1244-5.

# VARIABLES:

T/K = 311.2P/kPa = 101.3

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

l	Solvent	Number of samples	Density	Density M.pt /g cm <sup>-3</sup> /°C		oility of C	O <sub>2</sub> *	
		sampres	/ g Cm / C	cm³ g <sup>-1</sup>	α /m	H mol kg⁻¹	mmHg <sup>-1</sup>	
	Dog fat	9	0.9155	30	0.9405 ±0.0140	0.8609 ±0.0129	0.0556	
	Rat fat (	A) 9	0.9154	19	0.9738 ±0.0092	0.8917 ±0.0077	0.0576	
	Rat fat (	в) 10	0.9154	19	0.9813 ±0.0089	0.8985 ±0.0082	0.0578	
İ	Human fat	8	0.9110	18	0.9306 ±0.0483	0.8476 ±0.0447	0.0550	
ı	m / 122 24 4	0. D 10	4 2 1-0-					

T/K = 311.2;  $P_{CO_2} = 101.3$  kPa

\* volume of gas corrected to 273.15 K, 101.3 kPa;  $\alpha$  is the Bunsen coefficient; H is Henry's constant defined as millimoles of  $CO_2$  dissolved per kilogram of fat per mmHg partial pressure of  $CO_2$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Fatty tissue homogenized with sand at 30-35 °C in a buffer solution at pH 4.0 or, in the case of one rat sample, at pH 7.40. Fat removed by centrifuging. Dry air mixed with 23.5-24.9% CO<sub>2</sub> passed for 2.5 to 5 h through samples of volume 3-5 cm³. Solutions then analysed by use of a van Slyke apparatus. Concentrations of CO<sub>2</sub> corrected to a partial pressure of 101.3 kPa.

# SOURCE AND PURITY OF MATERIALS:

- 1. No information
- 2. Depot fat from the following
  sources:

Dog - perirenal and subcutaneous fat from an adult mongrel dog 2 h after death by exsanguination under anesthesia.

Rat - perirenal, subcutaneous and retroperitoneal fat from six 200-day old Wistar rats killed by a blow on the head followed by exsanguination. Samples pooled and divided in two parts, A and B.

Human - omental fat from an 86-year old woman 5 h after death.

Negligable water content - no loss of weight from any sample during 48 h in a dessicator

ESTIMATED ERROR:

See above

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Dog Fat

# ORIGINAL MEASUREMENTS:

Yeh, S. Y.; Peterson, R. E.

J. Pharm. Sci. 1963, 52, 453 - 458.

VARIABLES:

T/K = 298.15 - 318.15P/kPa = 101.325 (1 atm) PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

<i>T</i> /K	Bunsen Coefficient α/cm³ (STP) cm⁻³ atm⁻¹ ± Std. Dev.	Ostwald Coefficient L/cm <sup>3</sup> cm <sup>-3</sup>
298.15	1.3411 ± 0.0022	1.4638
303.15	1.2491 ± 0.0015	1.3862
310.15	1.1283 ± 0.0014	1.2822
318.15	1.0122 ± 0.0011	1.1790

The Bunsen coefficients are the average of three measurements. The Ostwald coefficients were fitted by the method of least squares to the equation  $\log L = A/T + B$  by the authors. The same line fitted olive oil and the fats. From the slope and intercept they obtained

 $\Delta H^{\circ}/\text{cal mol}^{-1} = -1273 \pm 30 \text{ and } \Delta S^{\circ}/\text{cal } K^{-1} \text{ mol}^{-1} = -8.5 \pm 0.1.$ 

The thermodynamic values are for the transfer of one mole of carbon dioxide from the gas phase at a concentration of one mole  $dm^{-3}$  to the solution phase at a concentration of one mole  $dm^{-3}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Fat was dried and degassed by stirring under vacuum at 80°C for about 12 hr. A 50 ml. sample was placed in an absorption flask attached to a Geffken gas buret (1). The fat was constantly stirred and equilibrated with increments of gas until no change was observed in a differential oil manometer for 1/2 hr. Difference between initial and final buret readings indicated amount of gas absorbed. Absorption at successively lower temperatures was determined. The authors also measured the viscosity and surface tension of the liquid.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Matheson Co. Research grade, maximum impurity 0.3 mole per cent N<sub>2</sub> or CO.
- (2) Dog perineal, mesenteric, omental, and other adipose fats were extracted with petroleum ether (b.p. 309-338 K). The ether was evaporated at 353 K under vacuum for several hours. Stored under refrigeration until use.

# ESTIMATED ERROR:

 $\delta T/K = 0.05$   $\delta P/mmHg = 0.5$   $\delta \alpha/\alpha = 0.005$ 

- 1. Geffken, G.
  - Z. Physik Chem. 1904, 49, 257.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Rat-pooled Fat

# ORIGINAL MEASUREMENTS:

Yeh, S. Y.; Peterson, R. E.

J. Pharm. Sci. 1963, 52, 453 - 458.

# VARIABLES:

T/K = 298.15 - 318.15P/kPa = 101.325 (1 atm) PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

<i>T</i> /K	Bunsen Coefficient α/cm³ (STP) cm⁻³atm⁻¹ ± Std. Dev.	Ostwald Coefficient _L/cm³cm-3
298.15	1.3363 ± 0.0073	1.4586
303.15	1.2344 ± 0.0051	1.3700
310.15	1.1125 ± 0.0035	1.2643
318.15	0.9989 ± 0.0041	1.1635

The Bunsen coefficients are the average of three measurements. The Ostwald coefficients were fitted by the method of least squares to the equation  $\log L = A/T + B$  by the authors. The same line fitted olive oil and the fats. From the slope and intercept they obtained

 $\Delta H^{\circ}/\text{cal mol}^{-1} = -2713 \pm 30 \text{ and } \Delta S^{\circ}/\text{cal } K^{-1} \text{ mol}^{-1} = -8.5 \pm 0.1.$ 

The thermodynamic values are for the transfer of one mole of carbon dioxide from the gas phase at a concentration of one mole  $\rm dm^{-3}$  to the solution at a concentration of one mole  $\rm dm^{-3}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Fat was dried and degassed by stirring under vacuum at 80°C for about 12 hr. A 50 ml. sample was placed in an absorption flask attached to a Geffken gas buret (1). The fat was constantly stirred and equilibrated with increments of gas until no change was observed in a differential oil manometer for 1/2 hr. Difference between initial and final buret readings indicated amount of gas absorbed. Absorption at successively lower temperatures was determined. The authors also measured the viscosity and surface tension of the liquid.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Matheson Co. Research grade, maximum impurity 0.3 mole per cent  $\rm N_2$  or CO.
- (2) Rat retroperitoneal, mesenteric, omental, and hair clipped skin was cut into about 2.5 cm squares, dried at 353 K under vacuum, coarsely crushed and then extracted with petroleum ether (b.p. 308-338 K) in a Soxhlet extractor. The ether was evaporated at 353 K for several hours under vacuum. Stored under refrigeration until use.

ESTIMATED ERROR:  $\delta T/K = 0.05$   $\delta P/\text{mmHg} = 0.5$  $\delta \alpha/\alpha = 0.005$ 

- 1. Geffken, G.
  - Z. Physik Chem. 1904, 49, 257.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Human Fat

# ORIGINAL MEASUREMENTS:

Yeh, S. Y.; Peterson, R. E.

J. Pharm. Sci. 1963, 52, 453 - 458.

VARIABLES:

T/K = 298.15 - 318.15P/kPa = 101.325 (1 atm) PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

EXPERIMENTA	AL VALUES:				
	Human fat l			Human fat 2	
T/K	Bunsen	Ostwald	T/K	Bunsen	Ostwald
	Coefficient <sup>1</sup>	Coefficient		Coefficient <sup>1</sup>	Coefficient
_	± Std. Dev.	$L/\mathrm{cm}^3\mathrm{cm}^{-3}$		_ ± Std. Dev	$L/cm^3cm^{-3}$
298.15	$1.3589 \pm 0.0015$	1.4833	298.15	$1.3376 \pm 0.0044$	1.4600
303.15	$1.2471 \pm 0.0015$	1.3840	303.15	1.2448 ± 0.0044	1.3815
310.15	$1.1359 \pm 0.0018$	1.2897	310.15	$1.1254 \pm 0.0014$	1.2789
_318.15	$1.0153 \pm 0.0020$	1.1826	318.15	$1.0122 \pm 0.0009$	1.1790

 $^{1}$   $\alpha/\text{cm}^{3}$  (STP) cm $^{-3}$  atm $^{-1}$ 

The Bunsen coefficients are the average of three measurements. The Ostwald coefficients were fitted by the method of least squares to the equation  $\log L = A/T + B$  by the authors. The same line fitted olive oil and the fats. From the slope and intercept they obtained

 $\Delta H^{\circ}/\text{cal mol}^{-1} = -2713 \pm 30 \text{ and } \Delta S^{\circ}/\text{cal K}^{-1} \text{ mol}^{-1} = -8.5 \pm 0.1.$ 

The thermodynamic values are for the transfer of one mole of carbon dioxide from the gas phase at a concentration of one mole  $dm^{-3}$  to the solution at a concentration of one mole  $dm^{-3}$ .

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Fat was dried and degassed by stirring under vacuum at 80°C for about 12 hr. A 50 ml. sample was placed in an absorption flask attached to a Geffken gas buret (1). The fat was constantly stirred and equilibrated with increments of gas until no change was observed in a differential oil manometer for ½ hr. Difference between initial and final buret readings indicated amount of gas absorbed. Absorption at successively lower temperatures was determined. The authors also measured the viscosity and surface tension of the liquid.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Matheson Co. Research grade, maximum impurity 0.3 mole per cent N<sub>2</sub> or CO.
- (2) Human omental fats obtained from two deceased patients (1 and 2). Extracted with petroleum ether (b.p. 309-338 K). The ether was evaporated at 353 K under vacuum for several hours. Stored under refrigeration until use. Fat 2 appeared to have more stearine precipitate than fat 1 at 296 K.

ESTIMATED ERROR:

 $\delta T/K = 0.05$  $\delta P/mmHg = 0.5$  $\delta \alpha/\alpha = 0.005$ 

# REFERENCES:

Geffken, G.
 Physik. Chem. 1904, 49, 257.

- (1) Carbon dioxide; CO2; [124-38-9]
- (2) Linseed oil

# ORIGINAL MEASUREMENTS:

Tomoto, N.

Miyazaki Daigaku Kogakubu Kenkyu Hokoku 1958, No. 4, 39 - 46.

[Bull. Fac. Eng., Miyazaki Univ.]

# VARIABLES:

T/K = 303, 323 $p_1/kPa = 27.45 - 98.405$ 

(205.9 - 738.1 mmHg)

# PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

ature	Carbon Dioxide	Solubility		Bunsen
T/K	Partial Pressure  p <sub>1</sub> /mmHg	mg g <sup>-1</sup>	cm <sup>3</sup> (STP) g <sup>-1</sup>	Coefficient
303	205.9 235.4 300.8 328.8 406.7 510.0 608.8 728.8	0.678 0.777 0.951 1.077 1.346 1.635 1.919 2.228	0.343 0.393 0.481 0.545 0.681 0.827 0.971	1.169 1.172 1.122 1.163 1.176 1.137 1.115
				1.130 <sup>2</sup>
323	232.3 374.1 502.7 615.5 689.4 738.1	0.546 0.886 1.194 1.429 1.589 1.706	0.276 0.448 0.604 0.723 0.804 0.863	0.822 0.830 0.830 0.812 0.806 0.808
	T/K	T/K Partial Pressure  p_/mmHg  303	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$

<sup>&</sup>lt;sup>1</sup> Bunsen coefficient  $\alpha/\text{cm}^3$  (STP) cm<sup>-3</sup>atm<sup>-1</sup>.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a thermostated absorption flask, a gas reservoir, and a manometer and leveling bulb system.

The oil is placed in the absorption flask and both are weighed, the system (2) Linseed oil. is heated to 80°C and evacuated for six hours to degass the solvent. The gas is admitted to the system. The oil is stirred by a magnetic stirrer until equilibrium is attained.

The flask and contents are disconnected from the system and weighed. The amount of gas absorbed is calculated from the gain in weight. The loss of oil due to evaporation during the degassing is considered negligible.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Commercial cylinder. Passed through the purification train: stannous chloride, NaHCO3, CuSO4, conc. H<sub>2</sub>SO<sub>4</sub>, hot copper, and P<sub>2</sub>O<sub>5</sub>.
- Linseed oil. Iodine value 175, acid value 0.32, density  $\rho/g \text{ cm}^{-3}$ = 0.9232, 0.9163, and 0.9096 at 30, 40, and 50°C, respectively.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ 

 $\delta p_{1/\text{mmHg}} = \pm 0.5$   $\delta w/\text{mg} = \pm 0.5$ 

 $\delta \alpha / \alpha = \pm 0.03$  (compiler)

<sup>&</sup>lt;sup>2</sup> The author's values, probably from their Henry's law diagrams.

# 443 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] Tomoto, N.; Kusano, K. (2) Linseed oil Yukagaku 1967, 16 (3), 108 - 113. [Oil Chemistry] VARIABLES: PREPARED BY: T/K = 303, 323 $p_1/kPa = 20.3 - \sqrt{101}$ H. L. Clever (0.2 - about 1 atm) EXPERIMENTAL VALUES: Temperature Bunsen Coefficient t/°C T/K $\alpha/cm^3$ (STP) $cm^{-3}$ $atm^{-1}$ 30 303 1.142 50 323 0.818<sub>n</sub> Five to seven measurements were made at each temperature over the pressure interval of 0.2 to about 1.0 atm. A diagram of solubility (cm³ per g) vs. pressure was linear. Only the values of the Bunsen coefficient above were tabulated in the paper. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) Carbon dioxide. (2) Linseed oil. The oil had a saponification value of 191.2, an acid value of 0.23, an iodine value of 175.7. Density $\rho^{3}$ 0/g cm<sup>-3</sup> = 0.9232, mean mol wt = 880, mean molar volume $V^{\circ}/\text{cm}^{3}$ mol<sup>-1</sup> = 953.2. ESTIMATED ERROR:

# COMPONENTS: (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9] Tomoto, N.; Kusano, K. (2) Soybean oil Yukagaku 1967, 16 (3), 108 - 113. [Oil Chemistry] VARIABLES: T/K = 303.15 - 343.15 p<sub>1</sub>/kPa = 20.3 - ~101 (0.2 - about 1 atm) PREPARED BY: H. L. Clever

# EXPERIMENTAL VALUES:

Temperature t/°C T/K		Bunsen Coefficient α/cm³ (STP) cm-³ atm-1
30	303	1.018
40	313	0.901
50	323	0.8002
70	343	0.6348

Five to seven measurements were made at each temperature over the pressure interval of 0.2 to about 1.0 atm. A diagram of solubility (cm³ per g) vs. pressure was linear. Only the values of the Bunsen coefficient above were tabulated in the paper.

# AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	<ul> <li>SOURCE AND PURITY OF MATERIALS: <ul> <li>(1) Carbon dioxide.</li> </ul> </li> <li>(2) Soybean oil. The oil had a saponification value of 192.0, an acid value of 0.17, an iodine value of 128.5. Density ρ³ 0/g cm⁻³ = 0.9132, Mean mol wt = 877, mean molar volume yo/cm³ mol⁻¹ = 960.4.</li> </ul>
	ESTIMATED ERROR:
	REFERENCES;

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Soybean oil

# ORIGINAL MEASUREMENTS:

Tomoto, N.

Miyazaki Daigaku Kogakubu Kenkyu Hokoku 1958, No. 4, 39 - 46.

[Bull. Fac. Eng., Miyazaki Univ.]

VARIABLES:

$$T/K = 303 - 323$$
  
 $p_1/kPa = 26.28 - 110.66$   
 $(197.1 - 830.0 mmHg)$ 

PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

Temper	rature	Carbon Dioxide Partial Pressure $p_{1}/\mathrm{mmHg}$	Solubility		Bunsen
t/°C	T/K		mg g <sup>-1</sup>	cm <sup>3</sup> (STP) g <sup>-1</sup>	Coefficient $\alpha^1$
30	303	272.5 347.5 444.1 588.8 765.2	0.795 1.026 1.307 1.726 2.153	0.402 0.519 0.661 0.873 1.089	1.026 1.037 1.033 1.029 0.988
					1.0162
40	313	197.1 254.1 346.9 350.2 467.8 580.0 723.4	0.493 0.646 0.915 0.916 1.274 1.533 1.853	0.249 0.327 0.463 0.463 0.644 0.776	0.872 0.886 0.920 0.912 0.949 0.921 0.893
50	323	306.5 380.5 491.0 582.0 693.1 830.0	0.660 0.850 1.117 1.352 1.617	0.334 0.430 0.565 0.684 0.818 0.969	0.911 <sup>2</sup> 0.745 0.772 0.787 0.804 0.807 0.799
1 Bungar					0.8022

Bunsen coefficient  $\alpha/\text{cm}^3$  (STP) cm<sup>-3</sup> atm<sup>-1</sup> The author's values, probably from his Henry's law diagrams.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a thermostated absorption flask, a gas reservoir, and a manometer and leveling bulb system.

The oil is placed in the absorption flask, heated to 80 C and the system evacuated for six hours to degass the solvent. The gas is admitted to the system. The oil is stirred by a magnetic stirrer until equilibrium is attained.

The flask and contents are disconnected from the system and weighed. The amount of gas absorbed is calculated from the gain in weight. The loss of oil due to evaporation during the degassing is considered negligible.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Commercial cylinder. Passed through the purification train: stannous chloride, NaHCO3, CuSO4, conc. H<sub>2</sub>SO<sub>4</sub>, hot copper, and P<sub>2</sub>O<sub>5</sub>.
- (2) Soybean oil. Iodine value 128, acid value 0.33, density  $\rho/g$  cm<sup>-3</sup> = 0.9132, 0.9066, and 0.9001 at 30, 40, and 50  $^{\circ}$ C, respectively.

ESTIMATED ERROR:  $\delta T/K = \pm 0.5$ 

 $\delta p_1/\text{mmHg} = \pm 0.5$  $\delta \omega / mg = \pm 0.5$ 

 $\delta \alpha / \alpha = \pm 0.03$  (compiler)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbon dioxide; CO <sub>2</sub> ;	Vibrans, F. C.
[124-38-9]	0il and Soap <u>1935</u> , 12, 14 - 15.
(2) Cottonseed oil	200 and 200p <u>200</u> 3, 12, 11
Steam rendered lard	
VARIABLES:	PREPARED BY:
T/K = 296-299, 318 p/kPa = 101 (1 atm)	P. L. Long H. L. Clever
EXPERIMENTAL VALUES: T/K	Bunsen
	Coefficient 1 cm 3 (STP) cm 3 atm 1
Cottonseed oil	
296 - 299	140.0 130.5
	133.0
	130.8 _135.9_
	134.0 Av. σ ± 4.0
318	105.8 101.7
	98.9
	101.1
	102.2 101.2 Av. σ ± 2.9
Steam rendered la	
318	100.4
	101.0
	100.4 102.6
	101.4 Av. o ± 1.2
1 The author labeled his results as of	cm <sup>3</sup> (STP) per 100 cm <sup>3</sup> of oil.
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Van Slyke manometric method (1).	(1) Carbon dioxide. Commercial cylinder. Source and purity not stated.
	(2) Cottonseed oil. Commercial sample bought on market. Representative of its class.
	Lard. From a mixture of killing and cutting fats. Steam rendered.
	ESTIMATED ERROR:
1	$\delta T/K = \pm 3$ at room temperature,
1	$\begin{array}{cccccccccccccccccccccccccccccccccccc$
	REFERENCES:
	1. Van Slyke, D. D.; et al. J. Biol. Chem. 1924, 61, 523 and 575.

- (1) Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- (2) Cottonseed oil Butter oil

Lard

VARIABLES:

T/K = 313.15, 333.15 KPa = 101.3 (1 atm) p/kPa = 101.3

ORIGINAL MEASUREMENTS:

Schaffer, P. S.; Haller, H. S.

0il and Soap 1943, 20, 161 - 162.

PREPARED BY:

P. L. Long H. L. Clever

# EXPERIMENTAL VALUES:

<i>T</i> /K	Bunsen Coefficient <sup>1</sup> 10 <sup>2</sup> α/cm <sup>3</sup> (STP) cm <sup>-3</sup> atm <sup>-1</sup>		
Cottonse	ed oil		
313.15	87.6		
Butter o	il		
313.15	109.5		
333.15	91.0		
Lard			
313.15	100.3		

<sup>1</sup> The author labeled his solubility values as cm<sup>3</sup>gas (STP) per 100 cm<sup>3</sup> of fat. The unit is the same as 100 x Bunsen coefficient.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a reaction flask connected to a water jacketed gas buret, a mercury leveling bulb, and a differential manometer. The reaction vessel is attached to a shaking mechanism in an air bath.

A 50 cm<sup>3</sup> sample of oil is placed in the flask. Heat and vacuum are applied to remove dissolved gases. The sample is cooled to the temperature of the measurement. The gas is admitted, a zero reading is taken. The system is shaken until the sample takes up no more gas at a pressure of one atm. Three dterminations are made on each sample.

# SOURCE AND PURITY OF MATERIALS:

- (1) Carbon dioxide. Commercial cylinder. Source and purity not stated.
- (2) Cottonseed oil. Good grade commercial product.

Butter oil. Obtained from butter prepared in the lab from fresh cream.

Lard. Good grade commercial product.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ 

 $\delta\alpha/\alpha = \pm 0.003$  (authors,

error among three determinations).

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Polymeric Materials

### **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

### CRITICAL EVALUATION:

Solubility of carbon dioxide in polymeric materials

The solubility constant for dissolution of gas in a polymer has been defined (1) as

volume of gas absorbed (reduced to 1 atm, 273.15 K)

volume of polymer × pressure of gas/atm

Solubility in different samples of polyethylene has been measured by Michaels and Bixler (1) at 273.2 K; 101.3 kPa. Values of the solubility constant were unaffected by the magnitude of the number average relative molecular mass. Ash et al. (2) measured solubility in a single sample of polyethylene at 313.2-333.2 K. Values of the solubility constant are consistent with a value given by Michaels and Bizler for polyethylene tested at 273.2 K, if error limits are taken into account.

Solubility in orientated polyethylene terephthalate having an amorphous volume fraction of 0.49 has been measured by Vieth  $et\ al.(3)$  from 5.5 kPa to 130.5 kPa at 298.2 K and 313.2 K. The authors showed that the measurements were consistent with earlier measurements of solubility in samples of unorientated material having amorphous volume fractions of 0.58 and 1, reported by Michaels  $et\ al.(4)$ .

Michaels and Bixler (1) measured the dissolution of carbon dioxide in unvulcanised smoked sheet rubber. The solubility constant for this material at 273.2 K was found to be  $0.95~\rm atm^{-1}$ . This value may be compared with a solubility constant for unvulcanised smoked sheet rubber of  $1.02~\rm atm^{-1}$  at 293 K which was reported by Venable and Fuwa (5). Venable and Fuwa also reported the solubility in other samples of rubber.

Solubility in polyvinyl acetate has been measured by Liu and Prausnitz (6) and in Nylon 11 by Ash  $et\ al.(2)$ . Solubility in hydrogenated polybutadiene was measured by Michaels and Bixler. There is no reason to doubt the reliability of these sets of measurements but no other work on these systems is available to the evaluator for comparison.

- 1. Michaels, A.S.; Bixler, H.J. J. Polymer Sci. 1961, 50, 393-412.
- 2. Ash, R.; Barrer, R.M.; Palmer, D.G. Polymer, 1970, 11, 421-435.
- Vieth, W.R.; Alcalay, H.H.; Frabetti, A.J. J. Appl. Poly. Sci. 1964, 8, 2125-2138.
- Michaels, A.S.; Vieth, W.R.; Barrie, J.A. J. Appl. Phys. <u>1963</u>, 34, 1-12.
- 5. Venable, C.S.; Fuwa, T. *J. Ind. Eng. Chem.* 1922, 14, 139-142.
- 6. Liu, D.D.; Prausnitz, J.M. J. Polymer Sci. (Polymer Phys. Edn.) 1977, 15, 145-153.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Ethene, homopolymer, (polyethylene); (C<sub>2</sub>H<sub>4</sub>)<sub>x</sub>; [9002-88-4]
  Hydrogenated polybutadiene
  Natural rubber

# ORIGINAL MEASUREMENTS:

Michaels, A.S.; Bixler, H.J.

J. Polymer Sci. 1961, 50, 393-412.

# VARIABLES:

P/kPa = 101.3 T/K = 273.15

# PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

Polymer	Solubility constant, k' /atm <sup>-1</sup>	Volume fraction of amorphous polymer, $\alpha$
Polyethylene	0.451 ±0.023	0.22-0.65
Hydrogenated polybutadiene Natural rubber	0.577 0.95	0.71 1

The solubility constant, k, is defined as the ratio of volume of gas absorbed at a partial pressure of gas of 1 atm to volume of polymer, corrected to 273.15 K and 1 atm, . The authors state that the value of k depends upon the volume fraction of amorphous polymer in the sample. Constants k' given above refer to hypothetical amorphous polymers and are related to k by the equation

$$k' = \alpha k$$

where  $\alpha$  is the volume fraction of amorphous polymer. The authors measured the solubility of thirteen different gases in three different polyethylenes having different number average relative molecular mass. These polyethylenes were Grex,  $Alathon\ 14$  and  $Epolene\ C$ . These three polymers gave no significant differences between values of k' for a particular gas. The hydrogenated polybutadiene was a sample of Hydropol.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Two methods of measuring solubility are mentioned. One method, used for samples of polyethylene, involved equilibrating the gas under test at a pressure of about 1 atm with pellets of the polymer. Gas in the voids was then quickly pumped off during a period of about 10 secs. Gas which subsequently diffused from the polymer was taken to be dissolved gas. It was estimated that about 5% of the dissolved gas was lost during the rapid evacuation périod.

A second method was the time lag method based upon work by Barrer (1). Gas at pressures from 5 mmHg to 800 mmHg was brought into contact with a film of polymer in an evacuated section of the apparatus. The build up of gas at the other side of the film was monitored. this method was used for all the polymers under test with the exception of  $Epolene\ C$ .

# SOURCE AND PURITY OF MATERIALS:

- 1. From a cylinder, dried over calcium sulfate before use.
- 2. Grex. Manufactured by W.R. Grace & Co.  $\overline{M}_{R}$  = 40 000.  $\alpha$  = 0.22-0.31. Alathon 14. Manufactured by E.I. du Pont de Nemours & Co.  $\overline{M}_{R}$  = 26 000.  $\alpha$  = 0.57-0.59.

Epolene C Manufactured by Tennessee Eastman Co.  $\overline{M}_n=6~600$ .  $\alpha=0.65~Hydropol$  Manufactured by Phillips Petroleum Co. by hydrogenation of  $(41\,^\circ\text{F})$  emulsion polybutadiene.  $\overline{M}_n=100~000$ .  $\alpha=0.71$  Natural rubber Unvulcanised smoked sheet (Hevea)  $\overline{M}_n=400~000$   $\alpha=1$ .

 $(\overline{N}_n = \text{number average relative molecular mass})$ 

# REFERENCES:

 Barrer, R.M. Diffusion In and Through Solids, 1951 Cambridge University Press, Cambridge, UK.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Ethene, homopolymer,
   (polyethylene); (C<sub>2</sub>H<sub>4</sub>)<sub>x</sub>;
   [9002-88-4]

# ORIGINAL MEASUREMENTS:

Ash, R.; Barrer, R.M.; Palmer, D.G. Polymer, 1970, 11, 421-35.

# VARIABLES:

T/K = 293.2-333.2P/kPa = 0-33

# PREPARED BY:

P.G.T. Fogg

### EXPERIMENTAL VALUES:

T/K	Henry's law solubility constant/atm		
293.2	0.321		
303.2	0.301		
313.2	0.289		
323.2	0.283		
333.2	0.273		

Henry's law solubility constant was defined as :

volume of gas absorbed, reduced to 273.2 K and 1 atm

volume of polymer × pressure of gas/atm

Values of the solubility constant were found from the slopes of graphs of solubility against pressure.

1 atm = 101.325 kPa

# AUXILIARY INFORMATION

# METHOD APPARATUS/PROCEDURE:

The gas at a known temperature and pressure was allowed to reach equilibrium with a sample of the polymer. The gas phase was then flushed out by mercury and the dissolved gas allowed to desorb into a previously evacuated vessel of known volume. The pressure of the desorbed gas was measured with a McLeod gauge. The temperature of the desorbed gas was also measured and the quantity of gas calculated from its volume, pressure and temperature. Correction was made for the absorbed gas lost during the flushing process. Measurements were made at various initial pressures of gas to a maximum pressure of about 25 cmHg (33 kPa).

# SOURCE AND PURITY OF MATERIALS:

- Spectrally pure sample supplied by British Oxygen Company.
- From laminated tubing made by Messrs. Griflex Ltd.

# ESTIMATED ERROR:

 $\delta T/K < \pm 0.1$   $\delta (\text{solubility constant}) = \pm 2\%$ (authors)

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- Poly(oxy-1,2-ethanediyloxycarbonyl-1,4-phenylenecarbonyl),
   (poly(ethylene terephthalate));
   (C<sub>10</sub>H<sub>8</sub>O<sub>4</sub>)<sub>x</sub>; [25038-59-9]

# ORIGINAL MEASUREMENTS:

Vieth, W.R.; Alcalay, H.H.; Frabetti, A.J.

J. Appl. Poly. Sci. 1964, 8, 2125-2138.

# VARIABLES:

T/K = 298.2, 313.2P/kPa = 5.5-130.5

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

T/K	P/mmHg	P/kPa	Solubility*
298.2	41	5.5	0.118
	91	12.1	0.272
	129	17.2	0.378
	272	36.3	0.763
	395	52.6	1.002
	591	78.8	1.356
	787	105.0	1.687
	903	120.4	1.843
313.2	72	9.6	0.146
	147	19.7	0.275
	256	34.1	0.439
	419	55.9	0.650
	568	75.8	0.830
	700	93.3	0.996
	870	116.0	1.180
	979	130.5	1.283

Solubility is defined as the volume of gas, reduced to 101.3 kPa and 273.15 K, dissolved by one volume of polymer

Data were presented as points on two graphs. The compiler took measurements from these graphs to compile the co-ordinates of the experimental points

# AUXILIARY INFORMATION

# METHOD APPARATUS/PROCEDURE:

A static method was used. The apparatus is described in ref. (1). The polymer was in the form of film of thickness 1 mil (0.00254 cm).

# SOURCE AND PURITY OF MATERIALS:

- 1. Minimum purity 99.5%.
- Crystalline biaxially oriented Mylar supplied by the Mylar Laboratory of E.I. du Pont de Nemours & Co.; ρ = 1.394 g cm<sup>-3</sup>; amorphous volume fraction = 0.49; number average relative molecular mass = 15000-20000.

# ESTIMATED ERROR:

 $\delta$ (Solubility) =  $\pm 8\%$  (authors) Errors on transfering data from graphs:  $\delta$ (Solubility) =  $\pm 0.002$ ;  $\delta P/\text{mmHg} = \pm 2$  (compiler)

# REFERENCES:

 Michaels, A.S.; Vieth, W.R.; Barrie, J.A.
 J. Appl. Phys. 1963, 34, 1.

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Poly(oxy-1,2-ethenediyloxy carbonyl-1,4-phenylenecarbonyl),
   (poly(ethylene terephthalate));
   (C10H<sub>8</sub>O<sub>4</sub>)<sub>x</sub>; [25038-59-9]

# ORIGINAL MEASUREMENTS:

Michaels, A.S.; Vieth, W.R.; Barrie, J.A.

J. Appl. Phys. 1963, 34, 1-12

### VARIABLES:

 $P/kPa \simeq 5-1240$ T/K = 298-379

# PREPARED BY:

P.G.T. Fogg

# EXPERIMENTAL VALUES:

Absorption of carbon dioxide in various samples of polyethylene terephthalate of different degrees of crystallinity and thicknesses were measured by time-lag solubility measurements and by static measurements. Absorption isotherms for glassy amorphous polymer were explained by postulating that absorption took place by two concurrent mechanisms. One mechanism involved the filling of voids and the other an ordinary dissolution process. The shape of the isotherms was explained by assuming that the filling of the voids was consistent with a Langmuir mechanism and the dissolution was consistent with Henry's law.

 $C^*$  = volume of gas, reduced to 273.15 K and 101.3 kPa, taken up by one cm<sup>3</sup> of amorphous polymer.

 $C_{\rm D}^*$  = reduced volume of gas absorbed by a dissolution process

 $C_{H}^{*}$  = reduced volume of gas absorbed by a void-filling process

 $C_{\mu}^{*}$  = reduced volume of gas absorbed by saturation of voids

b = a constant

 $k_{\rm D}^{\, \star} \, = \, {\rm solubility}$  constant for dissolution defined as

reduced volume of gas dissolved

pressure × (volume of amorphous polymer)

 $k^*$  = solubility constant for adsorption of gas defined as the value at low pressures of

reduced volume of gas adsorbed in voids and by dissolution

pressure × (volume of amorphous polymer)

At a pressure of P it follows that

$$C^* = C_{\rm H}^* + C_{\rm D}^* \tag{1}$$

$$= C_{3}^{*} bP/(1+bP) + k_{5}^{*}P \tag{2}$$

At low pressures this equation may be written

$$C^* = (C_{H}^{*'}b + k_{D}^{*})P$$

$$= k^*P$$
(3)

At high pressures when the microvoids are all filled equation (2) may be written

$$C^* = C_{\rm H}^{*'} + k_{\rm D}^{*P} \tag{4}$$

The variation in absorption of gas at high pressure from by time-lag solubility measurements gave a value for the constant  $k_{\rm D}^*$  of 0.38 atm<sup>-1</sup> at 298.15 K. Absorption of gas at low pressures at 298.15 K measured by a static method fitted the equation

$$C^* = \frac{2.33P/\text{atm}}{1 + 0.44P/\text{atm}} + 0.38P/\text{atm}$$

$$k^* = 2.33 + 0.38 = 2.71 \text{ atm}^{-1}$$

Samples of partially crystalline polymer with an amorphous volume fraction less than 1 absorbed less gas. The authors interpreted this by assuming that the crystalline fraction could only take up gas in the microvoids and not by a dissolution process.

Values of the solubility constant for the amorphous polymer,  $k^*$ , at other temperatures were displayed on a small scale graph. Approximate values for the amorphous polymer from the graph are as follows

T/K	solubility	constant	for
	amorphous	polymer,	$k*/atm^{-1}$

298	2.71 +
	_ • · ·
320	1.42
337	0.89
342	0.63
341	0.57

† from the text

The solubility constant for samples of crystalline polymer, k, were defined as the value at low pressure of

> reduced volume of gas absorbed in voids and by dissolution pressure × (total volume of polymer)

Solubility constants, k, for samples of partially crystalline polymer with an amorphous volume fraction of 0.58, taken from a small scale graph, are as follows

T/K	solubility constant for crystalline polymer $k/atm^{-1}$		T/K	solubility constant for crystalline polymer $k/\text{atm}^{-1}$		
297	2.02	s	349	0.34	s	
312	1.81	t	357	0.34	t	
312	1.70	t	373	0.37	t	
312	1.25	s	373	0.30	t	
327	0.65	S	387	0.30	t	
338	0.48	s	403	0.21	t	
343	0.45	t	402	0.20	t	

Glass transition zone approximately 355-368 K s - static measurements; t - time-lag measurements

# AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Low pressure static absorbtion measurements were carried at pressures up to about 170 kPa in glass apparatus using sheets of polymer film. The system was evacuated and a measured quantity of gas admitted. The amount of gas absorbed was calculated from the initial and final pressures.

Time-lag solubility measurements were carried out to pressures of about 1240 kPa using apparatus similar to that described earlier. (1,2).

- SOURCE AND PURITY OF MATERIALS:
  1. Dried with CaSO4; minimum purity 99.5%
- 2. Amorphous polyethylene terephthalate supplied by the Mylar laboratory of E.I. du Pont de Nemours & Co. Number average relative molecular mass 15-20 000. Crystalline samples prepared by annealing the amorphous polymer at 120°C to 150°C. Densities of samples were measured with density gradient columns and the amorphous volume fraction determined assuming that the fully crystalline polymer has a density of 1.455 g  $cm^{-3}$ . (3)

# ESTIMATED ERROR:

Static measurements - precision limits ±3.5% at the 95% confidence level. Time-lag measurements - precision limits of ±10% (authors)

- 1. Michaels, A.S.; Parker, R.B. J. Polymer Sci. 1959, 41, 53
- 2. Michaels, A.S.; Bixler, H.J. J. Polymer Sci. 1961, 50, 413.
- 3. Daubeny, R. de P.; Bunn, C.W.; Brown, C.J. Proc. Roy. Soc. 1954, A226,

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Carbon dioxide; CO₂; [124-38-9]	Venable, C.S.; Fuwa, T.  J. Ind. Eng. Chem. 1922, 14,
2. Rubber	139–142.
VARIABLES:	PREPARED BY:
T/K = 289-373	P.G.T. Fogg

### EXPERIMENTAL VALUES:

Grade of rubber	T/K	Solubility /cm <sup>3</sup> of gas per 100cm <sup>3</sup> of rubber
I	294	90
	293	92 <i>a</i>
II	289	108
	293	102 <i>a</i>
III	297	92
	293	99 <i>a</i>
IV	292	103.5
	293	101a
	331	58 <i>b</i>
	373	28 <i>b</i>
	373	34.0 <i>c</i>

a estimated by the authors; b values from a graph given by the authors
c value given in a table by the authors
I - pale crepe (raw); II - smoked sheet (raw);
III - smoked sheet (vulc. coeff. = 2.56);
IV - smoked sheet (vulc. coeff. 3.2)

Solubility in  ${\bf IV}$  was shown to be proportional to pressure to at least 128 kPa at 373 K , within experimental error.

The solubility was measured as the volume of gas reduced to 273.15 K and 101.3 bar which was dissolved by  $100~\rm{cm}^3$  of rubber. In the case of compounded samples (III & IV) the solubility was calculated on the basis of the actual rubber present in the sheet.

# AUXILIARY INFORMATION

Weighed samples of rubber were kept under high vacuum for 48 hrs to remove dissolved gases. They were then put into contact with carbon dioxide or other gas under test for 2 to 24 hrs until equilibrium was reached. The dissolved gas was then pumped off and measured.

- 1. From a cylinder; 97.55 pure.
- 2. I 3 to 4 years old;

II - from Akron;
III - composition by weight:
 smoked sheet 100
 zinc oxide 10
 thiocarbanilide 3
 combined sulfur 3.2% of
 smoked sheet present.

TV - composition by weight:
 smoked sheet 100
 zinc oxide 10
 free sulfur 10
 thiocarbanilide 0
 combined sulfur 2.56% of
 smoked sheet present.

## ESTIMATED ERROR:

δ(solubility) = ±5% (authors) (note the discrepancies in the data reported for 373 K)

- Carbon dioxide; CO₂; [124-38-9]
- Acetic acid ethenyl ester homopolymer, (polyvinyl acetate); (C<sub>4</sub>H<sub>6</sub>O<sub>2</sub>)<sub>x</sub>; [9003-20-7]

# VARIABLES:

T/K = 398-473

## ORIGINAL MEASUREMENTS:

Liu, D.D.; Prausnitz, J.M.

J. Polymer Sci. (Polymer Phys. Edn.) 1977, 15, 145-153.

## PREPARED BY:

P.G.T. Fogg

## EXPERIMENTAL VALUES:

T/°C	т/к	Henry's la H/atm	w constant H/kPa*
125	398.15	990	100300
150	423.15	1200	121600
175	448.15	1500	152000
200	473.15	1700	172300

<sup>\*</sup> calculated by the compiler.

Henry's law constant, H, is defined as:

$$H = \lim_{w \to 0} \left[ \frac{f}{w} \right]$$

where f is the fugacity of the carbon dioxide and w the weight fraction of carbon dioxide in the polymer.

The polymer had a number average relative molecular mass of 8.34 × 104.

# AUXILIARY INFORMATION

## METHOD/APPARATUS/PROCEDURE:

Solubilities were measured by gas-liquid chromatography using helium as carrier gas and Chromosorb as support material. A weighed quantity of poly(vinyl acetate) was dissolved in a mixture of methanol and 1,2-dichloroethane at 80°C. This was then mixed with a weighed and preheated quantity of the support. The mixture was then heated in an oven until methanol and 1,2-dichloroethane had evaporated. and subsequently used in a steel chromatography column. The dead time of a chromatogram was found by injecting nitrogen. Retention volumes for carbon dioxide were found for various ratios of polymer to support material. This enabled correction to be made for surface adsorption of carbon dioxide. Henry's constants were calculated from the corrected retention volumes. Additional correction was made for the solubility of nitrogen.

# SOURCE AND PURITY OF MATERIALS:

- 1. Supplied by Matheson Gas Products; purity > 99%
  - 2. Supplied by Cellomer Associates.

# ESTIMATED ERROR:

 $\delta H = \pm 9\%$  at 125°C;  $\pm 16\%$  at 200°C.  $\delta T/K = \pm 0.1$ .

- Carbon dioxide; CO<sub>2</sub>;
   [124-38-9]
- 2. Poly[imino(1-oxo-1,11-undecanediy1)],  $(Ny1on\ 11)$ ;  $(C_{11}H_{21}NO)_{x}$ ; [25035-04-5]

## ORIGINAL MEASUREMENTS:

Ash, R.; Barrer, R.M.; Palmer, D.G. Polymer, 1970, 11, 421-35.

# VARIABLES:

T/K = 313.2-333.2

## PREPARED BY:

P.G.T. Fogg

### **EXPERIMENTAL VALUES:**

T/K	Henry's law solubility constant/atm		
313.2	0.368	_	
323.2	0.314		
333.2	0.280		

Henry's law solubility constant was defined as :

volume of gas absorbed, reduced to 273.2 K and 1 atm  $\,$ 

volume of polymer × pressure of gas/atm

Values of the solubility constant were found from the slopes of graphs of solubility against pressure.

1 atm = 101.325 kPa

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The gas at a known temperature and pressure was allowed to reach equilibrium with a sample of the polymer. The gas phase was then flushed out by mercury and the dissolved gas allowed to desorb into a previously evacuated vessel of known volume. The pressure of the desorbed gas was measured with a McLeod gauge. The temperature of the desorbed gas was also measured and the quantity of gas calculated from its volume, pressure and temperature. Correction was made for the absorbed gas lost during the flushing process. Measurements were made at various initial pressures of The maximum pressure was not stated but measurements on the solubility of gases in polyethylene which are reported in the same paper were made to a maximum pressure of about 25 cmHg (33 kPa).

# SOURCE AND PURITY OF MATERIALS:

- Spectrally pure sample supplied by British Oxygen Company.
- From laminated tubing made by Messrs. Griflex Ltd.

## ESTIMATED ERROR:

δT/K < ±0.1
δ(solubility constant) = ±2%
 (authors)</pre>

COMPONENTS:	EVALUATOR:
<ol> <li>Carbon dioxide; CO₂;</li> <li>[124-38-9]</li> </ol>	Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London,
2. Liquid Gases	Holloway Road, London, N7 8DB, U.K.
	July 1991

## CRITICAL EVALUATION:

Solubility of solid carbon dioxide in liquid gases.

The solubility of solid carbon dioxide in liquid oxygen was measured by Amamchyan et al.(1) from 77 K to 95 K and by Rest et al.(2) from 89.5 K to 118.5 K. Equations for mole fraction solubility over the temperature ranges of measurement were given by each group of authors. Error limits in  $x_{\rm CO_2}$  were quoted as  $\pm 15-20$ % by Amamchyan and as  $\pm 21$ % by Rest. The two equations give the same value of  $x_{\rm CO_2}$  at 87.7 K. Values for  $x_{\rm CO_2}$  at 95 K from the two equations are as follows

Amamchyan et al.  $10.75 \pm 1.61 \text{ to } 2.15 \times 10^{-6}$ Rest et al.  $8.00 \pm 1.68 \times 10^{-6}$ 

The limits of error for the two values overlap. The two equations are therefore consistent with each other, within the limits of error given by the authors.

Rest et a1.(2) measured the solubility of solid carbon dioxide in liquid argon from 87.9 K to 120.5 K and published an equation for the variation of mole fraction solubility with temperature. Preston et a1.(3) also measured the solubility in argon at 109.0 K and 115.9 K. Mole fraction solubility at these two temperatures from the two sources are as follows

109.0 K Rest et al. 2.25  $\pm 0.47 \times 10^{-5}$  4.27  $\pm 0.90 \times 10^{-5}$  Preston et al. 7.97  $\pm 3.67 \times 10^{-5}$  20.59  $\pm 2.26 \times 10^{-5}$ 

The two sets of measurements are not compatible.

Rest et a1.(2) also measured the solubility of solid carbon dioxide in liquid nitrogen from 77.7 K to 117 K. No other measurements on this system are available for comparison.

Chang et al.(4) measured the solubility in liquid nitrogen oxide at partial pressures of carbon dioxide from 17.2 kPa to 67.8 kPa at 262.2 K to 293.2 K. Values of mole fraction solubility are close to 'ideal' or reference values from Raoult's law. Solubility of carbon dioxide gas in liquid chlorine was measured by Krieve and Mason (5) at partial pressures of carbon dioxide to 66.3 kPa at 273.2 K and 298.2 K. In this case experimental values of mole fraction solubility fall much lower than the reference values from Raoult's law. A selection of mole fraction solubilities in the two gases is given below.

Solvent	<i>T</i> /K	P <sub>CO₂</sub> /kPa	X <sub>CO<sub>2</sub></sub>	R.L.
liquid nitrogen oxide	262.15	58.49	0.02103	0.0228
	273.15	34.11	0.01018	0.0098
	293.15	63.07	0.01265	0.0110
liquid chlorine	273.15	78.2	0.0106	0.0225
		111	0.01593	0.0319
	298.15	111	0.00976	0.0173

(R.L. = reference value from Raoult's law)

The measurements on both systems are self-consistent but no other data on either system are available to the evaluator for comparison.

The solubilities of solid carbon dioxide in liquid methane, ethane, propane, butane, 2-methylpropane, ethene and propene have been measured. The data which are available have been discussed earlier (pages 1,8,10).

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Liquid Gases

# **EVALUATOR:**

Peter G.T. Fogg, School of Applied Chemistry, Polytechnic of North London, Holloway Road, London, N7 8DB, U.K.

July 1991

## CRITICAL EVALUATION:

- Amamchyan, R.G.; Bertsev, V.V.; Bulanin, M.O. Zh. Fiz. Khim. 1973, 47(10), 2665-2666.; Russian J. Phys. Chem. 1973, 47(10), 1496-1497.
- 2. Rest, A.J.; Scurlock, R.G.; Fai Wu, M. Chem. Eng. J. 1990, 43, 25-31.
- 3. Preston, G.T.; Funk, E.W.; Prausnitz, J.M. J. Phys. Chem. 1971, 75, 2345-2352.
- Chang, E.T.; Gocken, N.A.; Poston, T.M. J. Chem. Eng. Data 1971, 16, 404-408.
- 5. Krieve, W.F.; Mason, D.M. J. Phys. Chem. 1956, 60, 374.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Oxygen; O<sub>2</sub>; [7782-44-7] VARIABLES: T/K = 77-95 ORIGINAL MEASUREMENTS: Amamchyan, R.G.; Bertsev, V.V.; Bulanin, M.O. Zh. Fiz. Khim. 1973, 47(10), 2665-6. Russian J. Phys. Chem. 1973, 47(10), 1496-7. PREPARED BY: P.G.T. Fogg

EXPERIMENTAL VALUES:

The solubility of solid carbon dioxide in liquid oxygen was measured at six temperatures in the range 77 K to about 95 K. The following equation was given for the mole fraction solubility in this temperature range:

$$log_{10}x_{CO_2} = 2.40 - 700/(T/K)$$

The mole fraction solubility at 90 K was given as 4.3  $\pm$  0.5  $\times$  10<sup>-6</sup>

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Liquid oxygen and solid carbon dioxide were contained in an optical cryostat described previously (1,2). The solubility was calculated from optical density as measured by IKS-16 and IKS-21 spectrometers. The liquid was stirred vigorously before each measurement and then allowed to stand until the absorption band due to suspended solid carbon dioxide had disappeared. Measurements with step-wise increase in the temperature differed by less than 10% from measurements when the temperature was decreasing.

SOURCE AND PURITY OF MATERIALS:

No information

ESTIMATED ERROR:

 $\delta x_{\text{CO}_2} = \pm 15-20\%$ 

(authors)

# REFERENCES:

1. Bertsev, V.V. Pribory i Tekh.
Eksper. 1972, No.1, 255.
2. Bulanin, M.O.; Kolomiitsova, T.D.;
Mel'nik, M.G.; Tonkov, M.V. Zhur.
Friki. Spektrosk. 1967, 7, 118.

# COMPONENTS: 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9] 2. Oxygen; O<sub>2</sub>; [7782-44-7] Nitrogen; N<sub>2</sub>; [7727-37-9] Argon; Ar; [7440-37-1] VARIABLES: T/K = 77.7-120.5 ORIGINAL MEASUREMENTS: Rest, A.J.; Scurlock, R.G.; Fai Wu, M. Chem. Eng. J. 1990, 43, 25-31.

## EXPERIMENTAL VALUES:

Mole fraction solubilities of solid carbon dioxide in liquid gases were measured and, over the specified temperature ranges, fitted equations of the form  ${\sf G}$ 

$$\log_{10} x_{\text{CO}_2} = a - b/(T/K)$$

Solvent	Temperature range /K	a	b
Liquid oxygen	89.5-118.5	0.724	553
Liquid nitroge	en 77.7-117	0.552	512
Liquid argon	87.9-120.5	0.022	509

At a particular temperature the pressure was equal to the vapor pressure of liquid oxygen, nitrogen or argon.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Solid carbon dioxide was added to liquid oxygen, nitrogen or argon. Large particles of carbon dioxide were filtered off. The liquid containing carbon dioxide in solution and in suspension was introduced into a variable pressure infra-red absorption cell surrounded by a thermal shield chamber also containing liquid oxygen, nitrogen or argon. Temperature was varied by applying pressure to the solution from a gas cylinder or by supplying heat from a heating element at the bottom of the cell. Infra-red spectra were recorded at intervals until equilibrium was reached at a particular temperature. Concentrations of carbon dioxide were calculated from the intensities of bands due to carbon dioxide in solution but not due to carbon dioxide in suspension.

# SOURCE AND PURITY OF MATERIALS:

- 1. commercial sample of specified purity 99.999%
- 2. O<sub>2</sub>; specified purity 99.9997%
  N<sub>2</sub>; specified purity 99.999%
  Ar; specified purity 99.999%

## ESTIMATED ERROR:

$$\delta x_{\text{CO}_2} = \pm 21\% \text{ (O}_2 \& \text{Ar); } \pm 23\% \text{ (N}_2\text{)}$$
(authors)

- Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Methane; CH<sub>4</sub>; [74-82-8]
  Argon; Ar; [7440-37-1]

# ORIGINAL MEASUREMENTS:

Preston, G.T.; Funk, E.W.; Prausnitz, J.M.

J. Phys. Chem. 1971, 75, 2345-2352.

# VARIABLES:

T/K = 109.0-137.5 $P_{CO_2}/kPa = 0.00027-0.126$ 

## PREPARED BY:

P.G.T. Fogg

## EXPERIMENTAL VALUES:

Solvent	T/K	P <sub>CO2</sub> /kPa*	<sup>x</sup> CO₂
Methane	126.4	0.016	0.000732
	137.5	0.126	0.002366
Argon	109.0	. 0.00027	0.0000797
	115.9	0.0016	0.0002059

The above solubilities correspond to equilibria between solid carbon dioxide and solutions of carbon dioxide in liquid methane or argon.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Solubilities were measured in a vacuum cryostat held in a bath of liquid nitrogen. The temperature of the cryostat could be controlled by electric heating. Temperatures were measured by a calibrated copper-constantin theromocouple. Vapor from the cell was pumped from the top of the cell, cooled, passed into the base of the cell and bubbled through the liquid. speeded up the attainment of equilibrium. Samples of liquid from the cell were vaporized and analyzed by gas chromatography. Full details of the apparatus have been given by Preston (2) and Funk (3).

# SOURCE AND PURITY OF MATERIALS:

- Supplied by Matheson Co.; purity 99.8%
- 2. Supplied by Matheson Co.; purity
  99.97% (methane),
  99.995% (argon).

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$  (authors)

- Meyers, C.H.; van Dusen, M.S. Bur. Stand. J. Res. <u>1933</u>, 10, 381.
- Preston, G.T. Ph.D. Dissertation, 1970, University of California, Berkeley, USA.
- Funk, E.W. Ph.D. Dissertation, 1970, University of California, Berkeley, USA.

 $<sup>^</sup>st$  vapor pressure of solid CO2 from equation given in ref.(1).

- 1. Carbon dioxide; CO<sub>2</sub>; [124-38-9]
- 2. Nitrogen oxide; N<sub>2</sub>O<sub>4</sub>; [10544-72-6]

ORIGINAL MEASUREMENTS:

Chang, E.T.; Gocken, N.A.; Poston, T.M.

J. Chem. Engng. Data. 1971, 16, 404-8.

VARIABLES:

T/K = 262.15-293.15p/kPa = 17.23-67.79 PREPARED BY:

C.L. Young

# EXPERIMENTAL VALUES:

T/K	p <sup>+</sup> /atm	$p^+/kPa$	Mole fraction of carbon dioxide in liquid, $x_{\text{CO}_2}$
262.15	0.5773	58.49	0.02103
273.15	0.1700 0.3366	17.23 34.11	0.005276 0.01018
283.20	0.3495	35.41 67.79	0.008712 0.01642
293.15	0.1763	17.86	0.003742
	0.3175 0.6225	32.17 63.07	0.006524 0.01265

+ partial pressure of carbon dioxide

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus consisting of solvent vessel and buret with three calibrated bulbs. Pressure measured with mercury manometer and cathetometer. Solvent stirred with magnet enclosed in glass. Mole fraction absorbed calculated from knowledge of amount of gas before and after absorbtion. Solvent carefully degassed.

# SOURCE AND PURITY OF MATERIALS:

- Research grade gas, purity 99.995 mole per cent minimum.
- Research grade gas, purity 99.5 mole per cent minimum, further purified by bubbling oxygen through, degassed and distilled.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/kPa = \pm 0.01$ ;  $\delta x_{CO_2} < \pm 2\%$ 

# 463 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Carbon dioxide; $CO_2$ ; [124-38-9] Krieve, W. F.; Mason, D. M. J. Phys. Chem. 2. Chlorine; Cl<sub>2</sub>; [7782-50-5] 1956, 60, 374. VARIABLES: PREPARED BY: T/K = 273.15, 298.15C. L. Young $P_{\text{CO}_2} = 78.2 - 663$ **EXPERIMENTAL VALUES:** Mole fraction of carbon dioxide T/K $P^{\dagger}/10^{5}$ Pa in liquid, xCO2 0.0106 0.782 273.15 0.01593 1.11 0.02135 1.69 0.02983 2.32 2.94 0.03945 0.04950 3.64 4.15 0.05640 0.06582 4.84 0.00976 298.15 1.11 0.0142 1.52 0.0204 2.24 0.0298 3.07 0.0380 3.90 0.0474 4.86 0.0546 5.62 0.0643 6.63 † partial pressure of carbon dioxide. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Measured amount of gas added to 1. Matheson Co. sample, pure

Composition cell of known volume. of liquid determined from knowledge of total amounts of chlorine and carbon dioxide and assuming Raoult's law followed by chlorine in vapor.

- grade.
- 2. Commercial sample, fractionally distilled.

## ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/10^5 Pa = \pm 0.5%;$  $\delta x_{\text{CO}_2} = \pm 0.001$  (estimated by compiler).

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Page numbers preceded by E refer to evaluation texts whereas page numbers not preceded by E refer to compiled tables. Compounds are named as in Chemical Abstracts indexes (toluene appears under Benzene, methyl-).

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