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SOLUBILITY DATA SERIES

Volume 42

HYDROGEN HALIDES IN NON-AQUEOUS SOLVENTS

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES



Volume 42

HYDROGEN HALIDES IN NON-AQUEOUS SOLVENTS

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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of solubility data indeed existed, but they contained many errors, were in general uncritical, and were seriously out-of-date.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 evaluations 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;
 - (11) primary source of the data;
 - (iii) experimental variables;
 - (1v) 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;
- (v111) source and purity of materials used;
 - (1x) 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 principles 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 of hydrogen fluoride, hydrogen chloride, hydrogen bromide and hydrogen iodide in non-aqueous solvents. Information on about four hundred systems is included. Hydrogen halides take part, either as reactants or products, in many reactions of organic compounds. Measurements of solubilities of these gases have often been carried out during studies of such reactions.

There are few measurements of the solubility of hydrogen fluoride in non-aqueous solvents. The solubilities of each of the other gases show wide divergences from solvent to solvent under the same conditions of temperature and pressure. In many cases there are distinct non-linear variations of mole fraction solubility with change of partial pressure of gas at pressures less than 101.3 kPa. This must be borne in mind when attempts are made to predict solubilities at finite pressures from limiting values of Henry's law constants.

Reliance may be placed upon data when there is close agreement between measurements by different groups of workers. Unfortunately there are sometimes inconsistencies in the literature. Difficulties in attaining equilibria between gas and liquid phases are likely to be the chief cause of such discrepancies.

Equations relating mole fraction solubility at constant pressure with temperature have been derived if appropriate experimental data have been available. Errors may arise if these equations are used outside the temperature range of the original measurements.

The editors are grateful for help and encouragement from fellow members of the I.U.P.A.C. Commission on Solubility Data. In particular we should like to acknowledge the tremendous support given by the late Steven Kertes whose untimely death has caused great sorrow to members of the Commission.

Peter Fogg William Gerrard

London

July 1989

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

The Weight Per Cent Solubility, wt%

For a binary system this is given by

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

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_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(l) 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

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

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

is related to the Bunsen of
$$x(g, 1 \text{ atm}) = \frac{\alpha}{\alpha + \frac{273.15}{T} \frac{v^{\circ}(g)}{v^{\circ}(1)}}$$

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 α in the original publication and to make the necessary adjustments when calculating the mole fraction solubility.

The Kuenen Coefficient, S

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

The Ostwald Coefficient, L

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

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

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

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

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

The Absorption Coefficient,β

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

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

where P(1) is the partial pressure of the liquid in 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 K₂ and K₃ are constants, C the concentration, and (1) and (g) refer to the liquid and gas phases. Unfortunately, K₄, K₅ and K₆ 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 1s 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 =
$$\alpha(T/273.15)$$

 $C_{w} = \alpha/v_{o}\rho$
 $K_{H} = \frac{17.033 \times 10^{6}\rho(\text{soln})}{\alpha M(1)} + 760$
L = $C_{w}v_{t,gas}\rho$

where v_o is the molal volume of the gas in cm³ mol⁻¹ at 0°C, ρ the density of the solvent at the temperature of the measurement, ρ_{soln} the density of the solution at the temperature of the measurement, and $v_{t,gas}$ the molal volume of the gas (cm³ mol⁻¹) at the temperature of the measurement.

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Revised: December 1984 (CLY)

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сомро	NEMIS	EVALUATOR.
1.	Hydrogen Fluoride; HF; [7664-39-3]	Peter G. T. Fogg Department of Applied Chemistry and Life Sciences,
2.	Non-aqueous Solvents	Polytechnic of North London, Holloway, London, N7 8DB, U.K.
		January 1989

CRITICAL EVALUATION

The Solubility of Hydrogen Fluoride in Non-aqueous Solvents

Simons (1) measured the solubility of hydrogen fluoride in benzene over the temperature range 292.7 K to 345.9 K and pressure range 0.32 kPa to 89.2 kPa. Except at partial pressures of hydrogen fluoride below about 0.5 kPa the mole fraction solubility lies below the reference surface defined by the Raoult's law equation. i.e.

$$v_{HF} = P_{HF}/P_{HF}^{\circ}$$

where P_{HF} is the partial pressure of hydrogen fluoride and P_{HF}° the vapor pressure of liquid hydrogen fluoride. The behaviour differs from that of the other hydrogen halides. Mole fraction solubilities in benzene of these gases lie above this reference surface. Simons' data for hydrogen fluoride are self-consistent but there are no other data on this system available for comparison. They may be accepted on a tentative basis.

Simons also measured the solubility of hydrogen fluoride in octane in the range 298.3 K to 339.5 K at a total pressure equal to barometric. Mole fraction solubilities are very low. These measurements may also be accepted on a tentative basis until further studies have been made.

Matuszak (2) reported the solubility in 1,2-ethanediol, 1,2,3-propanetriol, 1,1'-oxybis[3-methylbutane] and in 1,1'-oxybisbenzene, each at a single temperature in the range 295.4 K to 304.3 K and single pressure of either 98.93 kPa (742 mmHg) or 99.59 kPa (747 mmHg). On the basis of analogy with the behaviour of the other hydrogen halides it is to be expected that the mole fraction solubility of hydrogen fluoride in these solvents should be high relative to the reference values based upon the Raoult's law equation. Mole fraction solubilities from Matuszak's measurements are as follows:

Solvent	P _{HF} /mmHg	т/к	^x HF	Reference value P _{HF} /P [°] HF
1,2-ethanediol	742	302.0	0.916	0.705
1,2,3-propanetriol	747	295.4	0.946	0.886
1,1'-oxybis[3-methylbutane]	742	297.6	0.799	0.820
1,1'-oxybisbenzene	742	304.3	0.583	0.653

This author's measurement of the solubility of hydrogen chloride in 1,2-ethanediol is consistent with measurements by Gerrard & Macklen. His values for the solubility of hydrogen chloride in 1,1'-oxybis[3-methylbutane] and in 1,1'-oxybisbenzene are lower than those reported by others. The evaluator recommends that these solubility data for hydrogen fluoride should be treated as semi-qualitative until they have been confirmed by other workers.

Hartman (4) reported the solubility in fluorosulfuric acid at four temperatures from 299.8 K to 333.2 K at a pressure of 101.3 kPa. Mole fraction solubilities are high, relative to the reference line based upon the Raoult's law equation, and are self-consistent. No experimental details were given. No other measurements are available for comparison and the reliability of these data cannot be judged.

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- 3. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1960, 10, 57-62.
- 4. Hartman, B. F. U. S. Patent 2,434,040 January 6, 1948.

- (1) Hydrogen fluoride; HF; [7664-39-3]
- (2) Octane; C₈H₁₈; [111-65-9]

ORIGINAL MEASUREMENTS:

Simons, J. H.

J. Am. Chem. Soc. 1931, 53, 83 - 87.

VARIABLES:

T/K: 298.3 - 339.5 HF P/kPa: 85.7 - 97.5

(643 - 741 mmHg)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Т/К	Pressure p ₁ /mmHg	Mol Fraction
[293.15	735	0.00372]
298.3		0.00338
[303.15	727	0.00305]
309.2		0.00276
[313.15	714	0.00253]
318.2		0.00235
[323.15	695	0.00213]
324.2		0.00194
[333.15	666	0.00181]
339.5	- 1	0.00170

The compiler calculated the smoothed values given in [].

The mole fraction values are from the equation $\ln x_1 = 1761.06/(T/K) - 11.6022$.

The HF vapor pressures were calculated by subtracting the octane vapor pressure at each temperature from the barometric pressure which was assumed to be 745 mmHg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Three vessels were connected by taps. Vessel X contained the liquid HF, and was furnished with an inlet tube passing to the bottom. The exit tube was flush with the top of X, and it then became the inlet tube for vessel Y which contained the octane. This inlet tube passed to the bottom of the absorption vessel, Y.

The outlet tube from Y was flush with the top of Y; but it was not clear where it went after that. These two vessels were immersed in separate thermostats. A vertical tube carrying a tap passed from the bottom of vessel Y, and was attached to a tapped vessel Z of about 20 cm³ capacity for the reception of a sample of solution for the determination of hydrogen fluoride by titration with sodium hydroxide (excess) and hydrochloric acid.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen fluoride. Prepared as described by Simons (1). It was distilled directly into the dry apparatus filled with nitrogen.
- (2) Octane. Self prepared. Dried with phosphorus pentoxide and sodium, and distilled directly into the apparatus.

ESTIMATED ERROR:

REFERENCES:

1. Simons, J. H. J. Am. Chem. Soc. <u>1924</u>, 46, 2179.

- (1) Hydrogen fluoride; HF; [7664-39-3]
- (2) Benzene; C₆H₆; [71-43-2]

Simons, J. H.

J. Am. Chem. Soc. 1931, 53, 83 - 87.

T/K	Pressure	Mol Fraction	T/K	Pressure	Mol Fraction
	$p_1/mmHg$	x_1		p_1 /mmHg	x_1
	rium vapor HF at 292.	pressure of 65 K			pressure of 15 K (continued)
[293.15	669	0.0673]	[323.15	214	0.0196]
294.6		0.0653	325.1		0.0181
294.7 295.1		0.0650 0.0648	329.4		0.0150
296.2		0.0530	[333.15	160	0.0117]
297.3 297.3 298.9		0.0625 0.0620 0.0596	334.3 338.2		0.0108 0.0084
300.3 302.4		0.0588 0.0556		rium vapor HF at 255.	pressure of 15 K
302.5		0.0548	[293.15	147	0.0385]
[303.15	625	0.0548]	293.9		0.0382
304.2 306.0		0.0525 0.0507	294.0 294.1		0.0381 0.0375
307.0		0.0495	296.1		0.0355
308.7		0.0510 0.0468	301.1		0.0327
309.8 312.2		0.0442	[303.15	137	0.0315]
312.3		0.0437	304.3		0.0306
312.5		0.0427	304.9 311.1		0.0323 0.0258
[313.15	561	0.0422]	[313.15	123	0.0244]
315.4 317.8		0.0394 0.0382	313.9	2-3	0.0244
317.9		0.0365	322.1		0.0184
319.1		0.0332	[323.15	104	0.0173]
[323.15	473.6	0.0298]	325.9		0.0161
324.1		0.0280	331.2		0.0117
327.1 327.2		0.0246 0.0248	[333.15	77.5	0.0102]
327.2		0.0243	333.7		0.0098
[333.15 334.1	354.9	0.0180] 0.0167	Equil:b	rium vapor HF at 196.	pressure of
335.5		0.0150	292.7		0.0249
335.6 345.9		0.0155 0.00395	[293.15	4.5	0.0248]
-				4.5	0.0248)
liquid	HF at 273.	pressure of 15 K	296.7 303.1		0.0208
[293.15	303	0.0432]	[303.15	4.2	0.0203]
		0.0435	311.4		0.0163
294.1 298.7		0.0425 0.0384	[313.15	3.8	0.0158]
300.6		0.0368	318.1	2.0	0.0128
[303.15	283	0.0355]	[323.15	3.2	0.0112]
			326.0	3.2	0.0098
303.3 306.0		0.0346 0.0330	329.1		0.0098
			[333.15	2.4	0.0071]
[313.15	254	0.0275]	333.9	-	0.0067
313.6		0.0277	338.1		0.00557
323.1		0.0201			

COMPONENTS: ORIGINAL MEASUREMENTS: Simons, J. H. (1) Hydrogen fluoride; HF; [7664-39-3]J. Am. Chem. Soc. 1931, 53, (2) Benzene; C₆H₆; [71-43-2] 83 - 87. VARIABLES: PREPARED BY: T/K: 296.1 - 345.9 P/kPa: 0.32 - 89.20 W. Gerrard (2.4 - 669 mmHq)

EXPERIMENTAL VALUES:

See preceeding page.

The mole fraction values in [] are smoothed values of the author.

The HF partial pressure values were calculated from the data below and the equation:

p₁/mmHg =[(p_{barometer}/mmHg - p₂⁰/mmHg)/p_{barometer}/mmHg] p₁⁰/mmHg

where p_1^{ρ} is the equilibrium vapor pressure of HF at the HF liquid temperature, and p_0^0 is the solvent equilibrium vapor pressure at the temperature of the solubility measurement. The author's values are below.

5.1	p2/mmHg	p barometer/mmHg
		750
		750
		130
166		740
342		742
760		745
768	75.6	
070	120.2	
470	183.6	
990	271.4	
630	390.1	
	342 760 768 070 470 990	342 760 768 75.6 070 120.2 470 183.6 990 271.4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Three vessels are connected by taps. Vessel I contains the liquid HF. is furnished with an inlet tube passing to the bottom. The exit tube is flush with the top of I, and passes to the bottom of vessel II. The outlet tube from II is flush with the top and can be opened to the atm. The two vessels are immersed in separate thermostats. Vessel I controls the partial pressure of HF, vessel II contains the solvent at the temperature of the solubility measurement. A vertical tube passes from the ESTIMATED ERROR: bottom of II to vessel III for the reception of a sample of solution for chemical titration. The sample is reacted with excess NaOH, and back titrated with HCl.

Vessel I is maintained at a chosen temperature of 292.65 K (normal b.p. of HF) or lower to control the HF

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen fluoride. Prepared as described by Simons (1). It was distilled directly into the dry apparatus filled with nitrogen.
- (2) Benzene. Thiophene free. Dried with phosphorus pentoxide and sodium, and distilled directly into the apparatus.

- 1. Simons, J. H. J. Am. Chem. Soc. 1924, 46, 2179.
- partial pressure. The partial pressure of HF above the saturated solution in II is calculated from the vapor pressure of HF in I, the vapor pressure of solvent in II, and the barometric pressure.

	Hydrog	jen Fluoride	in Non-Aqueous Sol	vents	
COMPONENTS:			ORIGINAL MEA	SUREMENTS:	
(1) Hydrogen fluo [7664-39-3]	ride; H	F;	Matuszak, M.		
(2) 1,2-Ethanedio 1,2,3-Propane 1,1'-Oxybis[3 1,1'-Oxybisbe	dıol -methyl	butane]	U.S. Patent September 5 Chem. Abstr.		1044g
VARIABLES: T/K: 295 P/kPa: 98.9 (7		59	PREPARED BY:		
EXPERIMENTAL VALUE	s:				
Tempera t/°F	ture T/K	Pressure P/mmHg	HF Absorbed* g HF per 100 g component 2	Mole Ratio*	* Mole Fraction** [*] HF
1,2-Ethanediol, (e C ₂ H ₆ O ₂ ; [107-21-1]	thvlene	glycol);			
2 6 2 84	302.0	742	350	10.86	0.916
1,2,3-Propanetriol C ₃ H ₈ O ₃ ; [56-81-5]					
72	295.4	747	382	17.6	0.946
1,1'-Oxybis[3-meth	ylbutan	e], (d11so	amv1 ether);		
C ₁₀ H ₂₂ O; [544-01-4	297.6	742	50.5	4.00	0.799
1,1'-Oxybisbenzene,		nvl ether)	;		
C ₁₂ H ₁₀ O; [101-84-8 88	304.3	742	16.4	1.396	0.583
* The author's s	tatemen	t was "HF	absorbed, weight	per cent of	
** calculated by	the com	pıler.			
	· · · · · · · · · · · · · · · · · · ·				

AUXILIAR	Y INFORMATION
METHOD/APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
No information	No information
	ESTIMATED ERROR:
	REFERENCES:
	REFERENCES;

COMPONENTS: (1) Hydrogen fluoride; HF; [7664-39-3] (2) Fluorosulfuric acid or fluosulfonic acid; FHO₃S;[7789-21-1] VARIABLES: T/K = 299.8 - 333.2 p/kPa = 101.325 (1 atm) ORIGINAL MEASUREMENTS: Hartman, B. F. U. S. Patent 2,434,040, Jan. 6, 1948. PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

Tempe	erature	Hydrogen Fluoride	Mol Fraction
t/ ⁰ F	<i>T</i> /K	$10^2 w_1/\text{wt}$ % dissolved in fluosulfonic acid at one atm	<i>x</i> ₁
80	299.8	58.0	0.874
100	310.9	33.0	0.711
120	322.0	18.0	0.523
140	333.2	11.0	0.382

The compiler calculated the mole fraction values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No information.	No information.
	ESTIMATED ERROR:
	REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanes

EVALUATOR:

H. Lawrence Clever Chemistry Department Emory University Atlanta, GA 30322 USA

1986, November

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Alkanes.

Seven papers (ref 1 - 7) report measurements of the solubility of hydrogen chloride in seven normal alkanes and one branched alkane. Some of the measurements were made as a function of pressure at partial pressures well below atmospheric pressure. Other measurements were made at only one pressure at or near atmospheric pressure. The measurements cover the temperature interval of 194.6 to 475 K.

Two trends have been observed in evaluating the solubility of gases in normal alkanes which are also expected for hydrogen chloride. The trends are:

(i) the temperature coefficient of solubility of a gas is the same for all alkanes at a given temperature. This is because a given gas has nearly the same enthalpy of solution in all normal alkanes.

 $(i\,i)$ at a given temperature and gas partial pressure the mole fraction solubility increases with normal alkane chain length. The increasing contact area of the alkane with carbon number will allow more solute molecules to contact the alkane which results in a larger mole fraction solubility.

Henry's law can be a helpful relationship in the evaluation of gas solubility data. The hydrogen halides are non-ideal gases, their solutions are non-ideal, and there is a question as to whether or not their solutions obey Henry's law over even a low partial pressure range, especially for solvents with some basic character. Of all the solvents the normal alkanes probably show the least basic character. The HCl + heptane solubility data of Brown and Brady (ref 3) and Strohmeir and Echte (ref 4) at eight temperatures between 194.6 and 272.9 K strongly indicate that Henry's law is a good approximation to the solubility behavior of the system. The evidence is presented in Figure 1. When Henry's law, in the form

 $(p_1/\mathrm{kPa}) = (k_H/\mathrm{kPa})x_1$, is put in logarithmic form $\ln(p_1/\mathrm{kPa}) = \ln k_H + \ln x_1$, it is seen that a plot of $\ln (p_1/\mathrm{kPa}) vs$. $\ln x_1$ should be linear and of unit slope. The HCl + heptane data plotted in Figure 1 is linear and averages within 2 percent of unit slope. The gas partial pressures range from 1.1 to 47.8 kPa. Thus the present evaluation will assume a Henry's law like model can be used to help evaluate the data. It is further assumed that the relationship is valid to 101.3 kPa (atmospheric pressure).

Both O'Brien and Kenny (ref 2) and Ryabov $et\ al.$ (ref 7) present pressure dependent solubility data for the HCl + hexane system. The Ryabov $et\ al.$ experiment appears to be seriously flawed. The data scatter badly, and the atmospheric pressure values at several temperatures appear to be too small when compared with other data. The O'Brien and Kenny data when plotted in logarithmic form are approximately linear, but the slope is 7 per cent larger than unity. Although these experiments do not support the Henry law model well, we believe the Strohmeir and Echte experiments on HCl + heptane are definitive, and accept Henry's law for all of the HCl + alkane systems.

The HCl + alkane mole fraction solubilities at 101.3 kPa are shown in Figure 2 and given in Table 1 as a function of temperature. In the figure is plotted $\ln x_1 vs$. 1000/(T/K). The HCl vapor pressure and Raoults law were used to construct an ideal solubility line at 101.3 kPa partial pressure (the line also represents the 101.3 kPa solubility predicted by the Gerrard reference line). Also given in Table 1 are Henry's constants in kPa. The Henry's constants reproduce the low pressure solubility values of the HCl + heptane system with an average deviation of 0.9 percent.

Figure 2 allows the expected trends of a similar temperature coefficient of solubility and of an increasing solubility with increasing chain length for the HCl + alkane systems to be checked. The results are disappointing. The figure indicates the HCl + alkane data do not make up a self-consistent set of solubility data. The figure shows that the HCl +

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanes

EVALUATOR:

H. Lawrence Clever Chemistry Department Emory University Atlanta, GA 30322

USA

1986, November

CRITICAL EVALUATION:

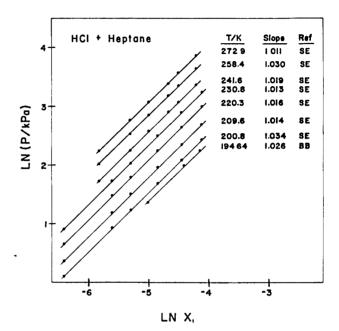
Figure 1.

Hydrogen chloride + Heptane

 $\ln (p_1/kPa) vs. \ln x_1$

The near unit slope indicates the system behaves in a Henry's law like manner.

BB = Brown, Brady (ref 3)



heptane data of Brown and brady (ref 3) and Strohmeir and Echte (ref 4), and the HCl + decane data of Gerrard, Mincer and Wyvill (ref 5) best represent the behavior of HCl in alkanes. The HCl + hexane data of Ryabov $et\ al.$ (ref 7) appear to be too low and of a different temperature coefficient of solubility. The HCl + hexadecane data of Tremper and Prausnitz (ref 6) do not fit the expected pattern well. Near 300 K the mole fraction solubility values are smaller than expected on comparison with the heptane and decane data. Above 400 K the values are nearer the expected magnitude. However, the temperature coefficient of solubility is quite different from that of the systems considered most reliable.

Not all of the data points of Bell (ref 1) and Ryabov et al. (ref 7) are shown on Figure 2. Bell reported one solubility value at 293.2 K for each of four hydrocarbons. From the location of Bell's solubility values on Figure 2 we believe his values are reliable with the possible exception of the hexadecane value.

Each HCl + alkane system is discussed further below.

1. Hydrogen chloride + Pentane; C₅H₁₂; [109-66-0]

Ryabov $et\ al.$ (Ref 7) report one mole fraction solubility value at 101.3 kPa and 298.2 K. It appears to be too small and is classified as doubtful.

2. Hydrogen chloride + Hexane; C₆H₁₄; [110-54-3]

Three papers report rather discordant measurements of the solubility of HCl in hexane. Probably the most reliable value is the single value reported by Bell (ref 1) at 101.3 kPa and 293.2 K. O'Brien and Kenny (ref 2) report four values measured at pressures between 2.10 and 10.84 kPa HCl at 298.2 K. The data recalculated as Henry's constant show some scatter and lead to an atmospheric pressure value that is nearly 20 per cent below the Bell value. Ryabov $et\ al.\ (ref\ 7)$ report solubility values at 101.3 kPa

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanes

EVALUATOR:

H. Lawrence Clever Chemistry Department Emory University Atlanta, GA 30322 USA

1986, November

CRITICAL EVALUATION:

at six temperatures between 283.2 and 313.2 K. It appears that they made measurements at a number of HCl partial pressures, but a complete data set is given for only the 298.2 K measurements. As discussed earlier their experiment appears to be flawed. The pressure dependent data at 298.2 K scatter badly, and all of their values appear to be low. The results are classed as doubtful.

Hydrogen chloride + Heptane; C₇H₁₆; [142-82-5]

The data reported by Brown and Brady (ref 3) and Strohmeir and Echte (ref 4) are classed as tentative. However, they may be the most reliable data available for HCl + alkane systems. Their pressure dependent data appears to obey Henry's law (Figure 1). The Henry's constants given in Table 1 regenerate the experimental data from these papers with an average deviation of 0.9 percent. The 101.3 kPa mole fraction solubilities calculated from these data are plotted in Figure 2. A single value at 101.3 kPa and 298.2 K of Ryabov $et\ al.$ (ref 7) appears to be too small and is classed as doubtful.

4. Hydrogen chloride + Octane; C₈H₁₈; [111-65-9]

Bell (ref 1) reports a single value at 101.3 kPa and 293.2 K which is classed tentative. Ryabov et al. (ref 7) report a single value at 101.3 kPa and 298.2 K which is classed doubtful.

5. Hydrogen chloride + 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]

One value at 101.3 kPa and 298.2 K is reported (ref 7). The branched alkanes do not always fit a predictable pattern of gas solubility. The present value is suspected of being low. It is classed doubtful.

6. Hydrogen chloride + Decane; $C_{10}H_{22}$; [124-18-5]

Gerrard, Mincer, and Wyvill (ref 5) report the only data on the system. They report eleven measurements at 101.3 kPa between the temperatures of 269.2 and 319.2 K. The data show some scatter (Figure 2), but they do show the expected trends in mole fraction solubility and temperature coefficient of solubility relative to the HCl + heptane data. The data are classed as tentative.

7. Hydrogen chloride + Dodecane; C₁₂H₂₆; [112-40-3]

Bell (ref 1) reports a single measurement at $101.3 \ \mathrm{kPa}$ and $293.2 \ \mathrm{K}$. The value fits the expected pattern of solubility in alkanes fairly well, and it is classed as tentative.

8. Hydrogen chloride + Hexadecane; $C_{16}H_{34}$; [544-76-3]

Bell (ref 1) reports a single solubility value at 101.3 kPa and 293.2 K. Tremper and Prausnitz (ref 6) report seven Henry's constant values at temperatures between 300 and 475 K. The Henry's constant values have been converted to mole fraction values at 101.3 kPa. They are shown in Figure 2 and given in Table I. At 293.2 K the extrapolated solubility value of Tremper and Prausnitz is 12 percent lower than the Bell value. Bell's value already appears to be low when compared with the solubility values of HCl in heptane and decane at 293.2 K.

Tremper and Prausnitz used modern equipment, established techniques, and took account of the non-ideality of the gas state in their calculations. They state their reproducibility is one percent. Thus, it is of concern to inspect Figure 2 and see that their data does not fit the overall pattern well. Their results near 300 K appear to be too small when compared to the HCl solubility in other alkanes. Their temperature coefficient of solubility differs from that of other systems. At this time it is not possible to decide whether the HCl + dodecane or the HCl + heptane and decane solubility curves (Fig 2) best represent the typical behavior of HCl in a normal alkane. New experimental results are needed.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanes

EVALUATOR:

H. Lawrence Clever Chemistry Department Emory University Atlanta, GA 30322 USA

1986, November

CRITICAL EVALUATION:

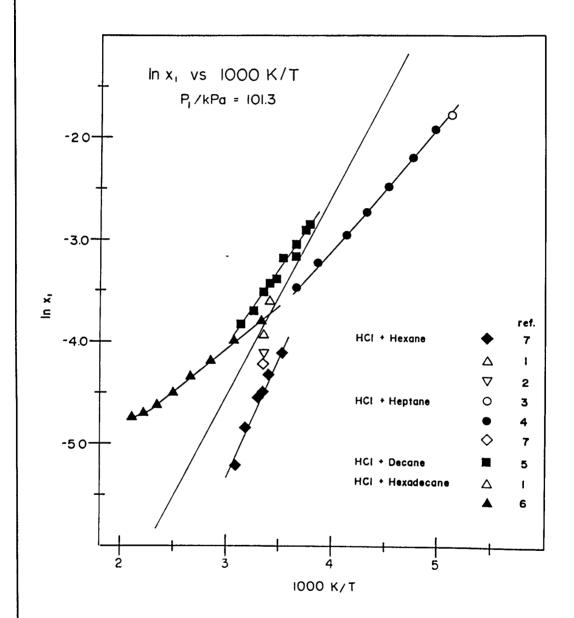


Figure 2. Hydrogen chloride + Normal Alkanes

 $\ln x_1 vs. 1000 K/T$

The plain line represents the "ideal" solubility as calculated assuming Raoults law. The HCl solubilities in heptane and decane follow expected trends. Except for the ref l value the solubilities in hexane appear to be too small. The solubilities in hexadecane are smaller magnitude than expected at the lower temperatures, but near expected magnitudes at the higher temperatures. The HCl + hexadecane slope agrees poorly with the slopes of the other systems.

Table 1.	Hydrogen o	chloride	+	alkanes		Henry's cor	nstant	and mole	fraction
	solubility	y at 101.	. 3	kPa as	а	function of	f tempe	erature.	

T/K	Pentane		Hexane		Heptane		Octane		Ref.
	k _H /kPa	x_1	k _H /kPa	x_1	k _H /kPa	x_1	k _H /kPa	ω_1	
194.6					600	0.169			3
200.8					689	0.147			4
209.6					901	0.1125			4
220.3					1206	0.0842			4
230.8					1554	0.0657			4
241.6					1941	0.0522			4
258.4					2572	0.0394			4
272.9					3206	0.0316			4
283.2			6220	0.0163					7
293.2			7680	0.0132					7
			5140	0.0197			3420	0.0296	1
298.2	21600	0.0047	9050	0.0112	6890	0.0147	6220	0.0163	7
			6220	0.0163					2
303.2			9560	0.0106					7
313.2			12840	0.00789					7
323.2			18730	0.00541					7

	2,2,4-T methylp		Decane		Dodecan	e	Hexadec	ane
	k _H /kPa	<i>x</i> ₁	k _H /kPa	x ₁	k _H /kPa	x 1	k _H /kPa	<i>x</i> ₁
264.2			1745	0.0581				
267.2			1865	0.0544				
273.2			2140	0.0473				
273.4			2170	0.0467				
279.2			2405	0.0421				
283.2			2465	0.0411				
288.4			3015	0.0336				
293.2					3230	0.0314	3750	0.0270
293.4			3155	0.0321				
298.2			3400	0.0298				
	6580	0.0154						
300							4565	0.0222
306.7			4100	0.0247				
319.2			4690	0.0216				
325							5505	0.0184
350							6665	0.0152
375							7915	0.0128
400							9210	0.0110
425							10340	0.00980
450							11250	0.0090
475							11750	0.0086

- 1. Bell, R. P. J. Chem. Soc. 1931, 1371-82.
- 2. O'Brien, S. J.; Kenny, C. L. J. Am. Chem. Soc. 1940, 62, 1189-92.
- 3. Brown, H. C.; Brady, J. D. J. Am. Chem. Soc. 1952, 74, 3570-82.
- 4. Strohmeir, W.; Echte, A. Z. Elektrochem. 1957, 61, 549-55.
- Gerrard, W.; Mincer, A. W. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89-93.
- 6. Tremper, K. L.; Prausnitz, J. M. J. Chem. Eng. Data 1976, 21, 295-99.
- 7. Ryabov, V. G.; Solomonov, A. B.; Ketov, A. N.; Bugaichuk, A. M. Zh. Fiz. Khim. 1979, 53, 2915-6; Russ. J. Phys. Chem. 1979, 53, 1667-8.

12 COMPONENTS: ORIGINAL MEASUREMENTS: Ryabov, V. G.; Solomonov, A. B.; Ketov, A. N.; Bugaichuk, A. M. (1) Hydrogen chloride; HCl; 7647-01-0 2h. Fiz. Khim. 1979, 53, 2915 - 6. (2) Alkanes; C_5H_{12} , C_6H_{14} , C_7H_{16} , and CaH18 Russ. J. Phys. Chem. 1979, 53, 1667 - 8. VARIABLES: PREPARED BY: T/K: 298.15 H. L. Clever P/kPa: 101.325 EXPERIMENTAL VALUES: Mol Fraction1 T/K Pentane; C₅H₁₂; [109-66-0]

Hexane; C₆H₁₄; [110-54-3]

298.15 0.0112 ± 0.0001 Heptane; C₇H₁₆; [142-82-5]

298.15 0.0147 ± 0.0003

Octane; $\vec{c}_8 H_{18}$; [111-65-9]

298.15 0.0163 ± 0.0004

2,2,4-Trimethylpentane or isooctane; $C_{8}H_{18}$; [540-84-1]

298.15

298.15

 0.0154 ± 0.0002

 0.0047 ± 0.0001

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen chloride was bubbled through a thermostated layer of the hydrocarbon.

Samples were removed at specified times, washed with distilled water, and the aqueous extract titrated with 0.1 N sodium hydroxide.

Saturation was confirmed by taking 2 to 3 more samples after the time concentration curve leveled.

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

The uncertainty is described by the authors as a fiducial probability of 0.99.

The authors reported the solubility as mole per cent. The compiler moved the decimal point and reports mole fraction.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanes; $C_{6}^{H}_{14}$, $C_{8}^{H}_{18}$, $C_{12}^{H}_{26}$, and C16H34

ORIGINAL MEASUREMENTS:

Bell, R. P.

J. Chem. Soc. 1931, 1371 - 1382.

VARIABLES:

T/K = 293.15P/kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Partition Coefficient	Mol	Fraction	
	c _{1,l} /c _{1,g}		I	

Hexane; C_6H_{14} ; [110-54-3]

293.15 3.64 0.0197

Octane; C₈H₁₈; [111-65-9]

293.15

4.50 0.0296

Dodecane; C₁₂H₂₆; [112-40-3]

293.15

3.42

0.0314

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

293.15

2.28

0.0270

The ideal gas concentration at $p_1 = 1$ atm is $c_{1,g}/mol dm^{-3} = n/V = p/RT = 0.0417$.

a named cetane in the original paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO2 free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, c/mol dm⁻³, was converted to a partition coefficient ESTIMATED ERROR: by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Alkanes. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Hexane; C₆H₁₄; [110-54-3]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Kenny, C. L.

J. Am. Chem. Soc. 1940, 62, 1189 - 1192.

VARIABLES:

T/K: 298.15

P/kPa:

2.09 - 10.87 (15.7 - 81.5 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Henry's Constant	Mol Ratio	Mol Fraction
	p1/mmHg	$m_1/mol kg^{-1}$	k ¹	n_1/n_2	x_1
298.15	15.7	0.0042	4.9	0.000362	0.000362
	28.3	0.0073	5.1	0.000629	0.000629
	49.2	0.0111	5.8	0.000956	0.000956
	81.5	0.020	5.4	0.00172	0.00172
	(760		5.3		0.0160)2

¹ k/atm mol-1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Hexane. Eastman Kodak Co. Attested by refractive index, 1.3741.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0146 to 0.0173 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Hexane; $C_{6}H_{14}$; [110-54-3]

ORIGINAL MEASUREMENTS:

Ryabov, V. G.; Solomonov, A. B.; Ketov, A. N.; Bugaichuk, A. M.

Zh. Fiz. Khim. 1979, 53, 2915 - 6.

Russ. J. Phys. Chem. <u>1979</u>, 53, 1667 - 8.

VARIABLES:

T/K: 298.15

P/kPa: 9.626 - 101.325 (0.095 - 1.00 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

т/к	Gas Phase HCl Mol % ¹	Order of Measurement	Mol Fraction ²	Standard Error	Confidence Interval
298.15	9.5	2	0.00027	0.001	±0.001
	22.1	6	0.00175	0.001	±0.004
	24.2	8	0.00208	0.005	±0.009
	35.5	9	0.0032	0.012	±0.02
	47.8	3	0.00252	0.002	±0.003
	56.7	5	0.00445	0.004	±0.006
	74.1	7	0.01018	0.003	±0.01
	76.3	10	0.0103	0.006	±0.01
	76.6	4	0.0089	0.029	±0.05
	88.0	12	0.01045	0.009	±0.019
	97.1	11	0.01099	0.003	±0.006
	100.0	1	0.0112	0.0024	±0.01

¹ The gas phase is HCl plus an inert gas. The inert gas is not identified.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen chloride was bubbled through a thermostated layer of the hydrocarbon.

Samples were removed at specified times, washed with distilled water, and the aqueous extract titrated with 0.1 N sodium hydroxide.

Saturation was confirmed by taking 2 to 3 more samples after the time concentration curve leveled.

The measurements were made in the random order given in the table above.

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

See table above for authors values of standard error and confidence interval.

²The original paper reports the HCl solubility as mole per cent. The compiler has moved the decimal point and reports mole fraction.

COMPONENTS: (1) Hydrogen chloride; HC1; [7647-01-0] (2) Hexane; C₆H₁₄; [110-54-3] VARIABLES: T/K: 283.15 - 323.15 P/kPa: 101.325 (1 atm) CRIGINAL MEASUREMENTS: Ryabov, V. G.; Solomonov, A. B.; Ketov, A. N.; Bugaichuk, A. M. Zh. Fiz. Khim. 1979, 53, 2915 - 6. Russ. J. Phys. Chem. 1979, 53, 1667 - 8. PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction #1
283.15	0.01630
293.15	0.01316
298.15	0.0112 ± 0.0001
303.15	0.01060
313.15	0.00789
323.15	0.00541

The authors fitted their results on a computer to the equation

$$Y(mo1 \%) = -2.577 + 403.143/(t + 50) - 9055.09/(t + 50)^{2}$$

The standard deviation was 0.029 mole per cent, and the variance was 0.003 (mole per cent) 2 . In the equation the temperature is $t/^0C$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen chloride was bubbled through a thermostated layer of the hydrocarbon.

Samples were removed at specified times, washed with distilled water, and the aqueous extract titrated with 0.1 N sodium hydroxide.

Saturation was confirmed by taking 2 to 3 more samples after the time concentration curve leveled.

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

VARIABLES: T/K:

194.64

P/kPa: 3.921 - 9.503 (29.41 - 71.28 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Equilibri	ım Mixture	Mol Fraction	Henry's Constant
	p ₁ /mmHg	n_1/mmol	n ₂ /mmol	x_1	$K/mmHg = p_1/x_1$
194.64	29.41	0.217	32.57	0.00662	4443
	55.30	0.402	32.57	0.01219	4537
	71.28	0.520	32.57	0.01571	4537
					4520 ¹ (5.947 atm)

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant for the mixtures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

By means of high precision high vacuum equipment and procedure the change of the pressure of the gas phase due to absorption was accurately measured at 194.64 к.

The mole fraction of hydrogen chloride in the liquid phase was calculated. The solubility was finally expressed as the Henry's constant, K/mmHg = HCl pressure/mole fraction.

Henry's constant is the pressure (numerically) at which $x_1 = 1$, and it may deviate widely from the reported value of $p_1^{\circ} = 1.4\overline{3}$ atm (1087 mmHg), the vapor pressure of pure liquid

hydrogen chloride at 194.64 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated, but may be taken as of high quality.
- (2) Heptane. Thoroughly attested as of high quality. Values of the boiling point and refractive index are in the paper.

ESTIMATED ERROR:

18 Hydrogen Chloride in Non-Aqueous Solvents COMPONENTS: ORIGINAL MEASUREMENTS: Strohmeir, W.; Echte, A. (1) Hydrogen chloride; HCl; [7647-01-0] Z. Elektrochem. 1957, 61, 549-555. (2) Heptane; C₇H₁₆; [142-82-5] VARIABLES: PREPARED BY: T/K: 200.8 - 272.9 T/K: 200.8 - 272 $p_1/mmHg$: 8.3 - 358.8W. Gerrard EXPERIMENTAL VALUES: 200.8 209.6 220.3 230.8 241.6 258.4 272.9 T/K p₁/mmHg Mole Fraction 10.8 14.5 18.7 0.001651 8.3 18.9 33.1 24.8 42.4 0.003677 33.9 0.005000 25.9 45.2 57.6 53.3 91.7 71.3 0.007823 40.8 60.5 79.3 105.8 85.6 111.4 150.5 0.011646 60.5 136.1 0.016478 192.1 42.2 71.0 0.002983 56.6 0.004964 71.4 94.8 119.0 0.006764 98.9 130.1 162.6 137.1 181.0 223.9 0.009337 0.011088 162.8 215.0 267.9 219.3 288.6 358.8 0.014766 Henry's constant for $x_1 + 0$ at 272.9 K was given as 24,000 mmHg. Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$. AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

1. Brown, H. C.; Brady, J. C. J. Am. Chem. Soc. 1952, 74, 3570.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Decane; C₁₀H₂₂; [124-18-5]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 264.15 - 319.15 Total P/kPc: 101.325 (1 atm) PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	n HC1/ n C $_{10}$ H $_{22}$	x HCl
264.15	0.0617	0.0581
267.15	0.0575	0.0544
273.15	0.0496	0.0473
273.35	0.0490	0.0467
279.15	0.0440	0.0421
283.15	0.0429	0.0411
288.35	0.0348	0.0336
293.95	0.0332	0.0321
298.15	0.0307	0.0298
306.65	0.0253	0.0247
319.15	0.0221	0.0216

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = -8.716 + 15.491/(T/100)$

Standard error about regression line = 1.03×10^{-3}

T/K	Mol Fraction
	xHCl
263.15	0.0591
273.15	0.0476
283.15	0.0390
293.15	0.0323
303.15	0.0272
313.15	0.0231
323.15	0.0198

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

For determination at temperatures below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method. A low temperature, Teddington-type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Decane. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 < 273 K$ $\delta x/x = 0.025$

COMPONENTS: (1) Hydrogen chloride; HC1; [7647-01-0] (2) Hexadecane; C₁₆H₃₄; [544-76-3] VARIABLES: T/K = 300 - 475 p₁/kPa < 133.3 (1000 mmHg) ORIGINAL MEASUREMENTS: Tremper, K. L.; Prausnitz, J. M. J. Chem. Eng. Data 1976, 21, 295 - 299. W. Gerrard

EXPERIMENTAL VALUES:			
	T/K	Partial Molar Entropy of Solution	Henry's Constant
		$\Delta \overline{s}_1/\text{cal } K^{-1} \text{ mol}^{-1}$	H _{1,2} /atm
	300	-4.06	45.0
	325	-5.06	54.3
	350	-5.14	65.8
	375	-4.81	78.3
	400	-4.22	90.7
	425	-3.47	102.0
	450	-2.52	111.0
	475	-1.61	116.

Henry's constant was defined as $H_{1,2}/\text{atm} = \lim_{\substack{x_1 \to 0 \\ \text{indicates the hexadecane.}}} (f_1/\text{atm})/x_1$

The partial molar entropy of solution is defined by:

$$\Delta \overline{s}_1 \equiv \overline{s}_1^L(T, x_1 = 1/H_{1,2}) - \overline{s}_{pure\ 1}^G(T, f_1 = 1 \text{ atm}) = -R(d \ln H_{1,2})/d \ln T$$

The partial molar enthalpy of solution is related by

 $\Delta \overline{h}_1 = T \Delta \overline{s}_1$.

The compiler states that caution should be exercized in using the expression 1/"Henry's constant" to calculate the mole fraction, x_1 , for 1 atm.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known amount of gas is added from a precision gas buret to a known amount of the hexadecane. Only the temperature and pressure need be measured to specify the system completely (1).

The experimental pressures were not stated. They were described as being low; "total pressures were always less than 1000 mmHg and usually much less."

The authors state that Henry's law was checked in some experiments, however, there is no definite statement that Henry's law was checked for HCl. Note compiler's caution below the table.

SOURCE AND PURITY OF MATERIALS:

Not specified; but may be deemed of acceptable purity.

ESTIMATED ERROR:

 $\delta x_1/x_1 = \pm 0.01$

REFERENCES:

 Cukor, P. M.; Prausnitz, J. M. Ind. Eng. Chem. Fundam. 1971, 10, 638.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Organic Solvents
- 3. Heptane; C₇H₁₆; [142-82-5]

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
Polytechnic of North London,
Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Mixtures of Heptane with Other Solvents.

Strohmeir & Echte (1) measured the solubility of hydrogen chloride in heptane at partial pressures from 1.1 kPa (8.3 mmHg) to 47.8 kPa (359 mmHg) in the temperature range 200.8 K to 272.9 K. Mixed solvents were prepared which, in most cases, consisted of 0.020 mole of heptane and 0.001 mole of a second solvent. The dioxane-heptane mixture under test however, consisted of 0.040 mole of heptane with 0.001 mole of dioxane. Solubility of hydrogen chloride was measured in each of the mixed solvents at 272.9 K and, in most cases, at other temperatures in the range 200.8 K to 272.9 K, over pressure ranges below barometric pressure. The variation of mole fraction solubility with partial pressure of hydrogen chloride deviates increasingly from linearity the greater the solubility of the gas in the mixed solvent.

The authors have calculated limiting values of Henry's constant, $k_{\rm H}$, for dissolution hydrogen chloride in the mixtures at 272.9 K from the variation of mole fraction solubility with pressure. These constants are defined by the relationship:

$$k_{H}/mmHg = lim. (P_{HC1}/x_{HC1})$$
 $x_{HC1} \rightarrow 0$

The evaluator has estimated mole fraction solubilities of hydrogen chloride in the mixtures for a temperature of 272.9 K and a partial pressure of 101.3 kPa. It has been assumed that the variation of partial pressure of hydrogen chloride with concentration in the solution can be represented by a Margules equation of the form :

$$P_{HC1} = P_{HC1}^{\circ} x_{HC1} \exp(\alpha(1-x_{HC1})^2)$$

The contribution of the heptane to the dissolution of the hydrogen chloride under these conditions has then been estimated. It has been assumed that this is given by the solubility of the gas in pure heptane multiplied by the mole fraction of heptane in the original mixed solvent i.e. 20/21 in most cases. The contribution of the second solvent in a mixture has been taken to be the difference between the total solubility and the contribution of the heptane. This has then been used to estimate the solubility of hydrogen chloride per mole of the second solvent and hence the apparent mole fraction solubility in this second solvent. Values are listed below.

For many of these second solvents there are independent values of mole fraction solubility at 273.15 K and a partial pressure of 101.3 kPa. These values are also listed below.

COMPONENTS. 1. Hydrogen Chloride; HCl;

- [7647-01-0]

 2. Organic Solvents
- 3. Heptane; C₇H₁₆; [142-82-5]

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
Polytechnic of North London,
Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION.

Solvent	Mixed solvent at 101.3 kPa (272.9 K)	Pure solvent *HCl at 101.3 kPa (273.15 K)
(Heptane)	(0.032)	0.032 (1)
1,1'-Oxybisethane	0.556	0.543 (2)
1,1'-Oxybispropane	0.502	(0.529)+
1,1'-Oxybisbutane	0.502	0.515 (3)
1,1'-0xybis[2-chloroethane]	0.235	0.229 (3)
Methoxybenzene	0.199	0.195 (3)
1,1'-Oxybisbenzene	0.175	0.105 (3)
1,1'-[Oxybis(methylene)]bisbenzene	0.413	<u>-</u>
Tetrahydrofuran	0.633	0.624 (3)
1,4-Dioxane	0.610	0.548 (3)
Tetrahydro-2H-pyran	0.552	-
1,1'-Thiobisethane	0.381	(0.397)¶(5)
Nitrobenzene	0.198	0.123 (4)
1-Methyl-2-nitrobenzene	0.193	(0.129)*(6)
Tetrachloromethane	0.017	0.022 §
Nitric acid, ethyl ester (ethyl nitra	ate) 0.092	_

- † mean of values for 1,1'-oxybisethane and 1,1'-oxybisbutane
- ¶ value for 1,1'-thiobispropane
- * estimated from the value at 298.15 K from measurements by O'Brien & Kenny on the assumption that the temperature coefficient of solubility at this temperature is the same as that for nitrobenzene
- § see page 236

Agreement is good, except in the case of nitrobenzene, 1-methyl-2-nitrobenzene and 1,1'-oxybisbenzene.

Brown & Brady (7) studied the solubility of hydrogen chloride in mixtures of heptane or methylbenzene with another solvent. In this case, however, the maximum partial pressure of hydrogen chloride was 9.67 kPa and extrapolation of solubilities to a partial pressure of 101.3 kPa is not justified. (see pages 38-40, 70-72)

- 1. Strohmeir, W.; Echte, A. Z. Elektrochem. 1957, 61, 549-555.
- Kapoor, K. P.; Luckcock, R. G.; Sandbach, J. A. J. Appl. Chem. Biotech. <u>1971</u>, 21, 97-100.
- Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1960, 10, 57-62.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109-119.
- 5. Frazer, M. J.; Gerrard, W. Nature, 1964, 204, 1299-1300.
- 6. O'Brien, S. J.; Kenny, C. L. J. Am. Chem. Soc. <u>1940</u>, 62, 1189-1192.
- 7. Brown, H. C.; Brady, J. D. J. Am. Chem. Soc. 1952, 74,3570-3582.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybisethane or diethyl
 ether; C₄H₁₀O; [60-29-7]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549-555.

VARIABLES:

T/K: 200.8 - 272.9 p₁/mmHg: 0.1 - 479.6

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K 200.8 209.6 220.3 230.8 241.6 258.4 272.9

Mole Fraction				p ₁ /mmHg			
0.005	0.1	0.2	0.5	1.8	3.4	9.4	20.7
0.010	0.2	0.5	1.5	3.4	7.9	20.8	43.8
0.015	0.3	0.8	2.4	5.5	14.2	33.5	70.9
0.020	0.5	1.1	3.8	8.7	20.3	49.2	101.5
0.025	0.7	1.9	5.6	12.7	27.5	66.1	137.3
0.030	1.3	3.0	8.5	19.7	36.5	92.9	176.1
0.035	2.2	5.0	12.3	27.9	53.1	122.3	221.7
0.040	3.7	8.6	19.3	40.2	73.4	158.7	278.4
0.045	6.4	17.2	31.1	58.0	97.7	200.7	334.0
0.050	12.6	25.5	46.7	81.5	127.8	253.1	405.6
0.055	23.4	39.7	72.4	113.0	166.7	312.9	479.6

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 4000 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Diethyl ether. Treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybispropane or dipropyl ether; C₆H₁₄O; [111-43-3]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549-555.

VARIABLES:

T/K: 200.8 - 272.9 p_1/mmHg : 0.25 - 556.0

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K 200.8 209.6 220.3 230.8 241.6 258.4 272.9

Mole Fraction				p ₁ /mmHg			
0.005	0.25	0.5	1.2	2.1	5.3	15.8	27.0
0.010	0.4	1.0	2.6	5.4	11.7	29.3	58.1
0.015	0.6	1.7	4.2	8.9	19.3	47.9	92.1
0.020	0.9	2.5	6.1	13.5	29.4	69.1	130.7
0.025	1.4	3.7	8.7	19.1	41.2	93.7	174.2
0.030	2.1	5.2	12.5	26.9	56.8	123.9	222.3
0.035	3.4	7.8	18.2	38.5	76.6	159.8	276.8
0.040	5.7	12.5	27.0	54.0	101.6	198.0	336.9
0.045	10.5	20.6	39.7	72.9	130.3	245.7	404.0
0.050	18.1	31.3	57.1	97.3	164.4	297.0	474.0
0.055	28.0	46.0	77.8	127.5	208.6	349.0	556.0

Henry's constant for $x_1 + 0$ at 272.9 K was given as 5200 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Dipropyl ether. Treated with KOH; distilled, and treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybisbutane or dibutyl ether; C₈H₁₈O; [142-96-1]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

2. Elektrochem. 1957, 61, 549 - 555.

VARIABLES: T/K: 200.8 - 272.9 $p_{_{1}}$ /mmHg: 0.25 - 556.0

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K 200.8 209.6 220.3 230.8 241.6 258.4 272.9

Mole Fraction F ₁ /mmHg	
0.005 0.25 0.5 1.2 2.1 5.3 15.8 2	27.0
	8.1
0.015 0.6 1.7 4.2 8.9 19.3 47.9 9	92.1
0.020 0.9 2.5 6.1 13.5 29.4 69.1 13	30.7
0.025 1.4 3.7 8.7 19.1 41.2 93.7 17	74.2
0.030 2.1 5.2 12.5 26.9 56.8 123.9 22	22.3
0.035 3.4 7.8 18.2 38.5 76.6 159.8 27	76.8
0.040 5.7 12.5 27.0 54.0 101.6 198.0 33	36.9
0.045 10.5 20.6 39.7 72.9 130.3 245.7 40	04.0
0.050 18.1 31.3 57.3 97.3 164.4 297.0 47	74.0
0.055 28.0 46.0 77.8 127.5 208.6 349.0 55	56.0

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 5200 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Dibutyl ether. Treated with KOH, distilled, and treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybis[2-chloroethane] or 2,2'-dichloroethyl ether; C₄H₈Cl₂O; [111-44-4]
- (3) Heptane; C₇H₁₆; [142-82-5]

VARIABLES:

T/K: 258.4, 272.9 p₁/mmHg: 16.2 - 562.0

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549 - 555.

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Mol
	p ₁ /mmHg	Fraction $\frac{x_1}{}$
258.4	76.2 139.4 198.2 256.5 319.1 387.4	0.00613 0.01181 0.01689 0.02164 0.02766 0.03234
272.9	109.6 204.1 290.7 373.1 480.0 562.0	0.00613 0.01181 0.01689 0.02164 0.02766 0.03234

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 17,300 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) 1,1'-Oxybis[2-chloroethane].
 Distilled in a vacuum.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Methoxybenzene or methyl phenyl ether or anisole; C7H0O; [100-66-3]

(3) Heptane; C_7H_{16} ; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549-555.

VARIABLES:

T/K: 209.6 - 272.9 p₁/mmHg: 12.8 - 635.0

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	209.6	220.3	230.8	241.6	258.4	272.9
Mole			p ₁ /mmHg			
Fraction			F 17			
<u> </u>						
0.00547	12.8	21.2	32.3	48.6	74.1	101.8
0.01134	26.3	44.2	67.7	101.1	153.8	210.2
0.01471	34.3	58.7	88.8	132.5	200.6	273.9
0.01918	46.9	77.1	117.2	174.6	263.1	358.8
0.02294	57.2	94.1	143.9	209.7	315.5	430.0
0.02871	72.9	121.3	181.3	265.2	398.6	539.9
0.03441	92.6	149.2	221.9	321.6	481.9	635

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 18,500 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Methoxybenzene. Dried with CaCl2, distilled, and treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-0xybisbenzene or diphenyl ether; $C_{12}^{H}_{10}^{O}$; [101-84-8]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

2. Elektrochem. 1957, 61, 549 - 555.

VARIABLES: T/K:

T/K: 258.4, 272.9 p₁/mmHg: 71.5 - 496.7

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Mol Fraction
	p_{η}/mmHg	\boldsymbol{x}_{1}
258.4	71.5	0.00454
	176.3	0.01120
	271.8	0.01727
	371.6	0.02348
272.9	94.0	0.00454
	234.7	0.01120
	359.4	0.01727
	496.7	0.02348

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 21,100 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Diphenyl ether. Distilled in a vacuum.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-[Oxybis(methylene)]
 bisbenzene or dibenzyl ether;
 C₁₄H₁₄O; [103-50-4]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

2. Elektrochem. 1957, 61, 549 - 555.

VARIABLES:

T/K: 258.4, 272.9 p₁/mmHg: 36.9 - 534.5

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/I	Pressure	Mol Fraction
	$\frac{p_1}{mmHg}$	$\frac{x_1}{x_2}$
258.4	36.9 75.2 115.7 172.6 221.4 281.1 341.5	0.00610 0.01243 0.01813 0.02491 0.03102 0.03783 0.04335
272.9	63.3 131.9 197.3 278.8 361.8 454.9 534.5	0.00610 0.01243 0.01813 0.02491 0.03102 0.03783 0.04335

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 10,300 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Dibenzyl ether. Dried with CaCl₂, distilled, treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrahydrofuran; C₄H₈O; [109-99-9]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS: Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549-555.

VARIABLES:

200.8 - 272.9 T/K: $p_1/mmHg: 0.0 - 371.8$

PREPARED BY:

,/mmHg

0.8

1.7

2.4

3.6

5.5

W. Gerrard

5.1

10.2

16.4

24.4

36.4

11.7 24.3

39.3

57.9

80.4

1.9

3.4

5.6

9.0

13.6

EXPERIMENTAL VALUES:

200.8 209.6 220.3 230.8 241.6 258.4 272.9 T/K

Mole Fraction				р
1				_
0.005	0.0	0.1	0.1	
0.010	0.0	0.3	0.3	
0.015	0.1	0.5	0.7	
0.020	0.2	0.7	1.3	
0.025	0.3	1.0	2.2	
0.030	0.4	1.3	3.3	

20.3 52.3 108.1 8.2 4.9 12.1 29.1 72.1 144.6 0.5 1.8 0.035 43.0 99.3 188.2 2.7 7.3 18.4 0.7 0.040 4.4 28.0 62.0 133.6 239.3 12.0 2.0 0.045 297.3 88.3 176.3 44.4 0.050 5.1 7.9 19.4 66.2 127.8 228.1 371.8 10.7 28.9 0.055 17.2

Henry's constant for $x_{j} \rightarrow 0$ at 272.9 K was given as 2100 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (Heptane) for each measurement.

Henry's constant: $H/mmHg = (r_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Tetrahydrofuran. Treated with KOH, distilled, and treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Dioxane; C₄H₈O₂; [123-91-1]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549 - 555.

VARIABLES:

T/K: 230.8 - 272.9 p_1 /mmHg: 5.0 - 716.0

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

1	r/K	230.8	241.6	258.4	272.9
Mole		p ₁ /mmHg			
Fract	-ion	1/1111111111111111111111111111111111111			
x_j					
	!				
0.0	05	5.0	9.6	21.3	39.0
0.0	010	10.6	20.7	45.5	85.0
0.0)15	17.7	35.9	76.7	136.0
0.0	20	28.1	54.0	112.0	189.5
0.0)25	41.7	78.6	152.6	252.5
)30		110.0	202.5	320.5
	35		141.8	257.3	400.0
	040		177.9	315.4	488.5
)45		222.4	377.5	558.5
	050		270.8	441.5	637.0
0.0)55		320.0	506.0	716.0

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 7500 mmHg.

The solvent is 0.001 mole of component (2) + 0.040 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Dioxane. Treated with KOH, distilled, and treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrahydro-2H-pyran; C₅H₁₀O; [142-68-7]
- (3) Heptane, C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957,61, 549 - 555.

VARIABLES:

T/K: 200.8 - 272.9 p₁/mmHg: 0.0 - 403.8

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	200.8	209.6	220.3	230.8	241.6	258.4	272.9
Mole Fraction				p_1 /mmHg	ſ		
<u> </u>							
0.005	0.0	0.3	0.7	1.3	2.8	6.7	13.3
0.010	0.1	0.6	1.2	2.7	5.6	14.1	29.9
0.015	0.2	0.9	1.9	4.1	8.7	22.6	48.9
0.020	0.3	1.2	2.8	5.8	13.1	34.8	73.0
0.025	0.4	1.5	3.8	8.4	18.6	48.8	101.0
0.030	0.5	1.8	5.3	12.0	26.9	66.6	134.6
0.035	0.8	2.9	7.9	17.8	39.1	90.5	171.6
	1.7	4.7	12.4	27.5	57.3	122.9	220.2
0.040		8.5	20.1	46.1	80.0	161.3	277.8
0.045	3.4			64.3	106.0	209.6	343.3
0.050	8.0	16.2	32.4			270.2	403.8
0.055	16.7	27.4	48.6	92.1	138.5	2/0.2	403.8

Henry's constant for x_7 > 0 at 272.9 K was given as 2600 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: H/mmHg = $(p_1/\text{mmHg})/x_1$ valid only in the limit $x_1 \to 0$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Tetrahydro-2H-pyran. Treated with KOH, distilled, treated with Na-K alloy.
- (3) Heptane. Purified as for optical measurements. Dried over sodiumpotassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Thiobisethane or diethyl sulfide; C₄H₁₀S; [352-93-2]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549-555.

VARIABLES:

200.8 - 272.9 T/K: p_1/mmHg : 1.4 - 544.4

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

_	T/K	200.8	209.6	220.3	230.8	241.6	258.4	272.9
14-1-	. \				~ /mmlla			
Mole	tion				p_1 /mmHg			
	<u> 1 </u>							
0.0	0655	1.4	3.0	6.3	12.0	22.4	44.9	74.7
	1085	2.6	5.4	11.0	21.1	39.3	70.0	126.7
0.0	1654	4.3	8.5	18.2	35.8	64.5	123.2	200.8
0.0	2075	6.0	12.5	24.7	47.2	85.1	159.1	252.2
0.0	2593	8.5	16.7	35.7	64.5	111.1	207.7	324.6
0.0	3039	11.7	21.9	44.3	79.9	137.3	250.3	389.1
0.0	3596	15.9	30.0	58.6	102.1	175.6	309.7	470.3
0.0	04131	21.6	39.1	74.2	129.9	210.9	365.8	544.4

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 11,400 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

- SOURCE AND PURITY OF MATERIALS:
 (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Diethyl sulfide. Treated with HgO, P_2O_5 , and distilled.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549 - 555.

(3) Heptane; C₇H₁₆; [142-82-5]

VARIABLES:

272.9 T/K: p_1/mmHg : 76.2 - 549.7 PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

	Mol
T/K Pressure	raction
p ₁ /mmHg	x ₁
272.9 76.2	0.00413
122.6	0.00660
203.6	0.01148
284.2	0.01580
375.4	0.02045
460.6	0.02514
549.7	0.02955

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 18,300 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Nitrobenzene. Dried with CaCl2, and distilled, in a vacuum.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

- (2) l-Methyl-2-nitrobenzene or o-nitrotoluene; C₇H₇NO₂; [88-72-2]
- (3) Heptane; C₇H₁₆; [142-82-5]

PREPARED BY:

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

W. Gerrard

2. Elektrochem. 1957, 61, 549 - 555.

VARIABLES:

T/K: 258.4, 272.9 $p_1/mmHg$: 39.0 - 522.6

EXPERIMENTAL VALUES:

T/K	Pressure	Mol Fraction
	p ₁ /mmHg	$\frac{x_1}{x_2}$
258.4	39.0 90.6 149.4 211.6 261.1 319.1 378.0	0.00293 0.00697 0.01134 0.01596 0.01955 0.02378 0.02801
272.9	53.1 125.3 207.4 294.7 361.9 442.6 522.6	0.00293 0.00697 0.01134 0.01596 0.01955 0.02378 0.02801

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 18,100 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) o-nitrotoluene. Dried with CaCl₂ and distilled in a vacuum.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrachloromethane or carbon tetrachloride; CCl₄; [56-23-5]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

2. Elektrochem. 1957, 61, 549-555.

VARIABLES:

T/K: 200.8 - 272.9 p_1/mmHg : 22.3 - 498.4

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

200.8 209.6 220.3 230.8 241.6 258.4 272.9 T/K

Mole Fraction $p_1/mmHg$

$\frac{x_1}{}$							
0.00430	22.3	28.8	39.0	50.9	63.7	84.8	105.4
0.00831	42.9	56.1	75.3	96.8	124.6	163.8	203.3
0.01160	60.0	78.0	105.2	135.3	174.1	229.5	287.1
0.01663	85.4	110.4	150.5	193.7	249.2		407.7
0.02016	103.7	134.6	181.5	234.4	300.7	399.3	498.4

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 24,600 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Carbon Tetrachloride. Dried with P₂O₅.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- Hydrogen chloride; HCl; [7647-01-0]
- (2) Nitric acid ethyl ester or ethyl nitrate; $C_2H_5NO_3$; [625-58-1]
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Strohmeir, W.; Echte, A.

Z. Elektrochem. 1957, 61, 549-555.

VARIABLES:

T/K: 200.8 - 272.9 p_1/mmHg : 13.7 - 659.0

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K 200.8 209.6 220.3 230.8 241.6 258.4 272.9

Mole	
Fract	ion
~	

$p_1/mmHg$

Fraction x_{\perp}				1			
1							
0.00417	13.7	18.4	26.5	35.0	49.5	69.3	93.2
0.00905	28.3	40.4	59.1	80.7	108.3	151.0	196.5
0.01037	31.3	44.5	66.3	91.8	125.3	172.9	233.9
0.01373	43.0	63.4	91.0	123.3	165.9	230.3	298.0
0.01755	57.4	80.6	115.8	157.4	211.4	291.7	376.8
0.02342	76.0	109.0	156.3	212.4	285.5	394.7	507.3
0.03000	96.8	136.5	200.4	270.4	365.1	503.3	659.0

Henry's constant for $x_1 \rightarrow 0$ at 272.9 K was given as 21,900 mmHg.

The solvent is 0.001 mole of component (2) + 0.020 mole of component (3) (heptane) for each measurement.

Henry's constant: $H/mmHg = (p_1/mmHg)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The same in principle as the high vacuum technique of Brown and Brady (1), except that the temperature was increased and the corresponding pressure of the gas phase measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not specified; but may be taken as of good quality.
- (2) Ethyl nitrate. Not stated.
- (3) Heptane. Purified as for optical measurements. Dried over sodium-potassium alloy.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen Chloride; HCl;
 - [7647-01-0]
- (2) Hydrocarbons and halogenated hydrocarbons
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. <u>1952</u>, 74, 3570 - 3582.

VARIABLES:

T/K: 194.64

p₁/kPa: 1.020 - 9.666 (see below)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES: Temperature = 194.64 K

Component (2)	P/mmHg	Equil	Equilibrium mixture			Henry's Constant
, = ,		n ₁ /mmol	n ₂ /mmol	n ₃ /mmol	Fraction *1	K/mmHg
Benzene; C ₆ H ₆ ;						
[71-43-2]	35.10	0.344	0.629	32.57	0.00996	3524
Į.	47.40	0.461	1.629	32.57	0.01330	3564
	72.50	0.723	1.629	32.57	0.02070	3502
j						3500¹
					(4	1.605 atm)
Methylbenzene; [108-88-3]	CaHa:				•	,
[108-88-3]	31.45	0.343	1.629	32.57	0.00993	3167
	49.05	0.538	1.629	32.57	0.01549	3167
	61.10	0.668	1.629	32.57	0.01916	3189
	01.10	0.000	1.025	32.37	0.01310	3170 ¹
					(4	1.171 atm)
	11.05	0-140	2.500	32.62 ²	0.00397	2783
	25.32	0.320	2.500	32.582²	0.00904	2801
	38.26	0.487	2.500	32.59 ²	0.01369	2795
	30.20	0.107	2.300	32.33	0.00	2790¹
					13	3.671 atm)
					(-	0.0/1 acm)

- The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.
- 2 Values calculated by the compiler. These experiments were carried out at a constant 2.5 mmol of component 2 in sufficient heptane to make a total volume of 4.803 ${\rm cm}^3$ of solution.

The compiler calculated the values of Henry's constant for the mixtures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

By means of high precision high vacuum equipment and procedure the change of the pressure of the gas phase due to absorption was accurately measured at 194.64 K.

The mole fraction of hydrogen chloride in the liquid phase was calculated. The solubility was finally expressed as the Henry's constant, K/mmHg = HCl pressure/mole fraction, p_1/x_1 .

Henry's constant is the pressure, (numerically) at which $x_1 = 1$, and it may deviate widely from the reported value of $p_1^{\circ} = 1.43$ atm (1087 mmHg), the vapor pressure of pure liquid hydrogen chloride at 194.64 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated, but may be taken as of high quality.
- (2,3) Thoroughly attested as of high quality. Values of the boiling points and refractive indices are given in the paper.

ESTIMATED ERROR:

- (1) Hydrogen Chloride; HCl; [7647-01-0]
- (2) Hydrocarbons and halogenated hydrocarbons
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS: Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

EXPERIMENTAL VALUES:

Temperature = 194.64 K

Component (2)	P/mmHg	Equil	ibrium mi:	xture	Mole Fraction	Henry's Constant
(2)		n_1/mmol	n ₂ /mmol	n ₃ /mmol	×1	K/mmHg
Ethylbenzene;						
C_8H_{10} ; [100-41-4]	12.22	0.167	2.500	32.64 ²	0.00473	2584
8 10	24.80	0.328	2.500	32.59 ²	0.00926	2678
	40.42	0.537	2.500	32.60²	0.01507	2682
						2680¹
1,3-Dimethylbenzen					(3	.526 atm)
C ₈ H ₁₀ ; [108-38-3]	25.00	0.300	1.629	32.57	0.00869	2877
8.10, 1.00 00 0,	39.99	0.468	1.629	32.57	0.01350	2962
	45.95	0.537	1.629	32.57	0.01545	2974
i						2980¹
}						.921 atm)
	13.53	0.193	2.500	32.59 ²	0.00547	2473
	30.86	0.441	2.500	32.592	0.01241	2487
	46.82	0.678	2.500	30.79²	0.01996	2346 2460¹
i	•				13	.237 atm)
1,3,5-Trimethylben	zene. (m	esitvlene):		()	.23/ acm;
C ₉ H ₁₂ ; [108-67-8]	12.11	0.113	0.326	32.57	0.00342	3541
9.12, [100 0, 0]	34.64	0.300	0.326	32.57	0.00903	3836
ĺ	44.79	0.381	0.326	32.57	0.01144	3915
1	62.83	0.531	0.326	32.57	0.01588	3957
[3910¹
						.145 atm)
	20.50	0.195	0.651	32.57	0.00583	3516
	30.79	0.292	0.651	32.57	0.00871	3535
	40.55	0.386	0.651	32.57	0.01148	3532 3510¹
					1.4	.618 atm)
Į.	30.25	0.415	1.629	32.57	0.01199	2523
	41.46	0.562	1.629	32.57	0.01617	2564
	49.92	0.676	1.629	32.57	0.01938	2576
						2550¹
					(3	.355 atm)
	7.65	0.126	2.500	32.67 ²	0.00357	2143
	19.16	0.309	2.500	32.59 ²	0.00873	2195
1	32.65	0.524	2.500	32.53 ²	0.01474	2215
						2210¹
/1 Math. 1 ath. 1 \ 1 = =	(:	1 -			(2	.908 atm)
(1-Methylethyl)ben C ₉ H ₁₂ ; [98-82-8]	15.30	0.217	2.500	32.63 ²	0.00614	2492
9"12' [90-02-0]	26.96	0.384	2.500	32.61 ²	0.01082	2492
i	38.69	0.556	2.500	32.59 ²	0.01560	2480
1						2490¹
					(3	.276 atm)
1						

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant for the mixtures.

 $^{^2}$ Values calculated by the compiler. These experiments were carried out at a constant 2.5 mmol of component 2 in sufficient heptane to make a total volume of 4.803 $\rm cm^3$ of solution.

- Hydrogen Chloride; HCl; (1) [7647-01-0]
- (2) Hydrocarbons and halogenated hydrocarbons
- (3) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS: Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

EXPERIMENTAL VALUES:

Temperature = 194.64 K

Component (2)	P/mmHg	Equil	ibrium mi	kture	Mole Fraction	Henry's Constant
(2)		n ₁ /mmol	n ₂ /mmol	n ₃ /mmo1	*1	K/mmHg
(2-Methylpropyl)be	enzene, (22.602	0.00600	2204
C ₁₀ H ₁₄ ; [538-93-2]	25.15	0.219 0.378	2.500 0.500	32.60 ² 32.58 ²	0.00620 0.01066	2384 2359
	39.56	0.589	2.500	32.59²	0.01651	2396 2380¹
Fluorobenzene;					(3	.132 atm)
C ₆ H ₅ F; [462-06-6]	14.21	0.162	2.500	32.632	0.00459	3096
	26.37 39.64	0.288 0.426	2.500 2.500	32.59^{2} 32.60^{2}	0.00814 0.01199	3240 3306
	33.51	0	2,300	32.00		3260 ¹ .289 atm)
Trifluoromethylben		0 051	1 (22	22.53	0.00730	4162
C ₇ H ₅ F ₃ ; [98-08-8]	30.30 45.66	0.251 0.368	1.629 1.629	32.57 32.57	0.00728 0.01064	4162 4291
	64.60	0.529	1.629	32.57	0.01523	4242
		•			(5	4220 ¹ .553 atm)
Chlorobenzene;	12.40	0 117	1 620	22 57	0 00341	2060
C ₆ H ₅ Cl; [108-90-7]	39.75	0.117 0.346	1.629 1.629	32.57 32.57	0.00341 0.01001	3960 3971
	72.32	0.628	1.629	32.57	0.01803	4011
					(5	4000 ¹ .263 atm)
	14.53	0.145	2.500	32.632	0.00411	3535
	26.23 41.67	0.258 0.413	2.500 2.500	32.58 ² 32.60 ²	0.00730 0.01163	3593 3583
	11.07	0.1.5	2,300	32.00		3570¹
Bromobenzene;					(4	.697 atm)
C ₆ H ₅ Br; [108-86-1]	10.50	0.101	2.500	32.59 ²	0.00287	3658
0 3	21.30 33.90	0.201 0.325	0.500 0.500	32.62 ² 32.58 ²	0.00569 0.00918	3743 3693
	33.70	0.525	0.300	32.30		3660¹
Todohongonos					(4	.816 atm)
Iodobenzene; C ₆ H ₅ I; [591-50-4]	11.58	0.111	2.500	32.63 ²	0.00315	3676
U D	30.58 39.86	0.289 0.375	2.500 2.500	32.58 ² 32.60 ²	0.00817 0.01057	3743 3771
	37.00	0.3/3	2.500	32.00	0.0105/	3750¹
(1009 Hontono)					(4	.934 atm)
(100% Heptane)	29.41	0.217	_	32.57	0.00662	4443
	55.30	0.402	-	32.57	0.01219	4537
	71.28	0.520	-	32.57	0.01571	4537 4520¹
					(5	.947 atm)

 $^{^1}$ The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant for the mixtures.

 $^{^2}$ Values calculated by the compiler. These experiments were carried out at a constant 2.5 mmol of component 2 in sufficient heptane to make a total volume of 4.803 $\rm cm^3$ of solution.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Miscellaneous Hydrocarbons

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Miscellaneous Hydrocarbons.

Chesterman (1) found that the solubility in a sample of petroleum boiling between 333.2 K and 353.2 K. was 0.3 wt.% at 298.15 K and a total pressure of 100.9 kPa. This may be compared with the solubility in hexane (b.pt. 341.9 K) of 0.54 wt.% under the same conditions as estimated by the evaluator from measurements by O'Brien & Kenny (2).

Solubility in cyclohexane was reported by Bell (3) at 293.15 K for a partial pressure of 101.3 kPa, by Wiegner (4) at 292.99 K and 313.15 K for a partial pressures from 0.025 to 89.1 kPa and by Tsiklis & Svetlova (5) at 283.15 K to 313.15 K for partial pressures from 0.133 to 106.7 kPa. There are discrepancies between the measurements as may be seen by comparing mole fraction solubilities at a partial pressure of 101.3 kPa based upon data from the three sources.

Mole fraction solubilities in cyclohexane at a partial pressure of 101.3 kPa from different sources.

	292.99 K	293.15 K	313.15 K
Bell		0.0154	
Wiegner	0.0144		0.0106
Tsiklis & Svetlova	0.0180	0.0179	0.0133

Further measurements on this system are required before reliable solubility data can be established.

Brown & Brady (6) measured solubilities in 2,4,4-trimethyl-1-pentene and in 2,4,4-trimethyl-2-pentene at 194.64 K and at partial pressures of gas between 0.509 kPa and 1.432 kPa. The solubility is greater in the latter than the former. These measurements cannot be linearly extrapolated to give a meaningful estimate of the mole fraction solubility at a partial pressure of 101.3 kPa. Such an extrapolation would give values greater than unity. However if the variation of mole fraction solubility with pressure approximates to a Margules equation then mole fraction solubilities at this partial pressure would be about 0.74.

Rajalo and co-workers (7) have published equations for Henry's law constants for dissolution in mixtures of dienes and chlorides from reaction with hydrogen chloride. If it is assumed that the equations are valid for 298.15 K over the whole of the mole fraction range and that the Henry's law constants can be used to calculate solubilities at 101.3 kPa then mole fraction solubilities at this temperature in the compounds under test are as follows:

1,3-pentadiene 0.049
2-methyl-1,3-butadiene 0.062
2,3-dimethyl-1,3-butadiene 0.017
(or 2-methyl-1,3-pentadiene; see the compilation)

In view of the lack of numerical data in the papers and the uncertainties involved in their interpretation the mole fraction solubilities can only be considered to be of semi-quantitative significance.

Scher et al. (8) measured the solubility of hydrogen chloride in 1-hexadecene at pressures from 23.3 kPa to 100.0 kPa and at four temperatures from 298.15 K to 328.15. Values of Henry's constants were reported. The data are self consistent and appear to be reliable. The corresponding mole fraction solubility at 298.15 K and a partial pressure of 101.3 kPa is 0.0357. This may be compared with a value of 0.0225 for dissolution in hexadecane from measurements by Tremper & Prausnitz (9). The reference value for this temperature from the Raoult's law equation is 0.0218. No other data for 1-hexadecene are available for comparison.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Miscellaneous Hydrocarbons

EVALUATOR:

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Department of Applied Chemistry
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January 1989

CRITICAL EVALUATION:

- 1. Chesterman, D. R. J. Chem. Soc. <u>1935</u>, 906-910.
- 2. O'Brien, S. J.; Kenny, C. L. J. Am. Chem. Soc. 1940, 62, 1189-1192.
- 3. Bell, R. P. J. Chem. Soc. 1931, 1371-1382.
- 4. Wiegner, F. Z. Elektrochem. 1941, 47, 163-164.
- 5. Tsiklis, D. S.; Svetlova, G. M. Zh. Fiz. Khim. 1958, 32, 1476-1480.
- 6. Brown, H. C.; Brady, J. D. J. Am. Chem. Soc. 1952, 74, 3570-3582.
- 7. Savich, T. O.; Dement'eva, V.; Rajalo, G. Eesti NSV Tead. Akad. Toim. Keem. Geol. 1977, 26, 83-88; 1979, 28, 45-46; Volens, T.; Rajalo G. ib. 1981, 30 (2), 136-137.
- Scher, M.; Gill, W. N.; Jelinek, R. V. Ind. Eng. Chem., Fundam. 1963, 2, 107-112.
- Tremper, K. L.; Prausnitz, J. M. J. Chem. Eng. Data 1976, 21, 295-299.

	1
COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Hydrogen chloride; HCl; [7647-01-0]</pre>	Chesterman, D. R.
(2) Petroleum	J. Chem. Soc. <u>1935</u> , 906 - 910.
(2) reclotedin	
VARIABLES: T/K: 298.15	PREPARED BY:
Total P/kPa: 101 (∿l atm)	W. Gerrard
EXPERIMENTAL VALUES:	
T/K Observed	Solubility g HCl g ⁻¹ Solution
p/mmHg	g HCl g · Solution
298.15 757	0.003
	}
AUUTTTANU	TNEODWATTON
	INFORMATION
METHOD APPARATUS / PROCEDURE:	
The apparatus was that used for the	SOURCE AND PURITY OF MATERIALS:
	(1) Hydrogen chloride. Prepared from
conductivity. A sample of the saturated solution was removed,	(1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was	(1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure
conductivity. A sample of the saturated solution was removed,	(1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P ₂ O ₅ .
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium,
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium,
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium,
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.
conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a	 (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅. (2) Petroleum. Was stated to be the purest obtainable. "Light petroleum," dried with sodium, b.p./°C (750 mmHg) = 60 - 80.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]

ORIGINAL MEASUREMENTS: Bell, R. P.

J. Chem. Soc. 1931, 1371 - 1382.

VARIABLES: T/K: 293.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Partition Coefficient c1,1/c1,g	Mol Fraction x1
293.15	3.42	0.0154

The ideal gas concentration at $p_1 = 1$ atm is $c_{1,q}/mo1 dm^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm^3 bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO, free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, $c/\text{mol dm}^{-3}$, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Cyclohexane. Good specimen was dried over calcium chloride, and distilled. Boiling point is given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

COMPONENTS: (1) Hydrogen chloride; HC1; [7647-01-0] (2) Cyclohexane; C₆H₁₂; [110-82-7] VARIABLES: T/K = 292.99, 313.15 p₁/kPa = 2.506 - 89.059 (18.8 - 668 mmHg) ORIGINAL MEASUREMENTS: Wiegner, F. 2. Elektrochem. 1941, 47, 163 - 164. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

Temp	erature	Hydrogen Chloride	Mol Fraction
t/°C	<i>T</i> /K	Partial Pressure p ₁ /mmHg	<i>x</i> ₁
19.84	292.99	18.8 176.9 263.0 372.6 473.9 566.9 668.0 (760.0	0.00039 0.00334 0.00480 0.00712 0.00878 0.01030 0.01230 0.0144) 1
40.00	313.15	58.0 164.9 271.5 366.3 465.4 543.4 (760.0	0.00094 0.00238 0.00401 0.00516 0.00681 0.00787 0.0106) 1

¹ By compiler's graphical extrapolation.

Between 293 and 313 K the enthalpy of solution was calculated to be $-2.19 \text{ kcal mol}^{-1}$ (-9.16 J mol⁻¹).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the cyclohexane until saturation was attained. The HCl content was determined by chemical titration.

The partial pressure, p_1 , appears to have been calculated by subtracting the vapor pressure of cyclohexane (over the pure liquid) from the measured total pressure, the vapor pressure lowering being deemed negligible for these small mole fraction, x_1 , values.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride was selfprepared.
- (2) Cyclohexane was rigorously
 purified. F.p./°C = 6.34,
 b. p. (1 atm)/°C = 80.05.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Cyclohexane; C₆H₁₂; [110-82-7]

ORIGINAL MEASUREMENTS:

Tsiklis, D. S.; Svetlova, G. M.

Zh. Hz. Khim. 1958, 32, 1476-1480.

VARIABLES: T/K: 283.15, 293.15, 313.15

 $p_1/mmHg:$ 100 - 800 PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K 283.15		T/K 25	T/K 293.15		T/K 313.15		
Pressure	Mole Fraction	Pressure	Mole Fraction	Pressure	Mole Fraction		
p ₁	<i>x</i> ₁	<i>p</i> ₁	<i>x</i> ₁	<i>p</i> ₁	x 1		
100	0.0028	100	0.0024	100	0.0018		
200	0.0055	200	0.0047	200	0.0035		
300	0.0083	300	0.0071	300	0.0053		
400	0.0111	400	0.0094	400	0.0071		
500	0.0131	500	0.0110	500	0.0088		
600	0.0166	600	0.0142	600	0.0105		
700	0.0194	700	0.0165	700	0.0123		
760	0.02091	760	0.01791	760	0.01331		
800	0.01222	800	0.0189	800	0.0141		

¹ Values at 760 mmHg read from graph prepared by compiler.

The authors smoothing equation for Henry's constant is

log (H/mmHg) = 6.608 - 580.5/(T/K) with H/mmHg = $(p_1/mmHg)/x_1$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The cyclohexane was frozen in the absorption vessel, and the air was pumped out. The vapor pressure, p_{g}^{u} , of the cyclohexane was determined.

The hydrogen chloride was admitted from a weighed vessel, and a second weighing gave (with certain adjustments) the amount of gas absorbed at the observed total pressure, p_t . The hydrogen chloride partial pressure, p, appeared to be obtained from the difference $p_t - p_s^0$.

The authors concluded that the mole fraction form of Henry's law was obeyed.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. The HCl was freed from water by cooling to about 213 K. It was then cooled by liquid nitrogen and distilled.
- (2) Cyclohexane. Purified by adsorption on silica gel and twice distilled.

ESTIMATED ERROR: The authors stated that they evaluated the error of their data by calculating the mean square deviation of the experimental data from those produced by interpolation of the curves. The deviation was stated to fluctuate from 10 to 15 per cent.

Probably in error for 0.0222.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2,4,4-trimethyl-1-pentene; C₈H₁₆; [107-39-1]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

VARIABLES: T/K:]

T/K: 194.64

P/kPa: 0.509 -

0.509 - 1.432 (3.82 - 10.74 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure P ₁ /mmHg	Equilibrium Mixture		Mol Fraction	Henry's Constant
		n ₁ /mmol	n ₂ /mmol	<i>x</i> 1	$K/mmHg = p_1/x_1$
194.64	3.82 5.95 10.74	0.325 0.490 0.840	44.96 44.96 44.96	0.00718 0.01078 0.01834	532 552 586
					550 ¹ (0.724 atm)

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant.

The authors estimated K/mmHg graphically; and stated that the graph showed slight curvature, possibly the result of a small quantity of a more basic impurity in the olefin.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

By means of high precision high vacuum equipment and procedure the change of the pressure of the gas phase due to absorption was accurately measured at 194.64 K.

The mole fraction of hydrogen chloride in the liquid phase was calculated. The solubility was finally expressed as the Henry's constant, K/mmHg = HCl pressure/mole fraction.

Henry's constant is the pressure (numerically) at which $x_1=1$, and it may deviate widely from the reported value of $p_1^\circ=1.43$ atm (1087 mmHg), the vapor pressure of pure liquid hydrogen chloride at 194.64 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated, but may be taken as of high quality.
- (2) 2,4,4-trimethyl-1-pentene. Thoroughly attested as of high quality. Values of the boiling point and refractive index are in the paper.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2,4,4-trimethy1-2-pentene; C₈H₁₆;
 [107-40-4]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

VARIABLES:

T/K: 194.64

P/kPa: 0.599 - 1.163

(4.49 - 8.72 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Equilibrium	Mixture	Mol Fraction	Henry's Constant
	p ₁ /mmHg	n ₁ /mmol	n ₂ /mmol	<i>x</i> ₁	$K/mmHg = p_1/x_1$
194.64	4.49	0.483	44.96	0.01063	422
	7.40	0.774	44.96	0.01693	437
	8.72	0.910	44.96	0.01984	440
					430 ¹ (0.566 atm)

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant.

The authors estimated K/mmHg graphically; and stated that the graph showed slight curvature, possibly the result of a small quantity of a more basic impurity in the olefin.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

By means of high precision high vacuum equipment and procedure the change of the pressure of the gas phase due to absorption was accurately measured at 194.64 K.

The mole fraction of hydrogen chloride in the liquid phase was calculated. The solubility was finally expressed as the Henry's constant, K/mmHg = HCl pressure/mole fraction.

Henry's constant is the pressure (numerically) at which $x_1 = 1$, and it may deviate widely from the reported value of $p_1^{\circ} = 1.43$ atm (1087 mmHg), the vapor pressure of pure liquid hydrogen chloride at 194.64 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated, but may be taken as of high quality.
- (2) 2,4,4-trimethyl-2-pentene. Thoroughly attested as of high quality. Values of the boiling point and refractive index are in the paper.

ESTIMATED ERROR:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Hydrogen chloride; HCl; [7647-01-0]	Savich, T. O.; Dement'eva, V. Rajalo, G.	
(2) 1,3-Pentadiene or piperylene; C ₅ H ₈ ; [504-60-9]	Eesti NSV Tead. Akad. Toim. Keem. Geol. <u>1977</u> , 26, 83 - 88.	
	Chem. Abstr. 1978, 88, 55542a	
VARIABLES:	PREPARED BY:	
	W. Gerrard	

EXPERIMENTAL VALUES:

The title of the paper is "Equilibrium Solubility of HCl in Piperylene and its Hydrochlorides." The authors used various mixtures of 1,3-pentadiene (piperylene), (E)-3-chloro-2-pentene (trans-2-chloro-3-pentene) [26423-61-0], and (Z)-3-chloro-2-pentene (cis-2-chloro-3-pentene) [26423-60-9]. There is a lack of definition in the quantities used. The pressure was not stated, presumably it was atmospheric. Numerical data were not given.

The solubility data were summarized by an equation which related Henry's constant, K/atm, to the temperature, T/K, and the 1,3-pentadiene mole fraction, x_2 : $\ln(K/\text{atm}) = 8.68 - 1760/(T/K) + 0.236 x_2.$

The low value of the term $0.236~x_2$ was deemed to show the small difference in solubility of HCl in 1,3-pentadiene and the chloro-hydrocarbons.

The heat of solution can be approximated from the temperature dependence of Henry's constant as-14630 J $mol^{-1}(-3495 \text{ cal } mol^{-1})$. There was deemed to be an insignificant difference in the heats of solution of HCl in 1,3-pentadiene and the chloro-hydrocarbons.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dried HCl was passed via a flowmeter into a jacketed bubbler tube reactor fitted with a sampling device. When constant conditions were attained, a sample was removed for titration with standard alkali. From this result, and by gas-liquid chromatography, the amounts of piperylene and its hydrochloride were determined.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride was obtained by the action of concentrated sulfuric acid, and dried calcium chloride.
- (2) "All components for the preparation of the initial mixtures were purified by rectification." Purity was stated to be greater than 99 per cent.

EXPERIMENTAL VALUES:

The title of the paper is "The Equilibrium Solubility of Hydrogen chloride in Systems Reacting with it and Consisting of Isoprene and Isopentenyl Chloride."

The authors stated that there is a negligible difference between the solubility of hydrogen chloride in isoprene and the isopentenyl chlorides. The authors conclude that there is absence of a statistical correlation between Henry's constant, K/atm, and the isoprene mole fraction, x_2 , and between ln (K/atm) and $x_2/T/K$. The authors obtained a correlation between Henry's constant, K/atm, and the temperature, T/K, which is given by the equation:

 $\ln (K/atm) = -6.12 - 996.6/(T/K)$.

The equation gives the approximate heat of solution of -8300 J mol^{-1} (-1980 cal mol⁻¹).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dried HCl was passed via a flowmeter into a jacketed bubbler tube reactor fitted with a sampling device. When constant conditions were attained, a sample was removed for titration with standard alkali. From this result, and by gas-liquid chromatography, the amounts of isoprene and the isopentenyl chlorides were determined.

See the authors earlier paper (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride was obtained by the action of concentrated sulfuric acid, and dried calcium chloride.
- (2) "All components for the preparation of the initial mixtures were purified by rectification." Purity was stated to be greater than 99 per cent.

ESTIMATED ERROR:

REFERENCES:

1. Savich, T. O.; Dement'eva, V.
Rajalo, G.
Eesti NSV Tead. Akad. Toim. Keem.
Geol. 1977, 26, 83.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2,3-Dimethy1-1,3-butadiene; C₆H₁₀; [513-81-5]

ORIGINAL MEASUREMENTS:

Volens, T.; Rajalo, G.

Eesti NSV Tead. Akad. Toim. Keem. 1981, 30 (2), 136 - 137.

VARIABLES:

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

The title of the paper is "Equilibrium solubility of hydrogen chloride in systems reacting with it consisting of 1,3-dimethylbutadiene and 1,3-dimethylbutadiene hydrochlorides."

The compiler assumes the title compound is 2,3-dimethyl-1,3-butadiene [513-81-5] however, 2-methyl -1,3-pentadiene [1118-58-7]is also possible.

Numerical data were not given. By using a regression analysis the authors related Henry's constant, K/atm, to the temperature, T/K, and the 2,3-dimethyl-1,3-butadiene mole fraction, x_2 :

ln (K/atm) = $8.26 - 1540/(T/K) + 0.997 x_2$.

The enthalpy of solution of hydrogen chloride in the hydrocarbon can be approximated from the temperature coefficient of the Henry's constant as $-12.8 \text{ kJ mol}^{-1}$ ($-3.06 \text{ kcal mol}^{-1}$).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dried HCl was passed via a flowmeter into a jacketed bubbler tube reactor fitted with a sampling device. When constant conditions were attained, a sample was removed for titration with standard alkali. From this result, and by gas-liquid chromotography, the amounts of the butadiene and its hydrochlorides were determined.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride was obtained by the action of concentrated sulfuric acid and dry calcium chloride.
- (2) "All components for the preparation of the initial mixtures were purified by rectification." Purity was stated to be greater than 99 per cent.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Hexadecene; C₁₆H₃₂; [629-73-2]

ORIGINAL MEASUREMENTS:

Scher, M.; Gill, W. N.; Jelinek, R. V.

Ind. Eng. Chem., Fundam. <u>1963</u>, 2, 107 - 112.

VARIABLES:

T/K: 298.15 - 328.15 P/kPa: 23.33 - 99.99 (175 - 750 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Henry's Constant		Number	Percent	Mol Fraction
	K'/mmHg dm ³ mol ⁻¹	K/mmHg	of Points	Mean Deviation	x ₁
298.15	6000	21,310	5	±1.0	0.0357
303.15	6990	24,470	7	±1.4	0.0311
313.15	7920	27,600	13	±1.6	0.0275
328.15	8680	29,820	4	±2.1	0.0255

Henry's constants:

 $K'/mmHg dm^3 mol^{-1} = (p_1/mmHg)/(c_1/mol dm^{-3})$

 $K/mmHg = (p_1/mmHg)/x_1$

The compiler calculated the mole fraction solubility value at 101.325 kPa (760 mmHg).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was measured in an apparatus designed to determine the kinetic rate of catalyzed hydrochlorination of 1-hexadecene in the presence of ferric chloride. The volume of gas absorbed by the pure liquid at increasing pressures, 175 - 750 mmHg, was measured. The individual solubility values are presented in a graph. The Henry's constants were tabulated.

The heat of solution was stated to be -3.00 kcal mol⁻¹ (-12.55 kJ mol⁻¹) at 303 K and -0.20 kcal mol⁻¹ (0.84 kJ mol⁻¹) at 328 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Matheson Co.
 Sublimed at high vacuum and
 liquid air temperature, and
 distilled into storage and
 supply system.
- (2) 1-Hexadecene. Purified by refluxing with potassium for 24 hours, and then distilled in a vacuum, and stored under nitrogen.

ESTIMATED ERROR:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Aromatic Hydrocarbons

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
Polytechnic of North London,
Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Aromatic Hydrocarbons.

The solubility of hydrogen chloride in benzene was measured over a pressure range by Saylor (1) and by O'Brien et al.(2). Approximate values of the solubility at a partial pressure of 101.3 kPa were estimated by the evaluator by use of the Krichevskir-Il'inskaya equation. Measurements were made at a total pressure equal to barometric pressure by Knight & Hinshelwood (3), Bell (4), Parande et al.(5), Chesterman (6) and by Zetkin et al.(7). Data by Paranda et al. differ by a factor of about 100 from other data and should be rejected. The solubility reported by Chesterman is high compared with values given by other workers and should be rejected because the method used may be unreliable. Mole fraction solubilities at a partial pressure of 101.35 bar fit the equation: $\ln x_{\rm HCl} = -358.42 + 17853.6 / ({\rm T/K}) + 51.818 \ln ({\rm T/K})$

The standard deviation in values of $x_{\rm HCl}$ is 0.00312. This equation is based upon measurements made from 283.15 KHCl to 323.15 K.

The solubility in benzene saturated with water was measured over pressure ranges below 101.3 kPa by Wynne-Jones (8) at 298.15 K and by Saylor (1) at 303.15 K. Extrapolation to a partial pressure of 101.3 kPa and comparison with the mole fraction solubility in dry benzene given by the above equation indicate an apparent increase in the mole fraction solubility from addition of water in the first case and an apparent decrease in the second case. However the difference between solubilities in benzene saturated with water and those in dry benzene are less than those between different values for solubility in dry benzene.

The solubility in methylbenzene was measured by Bell (4), by Parande et al.(5) and by Mirsaidov et al.(9) at barometric pressure, by O'Brien & Bobalek (10) at pressures to 28 kPa and by Brown & Brady (11) at pressures to 0.8 kPa. Measurements by Parande et al. should again be rejected because they are grossly out of line with other data. Extrapolation of measurements by O'Brien to a partial pressure of 101.3 kPa by use of a Krichevskii-Il'inskaya equation indicates a mole fraction solubility at 298.15 K of 0.0428. This is in contrast to the lower value of 0.0334 from measurements by Mirsaidov et al. Four values of mole fraction solubilities at a partial pressure of 101.3 kPa estimated by the evaluator from measurements by Bell, by Mirsaidov et al. and by O'Brien & Bobalek in the temperature range 273.15 K to 298.15 K fit the equation: $\ln x_{\rm HCl} = -9.383 + 1837/({\rm T/X})$

The standard deviation in values of $x_{\rm HCl}$ is 0.006.

Measurements by Brown and Brady at 194.64 K were at low pressures and reliable extrapolation to 101.3 kPa is not possible.

Solubilities in the three dimethylbenzenes at a total pressure equal to barometric pressure were measured over temperature ranges by Ahmed, Gerrard and Maladkar (12). These can be accepted on a tentative basis but no other measurements in pure dimethylbenzenes are available for comparison.

Mole fraction solubilities at 298.15 K and a partial pressure of gas of 101.3 kPa are, according to the data discussed above, in the order: benzene (0.0366) < methylbenzene (0.0399) < 1,2-dimethylbenzene (0.0515) < 1,4-dimethylbenzene (0.0529) < 1,3-dimethylbenzene (0.0570)

This series is close to that found by Brown & Brady except that the order of 1,2- and 1.4-dimethylbenzene is reversed. These authors measured the solubility of hydrogen chloride at 194.64 K and pressures to 0.84 kPa (6.4 mmHg) in mixtures of organic compounds (mostly aromatic) and methylbenzene in the ratio 4.515 moles to 44.96 moles. Similar measurements at the same temperature were also made of the solubility in mixtures of organic compounds and heptane. In this case measurements were carried out up to a pressure of 9.6 kPa (72 mmHg). Henry's constants, K, based on measurements at low pressures, were defined as:

 $K = P_{HC1}/x_{HC1}$

Values of K/mmHg are given in brackets. (The higher the value of K the lower is the mole fraction solubility at a fixed pressure.)

- Hydrogen Chloride; HCl; [7647-01-0]
- 2. Aromatic Hydrocarbons

EVALUATOR:

Peter G. T. Fogg Department of Applied Chemistry and Life Sciences, Polytechnic of North London, Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

Relative solubilities of HCl in mixtures containing methylbenzene and another solvent in the ratio 44.96 moles to 4.515 moles:

heptane (335) < (trifluoromethyl)-benzene (332) = tetrachlorethene (332)

- < chlorobenzene (318) < thiophene (316) < benzene (308) < 1-octene (306)</pre> < [methyl benzene] (299) < 1,4-dimethylbenzene (294) < cyclohexene (290)</pre>
- < 2,4,4-trimethyl-2-pentene (288) = 2,4,4-trimethyl-1-pentene (288)

- 1,2-dimethylbenzene (286) < 1,3-dimethylbenzene (278)
 1,2,4-trimethylbenzene (272) < 1,2,3-trimethylbenzene (265)
 1,3,5-trimethylbenzene (254) < 1,2,3,4-tetramethylbenzene (250)</pre>
- < 1,2,3,5-tetramethylbenzene (246)

Relative solubilities in mixtures containing heptane and another solvent in the ratio 32.57 moles to 1.629 moles :

[heptane] (4520) < trifluoromethylbenzene (4220) < chlorobenzene (4000)

- < benzene (3500) < fluorobenzene (3260) < methylbenzene (3170)</pre>
- < 1,3-dimethylbenzene (2980) < trimethylbenzene (2550)

Relative solubilities in mixtures containing heptane and another solvent in the ratio 32.67 moles to 2.5 moles :

[heptane] (4520) < lodobenzene (3750) < bromobenzene (3660)

- < chlorobenzene (3570) < fluorobenzene (3260) < methylbenzene (2790)
 < ethylbenzene (2680) < (1-methylethyl)-benzene (2490)</pre>
- < 1,3-dimethylbenzene (2460) < (2-methylpropyl)-benzene (2380)
- < 1,3,5-trimethylbenzene (2210)

The solubility of hydrogen chloride was also measured at two other concentrations of 1,3,5-trimethylbenzene in heptane. A plot of the reciprocal of the Henry's law constant against the mole fraction of 1,3,5-trimethylbenzene in the mixture lies close to a straight line (see fig. 1)

The data presented by Brown and Brady are self-consistent and appear to be reliable and enable useful comparisons with measurements of solubilities in single solvents at higher temperatures. The two authors explained the orders for the aromatic compounds indicated above in terms of relative basicities of aromatic nuclei and showed that there was good correlation with other measures of relative basicities.

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712-1714.
- O'Brien, S. J.; Kenny, C. L.; Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2 -2504-2507.; O'Brien, S. J. J. Am. Chem. Soc. 1941, 63, 2709-2712.
- Knight, R. W.; Hinshelwood, C. N. J. Chem. Soc. 1927, 466-472. 3.
- 4. Bell, R. P. J. Chem. Soc. 1931, 1371-1382.
- 5. Parande, M. G.; Kshirsagar, S. N.; Deshpande, A. B. Pet. Hydrocarbons 1969, 4, 17-18.
- 6. Chesterman, D. R. J. Chem. Soc. 1935, 906-910.
- Zetkin, V. I.; Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V. Khim. Prom. $\underline{1971}$, 47, 102-103. 7.
- Wynne-Jones, W. F. K. J. Chem. Soc. 1930, 1064-1071. 8.
- Mirsaidov, U.; Dzhuraev, Kh. Sh.; Semenenko, K.N. Dokl. Akad. Nauk. 9. Tadzh. SSR 1975, 18, 30-31.
- O'Brien, S. J.; Bobalek, E. G. J. Am. Chem. Soc. 1940, 62, 3227-3230. 10.
- Brown, H. C.; Brady, J. D. J. Am. Chem. Soc. 1952, 74, 3570-3582.
- 12. Ahmed W.; Gerrard W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109-115.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Aromatic Hydrocarbons

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
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January 1989

CRITICAL EVALUATION:

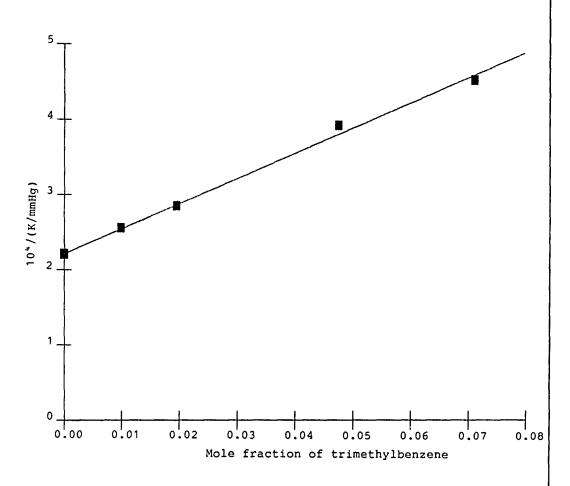


Figure 1

<u>Dissolution of hydrogen chloride in mixtures of</u>
1,3,5-trimethylbenzene and heptane - variation of the reciprocal of Henry's law constant, K, with the mole fraction of trimethylbenzene.

(see ref. 11)

- (1) Hydrogen chloride; HCl; [7647-01-1]
- (2) Benzene; C₆H₆; [71-43-2]

ORIGINAL MEASUREMENTS:

Knight, R. W.; Hinshelwood, C. N.

J. Chem. Soc. 1927, 466 - 472.

VARIABLES:

T/K: 293.15

Total P/kPa: 101.325

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total	Solubility
	Pressure p/mmHg	g dm ⁻³
293.15	760.4	16.80
	761.0	16.76
	760.4	16.82
	762.0	16.74
	761.4	16.79
	760.8	16.81
	759.4	16.80
	(760)	16.80 av.

The compiler assumes the density of solution to be the same as that of pure benzene at 293.15 K. He estimates the partial pressure of benzene above the solution to be 71.1 mmHg, and he assumes a linear change of mole fraction, x_1 , of hydrogen chloride with change in pressure for that range (689 - 760 mmHg). The estimated value of x_1 is 0.0433 for a partial pressure of HCl of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was a straight tube fitted with a gas inlet tube, and a capillary syphon tube for the withdrawal of samples of solution for chemical analysis. After the gas had been passed for many hours at 293.15 K, a sample of solution was allowed to pass into alkali, and the excess of the latter was back titrated. The total pressure in the absorption vessel was atmospheric.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. The HCl was prepared from sulfuric acid and ammonium chloride of attested purity.
- (2) Benzene. Analytical reagent standard. Purified and fractionated through a 6-foot column. M.p. 278.63 K.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Aromatic hydrocarbons; C6H6 and CyHo

ORIGINAL MEASUREMENTS:

Bell, R. P.

J. Chem. Soc. 1931, 1371 - 1382.

VARIABLES:

T/K: 293.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

Mol Fraction T/K Partition Coefficient x_1 c_{1,1}/c_{1,g} Benzene; C₆H₆; [71-43-2] 293.15 11.05 Methyl benzene or toluene; C_7H_8 ; [108-88-3]

293.15 11.9 0.0507

The ideal gas concentration at $p_1 = 1$ atm is $c_{1,q}/\text{mol dm}^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO2 free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, $c/\text{mol dm}^{-3}$, was converted to a partition coefficient by dividing by the ideal gas con-centration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Aromatic hydrocarbons. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

COMPONENTS: (1) Hydrogen chloride; HC1; [7647-01-0] (2) Benzene; C₆H₆; [71-43-2] VARIABLES: T/K: 298.15 Total P/kPa: 101 (~1 atm) ORIGINAL MEASUREMENTS: Chesterman, D. R. J. Chem. Soc. 1935, 906 - 910. W. Gerrard

EXPERIMENTAL VALUES:

T/K	Observed Pressure p/mmHg	Solubility g HCl g ⁻¹ Solution	Mol Fraction x1
298.15	767	0.02	0.042

The mole fraction solubility value was calculated by the compiler.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The apparatus was that used for the conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a standard acid solution.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅.
- (2) Benzene. Was stated to be the purest obtainable. Dried with sodium and distilled. B.p./°C (767 mmHg) = 79.5 - 80.0

ESTIMATED	ERROR:
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- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzene; C_6H_6 ; [71-43-2]

ORIGINAL MEASUREMENTS:

Saylor, J. H.

J. Am. Chem. Soc. 1937, 59, 1712 - 1714.

VARIABLES:

T/K: 303.15

P/kPa: 0.200 - 75.994 (1.5 - 570 mmHq)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Mole Ratio	Mol Fraction
	p ₁ /mmHg	$m_1/mol kg^{-1}$	n_1/n_2	x_1
303.15	1.5 6.2 51.4 78.0 211	0.0006 0.0022 0.0171 0.0391 0.111 0.172	0.0000468 0.000172 0.00133 0.00305 0.00866 0.0134	0.0000468 0.000172 0.00133 0.00304 0.00858 0.0132
	393 510 585 570	0.188 0.275 0.279 0.302	0.0147 0.0215 0.0232 0.0236	0.0145 0.0210 0.0226 0.0230
	(760			$0.027 - 0.029)^{1}$

¹ Estimated by the compiler from the uncertain plot of x_1 vs.

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consists of two glass bulbs which are separated by a tap. The lower bulb, $200~\rm{cm}^3$ capacity, contains the solvent and some gas space. The upper bulb, $292.6~\pm~0.02~\rm{cm}^3$ capacity, contains the gas.

The solvent in the lower bulb is saturated with HCl by bubbling the dry gas through the solvent. The bulbs are then "partially evacuated", the tap opened, and the whole apparatus put in a thermostat for 5 to 7 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated. The HCl partial pressure is calculated from the bulb volume and number of moles of HCl. A weighed solution sample is removed for the lower bulb and titrated with sodium hydroxide.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. The HCl was generated from sulfuric acid and good grade ammonium chloride.
- (2) Benzene. Both Baker Analyzed and Kahlbaum. Purified by fractional distillation, and stored over sodium.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

ORIGINAL MEASUREMENTS: COMPONENTS: O'Brien, S. J.; Kenny, C. L.; (1) Hydrogen chloride; HCl; [7647-01-0] Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504 - 2507. (2) Benzene; C₆H₆; [71-43-2] **VARIABLES:** PREPARED BY: T/K: 298.15 2.63 - 60.90W. Gerrard P/kPa: (0.026 - 0.601 atm)

EXPERIMENTAL VALUES:

T/K	Pressure p ₁ /atm	Molality m ₁ /mol kg ⁻¹	Mol Ratio	Mol Fraction $x_1^{'}$
298.15	0.026 0.078 0.100 0.111 0.197 0.211 0.391 0.601	0.014 0.040 0.047 0.048 0.096 0.112 0.191 0.273	0.00109 0.00312 0.00367 0.00374 0.00749 0.00874 0.0149 0.0213	0.00109 0.00311 0.00365 0.00373 0.00743 0.00866 0.0147 0.0209
	(1.00			0.0310)1

 $^{^1}$ Value from the compiler's graphical extrapolation of the plot of the above $x_1\ vs.\ p_1$ data.

The data are credited to unpublished M.S. theses of Schmelzle and Westfall, Creighton University, Omaha, NB.

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are almost identical to those of Saylor (1). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Benzene. Eastman Kodak Co. Used as received.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

REFERENCES:

Saylor, J. H.
 J. Am. Chem. Soc. 1937, 59,
 1712.

- Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzene; C_6H_6 ; [71-43-2]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.

J. Am. Chem. Soc. 1941, 63, 2709 - 2712.

VARIABLES:

T/K: 303.15, 313.15 0.77 - 61.73P/kPa: (5.8 - 463 mmHg)

PREPARED BY:

W. Gerrard

EXPER

T/K	Pressure P1/mmHg	Molality m ₁ /mol kg ⁻¹	Mol Ratio	Mol Fraction x1
303.15	47	0.0255	0.0020	0.0020
	65	0.0364	0.0028	0.0028
	72	0.0396	0.0031	0.0031
	246	0.145	0.0113	0.0112
	438	0.252	0.0197	0.0193
	463	0.263	0.0205	0.0201
	(760			0.0306)1
313.15	5.8	0.0026	0.000203	0.000203
	12.3	0.0061	0.00048	0.00048
	17.0	0.0074	0.00058	0.00058
	22.4	0.0110	0.00086	0.00086
	46.7	0.0204	0.00159	0.00159
	48.8	0.0221	0.00172	0.00172
	56.2	0.0284	0.00222	0.00221
	108	0.046	0.00359	0.00358
	159	0.076	0.00593	0.00590
	247	0.107	0.00835	0.00827
	(760			0.0214)1

 $^{^{1}}$ A graphical extrapolation of the plot of the actual x_{1} values vs. p, gives the stated value for 101.325 kPa (760 mmHg).

AUXILIARY INFORMATION

Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The HCl in the The tap is closed. upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

- METHOD/APPARATUS/PROCEDURE:

 The method and apparatus are those of (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
 - Stored over sodium. (2) Benzene. Distilled before use; m.p. 278.63 K.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzene; C₆H₆; [71-43-2]

ORIGINAL MEASUREMENTS:

Parande, M. G.; Kshirsagar, S. N.; Deshpande, A. B.

Pet. Hydrocarbons 1969, 4, 17 - 18.

VARIABLES:

T/K: 301.15 - 328.15

HCl P/kPa: 53.33 - 80.53 (400 - 604 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total	Approximate	Solubility	Mol Frac	tion x_1^2
,	Pressure p _t /mmHg	HC1 Pressure 1 p1/mmHg	g cm ⁻³	Experiment Pressure	
301.15	714	604	0.0001786	0.000439	0.000552
308.15	714	569	0.0001380	0.000342	0.000457
318.15	714	490	0.0001104	0.000278	0.000431
328.15	714	400	0.0000781	0.000199	0.000378

¹ The compiler calculated the approximate HCl partial pressure by subtracting the pure benzene vapor pressure from the total pressure at the specified temperature.

The mole fraction solubility at one atm HCl was obtained by the compiler assuming a linear change of x_1 with pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dry hydrogen chloride was bubbled into about $500\ \mathrm{cm}^3$ of solvent which was in a three-necked flask fitted with a stirrer. The pressure was stated to be atmospheric.

The passage of gas appeared to be stopped; the liquid was stirred for "some more time" to remove excess gas; a 5 cm3 sample of solution was removed for an acid-alkali titration

The liquid was then stirred 30 to 40 m at the next higher temperature, controlled by a thermostat, and another sample was removed for titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Chemically pure grade hydrochloric acid was added dropwise to chemically pure sulfuric acid.
- (2) Benzene. Source not given. Chemically pure sample distilled and stored over sodium.

ESTIMATED ERROR:

² The mole fraction solubility values were calculated by the compiler assuming the solubility represented g HCl with 1 cm3 of pure solvent. The density of pure solvent was used at each temperature.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzene; C_6H_6 ; [71-43-2]

ORIGINAL MEASUREMENTS:

Zetkin, V. I.; Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V.

Khim. Prom. 1971, 47, 102 - 103.

Soviet Chem. Ind. 1971, 3, 89 - 90.

VARIABLES:

T/K = 283.15 - 323.15p/kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Temp	erature	Mol Fraction
t/°C	<i>T</i> /K	x_1
10 20 30 40	283.15 293.15 303.15 313.15	0.0562 0.0417 0.0302 0.0224
50	323.15	0.0162

The measurements appear to have been carried out at a total pressure of one atm.

Smoothed Data: For use between 283.15 and 323.15 K

ln $x_1 = 34.3060 - 39.2708/(T/100 K) - 22.4004 ln (T/100 K)$ The standard error about the regression line is 2.53 x 10^{-4} .

<i>T</i> /K	Mol Fraction
283.15	0.0563
293.15	0.0415
298.15	0.0356
303.15	0.0305
313.15	0.0223
323.15	0.0162

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas absorbed at atmospheric pressure as described by Zetkin and Kosorotov (1). The amount of gas absorbed was determined by a chemical titration.

The author fitted the data to the linear equation

$$\log x_1 = -5.71 + 1270/(T/K)$$

However, the three constant equation above fits the data much better. The author's equation gives an enthalpy of solution of $-5.8 \text{ kcal mol}^{-1}$.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared from sodium chloride and concentrated sulfuric acid. Dried with sulfuric acid.
- (2) Benzene. Purity stated to be greater than 99 %. Dried with calcium chloride.

ESTIMATED ERROR:

REFERENCES:

Zetkin, V. I.; Kosorotov, V. I.
 Zh. Fiz. Khim. <u>1970</u>, 44, 830.

VARIABLES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzene; C₆H₆; [71-43-2]
- (3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Wynne-Jones, W. F. K.

J. Chem. Soc. 1930, 1064 - 1071.

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T/K: 298.15 $p_1/mmHg$: 2.95 - 28.1

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Water Phase	Benzene Phase	Henry's Constant	Mole Fraction 1
	p ₁ /mmHg	$m_1/\text{mol kg}^{-1}$	$m_1/\text{mol kg}^{-1}$	(Benzene) p ₁ /m ₁	(Benzene)
298.15	2.95	9.603	0.00213	1390 1370	0.000166
	5.72 10.74	10.508	0.00423	1350 1400	0.000330
	15.6	11.99	0.0110 0.0216	1420 1300	0.000858 0.00168

¹ The value of the mole fraction of HCl in benzene was calculated by the compiler.

Henry's constant: $H/mmHg \ kg \ mol^{-1} = (p_1/mmHg)/(m_1/mol \ kg^{-1})$.

 p_1/mmHg is the pressure common to both liquid phases, and based on the value for the aqueous solution, as given by Randall and Young (1). Notice that the maximum pressure is only 28.1 mmHg (0.0370 atm, 3.75 kPa).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

It was simply stated that the "two liquids" were shaken together in a stoppered bottle; but it must be presumed that hydrogen chloride had already been added to the water. The bottle was occasionally shaken over a period of 2 - 5 days. Then samples of each liquid were taken; and, by an acid-base titration, the amount of hydrogen chloride in a weighed amount of each sample was determined.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. The gas was obtained by dropping hydrochloric acid (analytical grade) into sulfuric acid.
- (2) Benzene. Not stated.
- (3) Water. Not stated.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$

REFERENCES:

1. Randall, M.; Young, L. E. J. Am. Chem. Soc. 1928, 50,

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Benzene; C_6H_6 ; [71-43-2]

ORIGINAL MEASUREMENTS:

Saylor, J. H.

J. Am. Chem. Soc. 1937, 59, 1712 - 1714.

VARIABLES:

T/K: 303.15

P/kPa: 14.49 - 77.21

(109 - 579 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Mole Ratio	Mol Fraction
	P ₁ /mmHg	m ₁ /mol kg ⁻¹	n ₁ /n ₃	x_1
303.15	109 244 395 579	0.0579 0.132 0.205 0.282	0.00452 0.0103 0.0160 0.0220	0.00450 0.0102 0.0157 0.0215
	(760			0.0266)1

¹ Estimated by the compiler. The actual plot of x_1 vs. p_1 is distinctly curved concave upward. Extrapolation from the highest pressure to 760 mmHg gives the value for x_1 .

The mole ratio and mole fraction values were calculated by the compiler.

Water-saturated benzene. The solution was prepared by bubbling HCl into a mixture of water and benzene. A sample of the benzene layer was transferred to the apparatus described below to determine the equilibrium vapor pressure of HCl.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consists of two glass bulbs which are separated by a tap. The lower bulb, 200 cm³ capacity, contains the solvent and some gas space. The upper bulb, 292.6 ± 0.02 cm³ capacity, contains the gas.

The solution is placed in the lower bulb. The bulbs are then partially evacuated, the tap opened, and the whole apparatus put in a thermostat for 5 to 7 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with carbonate free sodium hydroxide. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl. A weighed solution sample is removed from the lower bulb and titrated with carbonate free sodium hydroxide.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. The HCl was generated from sulfuric acid and a good grade ammonium chloride.
- (2) Water. No information.
- (3) Benzene. Both Baker Analyzed and Kahlbaum. Purified by fractional distillation, and stored over sodium.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Methylbenzene or toluene; C7H8; [108-88-3]

ORIGINAL MEASUREMENTS: O'Brien, S. J.; Bobalek, E. G.

J. Am. Chem. Soc. 1940, 62, 3227 - 3230.

VARIABLES:

298.15 T/K:

3.35 - 28.53P/kPa:

(25.1 - 214 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure P1/mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	25.1 25.7	0.0153 0.0167	2.16	0.00141 0.00154	0.00141 0.00153
	73.9	0.0465	2.09	0.00428	0.00426 0.00429
	73.3 120	0.0468 0.0762	2.07	0.0070	0.00696
	190 214	0.119 0.137	2.11 2.05	0.0109 0.0126	0.0108 0.0124
	(760	0.478	2.09 av	0.0444	0.0425)2

¹ k/atm mol -1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of (1) Hydrogen chloride. Prepared saylor (1) as modified by O'Brien et from chemically pure potassis The main difference is the al. (2). use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Toluene. Stated to be of good quality, stored over sodium, and distilled, $n_{\rm D}^{20}$, 1.4959.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0409 to 0.0436 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Methylbenzene or toluene; C₆H₅CH₃; [108-88-3]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

VARIABLES: T/K:

K: 194.64

P/kPa: 0.504 - 0.836 (3.78 - 6.27 mmHg)

.64 PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Pressure	Equilibrium	Mixture	Mol Fraction	Henry's Constant
	P1/mmHg	n ₁ /mmol	n ₂ /mmol	x_1	$K/mmHg = p_1/x_1$
194.64	3.78 4.84 6.27	0.640 0.824 1.061	49.475 49.475 49.475	0.01278 0.01639 0.02099	296 295 299
					299 ¹ (0.393 atm)

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

By means of high precision high vacuum equipment and procedure the change of the pressure of the gas phase due to absorption was accurately measured at 194.64 K.

The mole fraction of hydrogen chloride in the liquid phase was calculated. The solubility was finally expressed as the Henry's constant, K/mmHg = HCl pressure/mole fraction.

Henry's constant is the pressure (numerically) at which $x_1=1$, and it may deviate widely from the reported value of $p_1^\circ=1.43$ atm (1087 mmHg), the vapor pressure of pure liquid hydrogen chloride at 194.64 K.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not stated, but may be taken as of high quality.
- (2) Methylbenzene. Thoroughly attested as of high quality. Values of the boiling point and refractive index are in the paper.

ESTIMATED ERROR:

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Methylbenzene or toluene; C7Hg; [108-88-3]

ORIGINAL MEASUREMENTS:

Parande, M. G.; Kshirsagar, S. N.; Deshpande, A. B.

Pet. Hydrocarbons 1969, 4, 17 - 18.

VARIABLES:

T/K: 300.15 - 328.15 78.93 - 90.66 (592 - 680 mmHg) HCl P/kPa:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total	Approximate ,	Solubility	Mol Frac	tion x_1^2
	Pressure Pt/mmHg	HCl Pressure ¹	g cm ⁻³	Experiment Pressure	At One Atm
300.15	712	680	0.0002759	0.000809	0.000904
308.15	712	665	0.0001980	0.000586	0.000669
318.15	712	635	0.0001677	0.000502	0.000601
328.14	712	592	0.0001380	0.000423	0.000543

- 1 The compiler calculated the approximate HCl partial pressure by subtracting the pure toluene vapor pressure from the total pressure at the specified temperature.
- ² The mole fraction solubility values were calculated by the compiler assuming the solubility represented g HCl with 1 \mbox{cm}^3 of pure solvent. The density of pure solvent was used at each temperature.

The mole fraction solubility at one atm HCl was obtained by the compiler assuming a linear change of x_1 with pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dry hydrogen chloride was bubbled into about $500~{\rm cm}^3$ of solvent which was in a three-necked flask fitted with a stirrer. The pressure was stated to be atmospheric.

The passage of gas appeared to be stopped; the liquid was stirred for "some more time" to remove excess gas; a 5 cm³ sample of solution was removed for an acid-alkali titration.

The liquid was then stirred 30 to 40 m at the next higher temperature, controlled by a thermostat, and another sample was removed for titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Chemically pure grade hydrochloric acid was added dropwise to chemically pure sulfuric acid.
- (2) Methylbenzene. Chemically pure sample was distilled, and stored over sodium.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Methylbenzene or toluene; C₇H₈; [108-88-3]

ORIGINAL MEASUREMENTS:

Mirsaidov, U.; Dzhuraev, Kh. Sh.; Semenenko, K. N.

Dokl. Akad. Nauk Tadzh. SSR 1975, 18, 30 - 31.

VARIABLES:

T/K = 273.15, 298.15 $p_1/kPa = 101.325 (1 atm)$ PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Hydrogen Chloride	Mol Ratio	Mol Fraction
	wt%	$\frac{n_1/n_2}{}$	x ₁
273.15	2.8	0.0729	0.0679
298.15	1.3	0.0332	0.0322

The authors labeled the HCl as HCl, %. The compiler assumed this was weight per cent to calculate the mole ratio and mole fraction.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the liquid until the concentration remained constant. The amount dissolved was determined by an alkali titration. The final pressure was presumably a total pressure equal to the atmospheric pressure.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Obtained from its concentrated aqueous solution by treatment with concentrated sulfuric acid.
- (2) Methylbenzene. Not stated.

ESTIMATED ERROR:

- (1) Hydrogen Chloride; HCl;
 - [7647-01-0]
- (2) Various organic compounds
- (3) Methylbenzene, (toluene); C₇H₈; [108-88-3]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. <u>1952</u>, 74, 3570 - 3582.

VARIABLES:

T/K: 194.64

 $p_1/kPa: 0.120 - 0.855$ (see below)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES: Temperature = 194.64 K

Component (2)	P/mmHg	Equilibrium mixture			Mole Fraction	Henry's Constant
		n ₁ /mmol	n ₂ /mmol	n ₃ /mmol	[*] 1	K/mmHg
Cyclohexene;						
C ₆ H ₁₀ ; [110-82-7]	1.74	0.303	4.515	44.96	0.00609	286
6.10, 11, 32	3.38	0.588	4.515	44.96	0.01174	288
i	5.70	0.995	4.515	44.96	0.01971	289
1	3.	••••			• • • • • • • • • • • • • • • • • • • •	290¹
					(0	.382 atm)
Heptane;						
C ₇ H ₁₆ ; [142-82-5]	2.25	0.334	4.515	44.96	0.00671	335
7.16,	3.50	0.526	4.515	44.96	0.01052	333
	5.90	0.888	4.515	44.96	0.01763	335
]						335¹
		•			(0	.441 atm)
2,2,4-Trimethyl-1-	pentene;					
C ₈ H ₁₆ ; [107-39-1]		0.156	4.515	44.96	0.00314	287
8.16	3.33	0.574	4.515	44.96	0.01147	290
1	4.75	0.810	4.515	44.96	0.01611	295
						288¹
					(0	.379 atm)
					•	•

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant for the mixtures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

By means of high precision high vacuum equipment and procedure the change of the pressure of the gas phase due to absorption was accurately measured at 194.64 K.

The mole fraction of hydrogen chloride in the liquid phase was calculated. The solubility was finally expressed as the Henry's constant, K/mmHg = HCl pressure/mole fraction, p_1/x_1 .

Henry's constant is the pressure, (numerically) at which $x_1 = 1$, and it may deviate widely from the reported value of $p_1^{\circ} = 1.43$ atm (1087 mmHg), the vapor pressure of pure liquid hydrogen chloride at 194.64 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated, but may be taken as of high quality.
- (2,3) Thoroughly attested as of high quality. Values of the boiling points and refractive indices are given in the paper.

ESTIMATED ERROR:

COMPONENTS: (1)

Hydrogen Chloride; HCl; [7647-01-0]

(2) Various organic compounds

Methylbenzene, (toluene); (3) C_7H_8 ; [108-88-3]

ORIGINAL MEASUREMENTS: Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74,

3570 - 3582.

EXPERIMENTAL VALUES: Temperature = 194.64 K

Component (2)	P/mmHg	Equil	ibrium mi	xture	Mole Fraction	Henry's Constant
		n ₁ /mmol	n ₂ /mmol	n ₃ /mmol	^x 1	K/mmHg
2,4,4-Trimethyl-2-	pentene;					
C ₈ H ₁₆ ; [107-40-4]	1.30	0.228	4.515	44.96	0.00459	283
	2.75 4.58	0.476 0.772	4.515 4.515	44.96 44.96	0.00953 0.01537	289 298
						288¹
1-Octene;					(0	.379 atm)
C ₈ H ₁₆ ; [111-66-0]	1.95	0.317	4.515	44.96	0.00637	306
0 10	3.00	0.487	4.515	44.96	0.00975	308
	4.11	0.661	4.515	44.96	0.01320	311 306¹
					(0	.403 atm)
Benzene;	1.90	0.313	4.515	44.96	0.00629	302
C ₆ H ₆ ; [71-43-2]	3.67	0.601	4.515	44.96	0.00029	302
	5.80	0.947	4.515	44.96	0.01880	309
					(0	308 ¹
1,2-Dimethylbenzen	ne, (o-xy	lene);			(0	.405 acm)
C ₈ H ₁₀ ; [95-47-6]	1.40	0.245	4.515	44.96	0.00493	284
	3.65 5.15	0.636 0.902	4.515 4.515	44.96 44.96	0.01269 0.01791	288 288
	3.13	0.302	4.515	44.50	0.01731	286¹
	,				(0	.376 atm)
1,3-Dimethylbenzen C ₈ H ₁₀ ; [108-38-3]	1.99	1 <i>ene</i>); 0.359	4.515	44.96	0.00720	276
8.10	2.98	0.542	4.515	44.96	0.01084	275
	3.92	0.701	4.515	44.96	0.01397	281
					(0	278 ¹ 366 atm)
1,4-Dimethylbenzen	ne; (p-xy	lene);				
C ₈ H ₁₀ ; [106-42-3]	2.34	0.402	4.515	44.96	0.00806	290
	5.18 6.41	0.885 1.093	4.515 4.515	44.96 44.96	0.01757 0.02161	295 297
	0.1			1110	0,02,0.	2941
1 2 2 Marinoshirilban	mana (h	amima11:t			(0	.387 atm)
1,2,3-Trimethylben C _q H ₁₂ ; [526-73-8]	2.88	0.545	4.515	44.96	0.01090	264
1 -9.127 (020 70 01	4.45	0.838	4.515	44.96	0.01666	267
	5.61	1.065	4.515	44.96	0.02107	266 265¹
					(0	.349 atm)
1,2,4-Trimethylben						·
С ₉ н ₁₂ ; [95-63-6]	3.36 4.24	0.623 0.783	4.515 4.515	44.96 44.96	0.01244 0.01558	270 272
	5.49	1.011	4.515	44.96	0.02003	274
						272¹
					(0	.358 atm)

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant for the mixtures.

```
COMPONENTS:
(1) Hydrogen Chloride;
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- 1) Hydrogen Chloride; HCl; [7647-01-0]
- (2) Various organic compounds
- (3) Methylbenzene, (toluene); C₇H₈; [108-88-3]

ORIGINAL MEASUREMENTS:
Brown, H. C.; Brady, J. D.

J. Am. Chem. Soc. 1952, 74, 3570 - 3582.

EXPERIMENTAL VALUES: Temperature = 194.64 K

Component (2)	P/mmHg	Equil	ibrium mi	xture	Mole Fraction	Henry's Constant
		n ₁ /mmol	n ₂ /mmol	n ₃ /mmol	^x 1	K/mmHg
1,3,5-Trimethylben	zene, (m	esitylene	•);			
C_9H_{12} ; [108-67-8]	1.84	0.375	4.515	44.96	0.00752	245
9 12	2.78	0.547	4.515	44.96	0.01094	254
	4.40	0.852	4.515	44.96	0.01693	260
						254 ¹
4 2 2 4 Mahaamatha	14	/ - n - h			(0	.334 atm)
1,2,3,4-Tetramethy		., (prenni 0.276	tene); 4.515	44.96	0.00555	241
C ₁₀ H ₁₄ ; [488-23-3]	3.05	0.276	4.515	44.96	0.00555	255
	3.85	0.800	4.515	44.96	0.01158	248
	J.05	0.7,7	4.010	77.70	0.01333	250¹
					(0	.329 atm)
1,2,3,5-Tetramethy	lbenzene	, (isodur	ene);			
C ₁₀ H ₁₄ ; [527-53-7]	2.50	0.514	4.515	44.96	0.01028	243
10 1-1	3.61	0.733	4.515	44.96	0.01460	247
						2461
					(0	.324 atm)
(Trifluoromethyl)be		(benzotri			0.00073	222
C ₇ H ₅ F ₃ ; [98-08-8]	2.24	0.335	4.515 4.515	44.96 44.96	0.00673 0.01060	333
	3.50 5.43	0.530 0.824	4.515	44.96	0.01060	330 332
	3.43	0.024	4.010	44.70	0.01030	332 ¹
					(0	.437 atm)
Chlorobenzene;					• =	,,,,
C ₆ H ₅ Cl; [108-90-7]	1.88	0.299	4.515	44.96	0.00601	313
6 5	3.55	0.555	4.515	44.96	0.01109	320
	5.53	0.861	4.515	44.96	0.01711	323
						318 ¹
					(0	.418 atm)
Tetrachloroethene;	4 5 4	^ ^ ^ ^	A 515	44 06	0.00460	328
C ₂ Cl ₄ ; [127-18-4]	1.54 2.63	0.233 0.403	4.515 4.515	44.96 44.96	0.00469 0.00808	325 325
	2.03 5.15	0.403	4.515	44.96	0.00505	328
	J. 13	0.703	4.515	33.70	0.0137.	332¹
					(0	.437 atm)
Thiophene, (thiofus	ran);				-	
C4H4S; [110-02-1]	3.80	0.602	4.515	44.96	0.01202	316
4 4	4.92	0.783	4.515	44.96	0.01202	316
	5.89	0.939	4.515	44.96	0.01863	316
						316¹
(4000 N-th-1h-m-m	- 1				(υ	.416 atm)
(100% Methylbenzen	e) 3.78	0.640	_	49.475	0.01278	296
	4.84	0.824	-	49.475	0.01278	296 295
	6.27	1.061	-	49.475	0.02099	299
	0.27	1.001	_	47.473	0.02000	2991
					(0	.392 atm)
					()	· J / L a cm /

The authors' value. The plot of pressure vs. mole fraction was read as linear. The Henry's constant value should not be used indiscriminately to calculate values of mole fraction for pressures greater than the maximum recorded above.

The compiler calculated the values of Henry's constant for the mixtures.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybisethane or diethyl ether; $C_4H_{10}O$; [60-29-7]
- (3) Methylbenzene or toluene; $C_7^H_8$; [108-88-3]

ORIGINAL MEASUREMENTS:

Mirsaidov, U.; Dzhuraev, Kh. Sh.; Semenenko, K. N.

Dokl. Akad. Nauk Tadzh. SSR 1975, 18, 30 - 31.

VARIABLES:

T/K = 273.15, 298.15 $p_1/kPa = 101.325 (1 atm)$ PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Ether Methylbenzene Ratio	Hydrogen Chloride ² $10^2 w_1 / \text{wt}^{\$}$
273.15	1:0 1:1 3:7 1:3 0:1	26.5 20.1 12.7 11.04 2.8
298.15	1:0 3:1 1:1 1:3 0:1	17.0 19.0 13.5 81 1.3

From small graph. Note that the author's diagram showing plots of HCl, % vs. time is wrongly indexed; the line for 1:1 is labeled as for 1:3, and vice versa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the liquid until the concentration remained constant. The amount dissolved was determined by an alkali titration. The final pressure was presumably a total pressure equal to the atmospheric pressure.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Obtained from its concentrated aqueous solution by treatment with concentrated sulfuric acid.
- (2) 1,1'-Oxybisethane. Not stated.
- (3) Methyl benzene. Not stated.

ESTIMATED ERROR:

The authors labeled the HCl content as HCl, %. The compiler assumed this was weight per cent.

COMPONENTS: 1. Hydrogen chloride; HCl; Ahmed, W.; Gerrard, W.; Maladkar, V. K. 2. 1,2-Dimethylbenzene; C₈H₁₀; J. Appl. Chem. 1970, 20, 109 - 115. VARIABLES: PREPARED BY: T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm) VARIABLES: W. Gerrard

EXPERIMENTAL	VALUES:					
		T/K	Mol	Ratio	Mol	Fraction

	nHC1/nC3H10	X _{HC1}
253.15	0.188	0.158
263.15	0.136	0.120
273.15	0.103	0.0934
283.15	0.075	0.0698
293.15	0.061	0.0575

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -9.359 + 19.036/(T/100)$

Standard error about the regression line = 1.03×10^{-3}

T/K	Mol Fraction
	X _{HC1}
253.15 263.15 273.15 283.15 293.15	0.159 0.119 0.0917 0.0717 0.0570

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

 Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.

(smoothed data calculated by H.L. Clever)

 1,2-Dimethylbenzene. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.015$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972,
 22, 623 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. 1,3-Dimethylbenzene; C₈H₁₀;
 [108-38-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 203.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: T/K Mol Ratio Mol Fraction

_	n HC1 $/^{n}$ C $_{8}$ H $_{10}$	X _{HCl}
203.15	1.45	0.592
213.15	0.95	0.487
223.15	0.60	0.375
233.15	0.385	0.278
243.15	0.270	0.213
253.15	0.195	0.163
263.15	0.140	0.123
273.15	0.110	0.0991
283.15	0.085	0.0783
293.15	0.071	0.0663

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln x_{HC1} = 9.261 - 6.786/(T/100) - 9.026 \ln (T/100)$ Standard error about regression line = 1.42 x 10⁻²

T/K	Mol Fraction
	XHCl
203.15	0.621
213.15	0.471
223.15	0.359
233.15	0.275
243.15	0.212
253.15	0.165
263.15	0.129
273.15	0.101
283.15	0.0797
293.15	0.0632

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- 1,3-Dimethylbenzene. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.04$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972,
 22, 623 650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. 1,4-Dimethylbenzene; C₈H₁₀;
 [106-42-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARTABLES:

T/K: 273.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	"HC1/"C8H10	X _{HC1}
273.15	0.111	0.0999
283.15	0.080	0.0741
293.15	0.064	0.0602

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -9.752 + 20.313/(T/100)$

Standard error about regression line = 2.30×10^{-3}

T/K	Mol Fraction
3	X _{HC1}
273.15	0.0987
283.15	0.0759
293.15	0.0594

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- 1,4-Dimethylbenzene. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

$$\delta X/X = 0.015$$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Dimethylbenzene (mixture of isomers); C₈H₁₀; [1330-20-7]

ORIGINAL MEASUREMENTS:

Parande, M. G.; Kshirsagar, S. N.; Deshpande, A. B.

Pet. Hydrocarbons 1969, 4, 17 - 18.

VARIABLES:

T/K: 300.15 - 328.15

HCl P/kPa: 93.33 (700 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total	Approximate	Solubility	Mol Frac	tion x_1^2
	Pressure P _t /mmHg	HCl Pressure ¹	g cm ⁻³	Experiment Pressure	At One Atm
300.15	711	700	0.0005520	0.00187	0.00203
308.15			0.0004629		
318.15			0.0003750		
328.15			0.0003220		

The compiler calculated the approximate HCl partial pressure by subtracting the pure solvent vapor pressure from the total pressure at the specified temperature.

The mole fraction solubility at one atm HCl was obtained by the compiler assuming a linear change of x_1 with pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dry hydrogen chloride was bubbled into about $500~{\rm cm}^3$ of solvent which was in a three-necked flask fitted with a stirrer. The pressure was stated to be atmospheric.

The passage of gas appeared to be stopped; the liquid was stirred for "some more time" to remove excess gas; a 5 cm³ sample of solution was removed for an acid-alkali titration.

The liquid was then stirred 30 to 40 m at the next higher temperature, controlled by a thermostat, and another sample was removed for titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Chemically pure grade hydrochloric acid was added dropwise to chemically pure sulfuric acid.
- (2) Dimethylbenzene. Commercial grade sample was distilled, and stored over sodium.

ESTIMATED ERROR:

 $^{^2}$ The mole fraction solubility values were calculated by the compiler assuming the solubility represented g HCl with 1 ${\rm cm}^3$ of pure solvent. The density of pure solvent was used at each temperature.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alcohols

EVALUATOR:

H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA

1984, March; revised 1987, February

CRITICAL EVALUATION:

An Evaluation of the Solubility of Hydrogen Chloride in Alcohols.

Fifteen papers (ref 1 - 15) report the solubility of hydrogen chloride gas in fourteen linear primary alcohols, four branched primary alcohols, five linear secondary alcohols, and one branched secondary alcohol. Most of the measurements were carried out at a hydrogen chloride partial pressure of 101.3 kPa at several temperatures. Measurements at hydrogen chloride partial pressures less than atmospheric pressure (101.3 kPa) are reported for only methanol, ethanol, and 1-butanol. Seventy per cent of the data are in six papers (ref 5, 7, 8, 9, 13, 14) from the laboratory of Professor W. Gerrard, who has published extensively on the solubility of gases in liquids (ref 16, 17, and references therein).

The solutions saturated at 101.3 kPa partial pressure of hydrogen chloride are concentrated and non-ideal. A number of conductivity studies have been carried out on dilute hydrogen chloride-alcohol solutions, but few experiments have been carried out to characterize the departure from ideal behavior of the concentrated solutions. The nature of the interaction between hydrogen chloride and the alcohol lone pair electrons is still a matter of some controversy as to whether these are strong, moderate, or weak electrolyte interactions.

Table 1 compares the solubilities of hydrogen chloride in the various alcohol solutions liquid at 273.15 and 298.15 K and 101.3 kPa partial pressure hydrogen chloride in units of mole fraction (x_1) , molality $(m_1/\text{mol kg}^{-1})$, and concentration $(c_1/\text{mol dm}^{-3})$. The solubility of hydrogen chloride in water is included for comparison (ref 18). Table 2 contains a more extensive comparison of mole fraction solubilities for 24 alcohols at ten degree intervals over the experimental range reported.

The experimental data were treated by linear regressions to obtain equations of ln (mole fraction) as a function of temperature. The mole fraction values in Table 1 and 2 are from these equations. Several of the 273.15 K values were extrapolated from values at higher temperature. The mole fraction values in Table 1 are believed to be reliable to 0.5 percent or better. The molality values, calculated directly from the mole fraction values, should be equally reliable. However, the concentration values may be uncertain by several percent. They were approximated by estimating the solution volume to be the sum of the pure hydrogen chloride and alcohol volumes at 273.15 and 298.15 K. The density of liquid hydrogen chloride was taken from (ref 18).

The solubility data in Table 1 show several trends of interest. (i) The mole fraction solubility of hydrogen chloride is smaller in water than in any of the alcohols at 273.15 K, but larger in water than in the primary alcohols at 298.15. The secondary alcohols show a larger mole fraction solubility than in water at both temperatures. (ii) The mole fraction solubility of hydrogen chloride in the primary alcohols increases with increasing alcohol carbon number from methanol to 1-pentanol at 273.15 K, and from methanol to 1-heptanol at 298.15 K. The largest increase is between methanol and ethanol (5-7%); at higher carbon number alcohols the increase is about the magnitude of the uncertainty in the measurement. (iii) The mole fraction solubility is about four percent greater in the secondary alcohol than in the corresponding carbon number primary alcohol at these temperatures.

Individual hydrogen chloride + alcohol systems are discussed below under sections on the effect of hydrogen chloride partial pressure and temperature on the solubility.

 The solubility of hydrogen chloride in alcohols as a function of partial pressure.

The solubility of hydrogen chloride as a function of pressure

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Alcohols

EVALUATOR:

H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA

1984, March, revised 1987, February

Table 1. Solubility of hydrogen chloride in alcohols. Tentative values of the mole fraction (x_1) , molality $(m_1/\text{mol kg}^{-1})$, and concentration $(c_1/\text{mol dm}^{-3})$ solubilities at 273.15 and 298.15 K at a hydrogen chloride partial pressure of 101.3 kPa.

Alcohol	<i>T</i> /K	<i>x</i> ₁	m ₁ /mol kg ⁻¹	$c_1/\text{mol dm}^{-3}$
Water ^a	273.15 298.15	0.487 0.463	52.8 47.9	22.5 21.4
Linear (Normal) Primary	Alcohols			
Methanol	273.15 298.15	0.490 0.419	30.0 22.5	12.4 9.85
Ethanol	273.15 298.15	0.513 0.448	22.9 17.6	10.7 8.5
1-Propanol	273.15 298.15	0.513 0.449	17.5 13.6	9.2 7.3
1-Butanol	273.15 298.15	0.520 0.451	14.6 11.1	8.2 6.4
1-Pentanol	273.15 298.15	0.523	12.4 9.28	7.3 5.6
1-Hexanol	273.15 298.15	0.518	10.5	6.5 5.1
1-Heptanol	273.15 298.15	0.516 0.456	9.17 7.21	5.9 4.7
1-Octanol	273.15 298.15	0.511 0.452	8.02 6.33	5.3 4.2
1-Nonanol	273.15 298.15	0.449	5.65	3.85
1-Decanol	273.15 298.15	0.513 0.460	6.68 5.38	4.6 3.7
1-Dodecanol	273.15 298.15	0.424	3.95	2.9
Branched Primary Alcoho	ls			
2-Methyl-l-propanol	273.15 298.15	0.514 0.455	14.3 11.3	8.0 6.4
2-Methyl-1-butanol	273.15 298.15	0.526 0.471	12.6 10.1	7.4 6.0
3-Methyl-1-butanol	273.15 298.15	0.521	12.3	7.15
2,5,5-Trimethyl-1-hexand	298.15	0.517 0.457	7.42 5.83	5.0 3.95
Linear and Branched Seco 2-Propanol	273.15 298.15	0.530 0.472	18.8 14.9	9.4 7.6
2-Butanol	273.15 298.15 273.15	0.539 0.473 0.535	15.8 12.1 13.2	8.6 6.8
3-Pentanol 4-Heptanol	298.15 273.15	0.479 0.535	10.4 9.90	7.6 6.1 6.2
2-Octanol 4-Methyl-2-pentanol	298.15 273.15 273.15 298.15	0.478 0.535 0.547 0.476	7.88 8.83 11.8 8.89	5.0 5.7 7.0 5.4
a Ref 18				J • 3

was studied in methanol at 298.15 K, in ethanol at 298.15 K, and in 1-butanol at a number of temperatures between 235 and 326 K. One study estimated the hydrogen chloride solubility at a single small partial pressure from electrochemical measurements in methanol and ethanol at a temperature of 298.15 K. The temperatures, pressure intervals, and number of measurements are summarized below and in Figures 1, 2, and 3.

System	T/K	Pressure Interval	Number	Reference
HCl + Methanol	298.15	5.19-1.116x10 Pa	56	11
	298.15	0.11 Pa	1	6
HCl + Ethanol	298.15	14.4 - 625 Pa	5	2
	298.15	62 Pa	1	6
HCl + 1-Butanol	273.15	22.8 - 101.3 kPa	6	9
	278.15	28.3 - 116.9 kPa	6	9
	283.15	34.3 - 136.4 kPa	6	9
	288.15	41.2 - 157.7 kPa	6	9

1. Hydrogen chloride + 1-Butanol [71-36-3]

Gerrard, Mincer and Wyvill (ref 9) report the partial pressure of hydrogen chloride over six solutions as a function of temperature and pressure. There are over 60 measurements that range in temperature from 235.15 to 326.85 K and in hydrogen chloride partial pressure from 22.7 to 170.7 kPa (170 to 1281 mmHg). From these measurements data sets of the solubility of hydrogen chloride as a function of partial pressure were prepared at temperatures of 273.15, 278.15, 283.15, and 288.15. The data are displayed in Figure 1 as a plot of $\ln (p_1/k\text{Pa})vs$. $\ln (x_1)$. The plots were assumed to be linear, and the data were treated by a linear regression to obtain the intercepts and slopes below:

Intercept	Slope
8.6572	6.153
8.7605	6.044
8.7876	5.8575
8.8432	5.7146
	8.6572 8.7605 8.7876

The slopes are very near six. They show that the hydrogen chloride mole fraction solubility increases as about the (1/6) power of the partial pressure.

Professor Gerrard has long criticized both the concept and the application of Henry's law. He is correct in that Henry's law does not apply to the HCl + 1-butanol system at these temperatures and pressures. The partial pressure to the (1/6) power is quite different than the limiting first power dependence expected of Henry's law in the limit of low pressure and dilute solution.

At present we have no explanation of the linear $\ln \ (p_1) \ vs. \ln \ (x_1)$ relationship of slope near six. As an empirical relationship it appears to be useful. From a single measurement of the solubility at atmospheric pressure one can assume the slope of six and estimate the hydrogen chloride mole fraction solubility down to an HCl partial pressure of near 20 kPa. Figure 1 data do show a slight upward curvature. Thus, it is not advisable to use the relationship at either higher or lower pressures until the relationship is studied over greater pressure intervals.

The hydrogen chloride + 1-butanol data are classed as tentative. The equation $\ln (p_1/\text{kPa}) = \text{Intercept} + \text{Slope ln} (x_1)$ reproduces the data with an average deviation of less than 0.5 percent.

2. Hydrogen chloride + Ethanol [64-17-5]

Jones, Lapworth, and Lingford (ref 2) measured the solubility of hydroger chloride in ethanol and in a number of ethanol + water mixtures. Only the results for pure ethanol are presented and discussed in this volume. They measured the equilibrium pressure of HCl over solutions of known composition rather than measure directly the solubility. There are five duplicate measurements at hydrogen chloride partial pressures between 14 and 625 Pa. These values are presented in Figure 2 on a $\ln (p_{1}/\mathrm{kPa})$ vs. $\ln (x_{1})$ plot. Also on Figure 2 is a point for the accepted solubility at one atm (101.3 kPa) with a line of slope six drawn through it. The experimental data at

- (1) Hydrogen Chloride; HCl; [7647-01-0]
- (2) Alcohols

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pressures less than 1 kPa deviate from the line of slope six, but do appear to be approaching the line as the partial pressure increases.

The results are classed as tentative. The experimental values at $298.15 \, \mathrm{K}$ are given below:

HCl partial pressure, p_1/Pa 14.4 55.6 108. 351 625 Mole Fraction HCl, x_1 0.0159 0.0425 0.0651 0.1267 0.1642

The authors applied the Gibbs-Duhem relation to obtain an equation for the HCl partial pressure as a function of the solution mole ratio. It is interesting that the equation, when extrapolated to atmospheric pressure, gives a solution composition that is within 2 percent of the accepted HCl solubility in ethanol at that pressure.

3. Hydrogen chloride + Methanol [67-56-1]

Fritz (ref 6) estimated one solubility value at a partial pressure of 0.11 Pa from his analysis of emf results. Schmid, Maschka, and Sofer (ref 11) made 56 measurements of the HCl vapor pressure over HCl + methanol solutions of known composition. The partial pressures ranged from 5.19 to 11160 Pa at 298.15 K. The single value of Fritz does not agree well with the results of Schmid et al. The value was not considered further, but the lack of agreement is disturbing since Fritz's solubility value in ethanol appears to be reliable.

Nine of the Schmid $et\ al.$ values are plotted on the $\ln\ (p_1/\mathrm{kPa})\ vs.$ $\ln\ (x_1)$ scale of Figure 2. Also on the Figure is a point for the solubility of HCl in methanol at atmospheric pressure with a line of slope six through it. The solubility values at the lower pressures deviates greatly from the line, but the values at partial pressures of 3.08, 6.11, and ll.16 kPa fall almost on the line of slope six. This indicates the empirical observation of the slope six line for the HCl + 1-butanol system may be useful for other systems. For the HCl + methanol system it may allow a reasonable estimation of the solubility down to a partial pressure of 3 kPa.

A further test for Henry's law behavior is shown in Figure 3. All 56 measurements of Schmid et al. (ref 11) were used to prepare the Figure of ln (p_1/mmHg) ve. ln $(m_1/\text{mol kg}^{-1})$. The experimental values are compared with a Henry's law line of slope 2 (strong electrolyte assumption) estimated from literature emf measurements in ultradilute solutions. If our estimate is correct, the HCl + methanol system is not in agreement with Henry's law at the pressure of 5.19 Pa (0.0389 mmHg). For the HCl + methanol solutions the relationship for the HCl activity was taken to be $a_1 = a_+^2 = m_+^2 \gamma_+^2$.

The data of Schmid, Mashka, and Sofer (ref 11) are classed as tentative. The single value of Frizt (ref 6) is classed as doubtful. The behavior of HCl + methanol solutions at low HCl partial pressures needs further study.

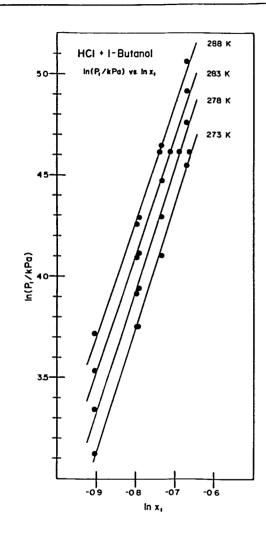


Figure 1. (+)

Hydrogen chloride + 1-Butanol

$$\ln (p_1/kPa)$$
 vs. $\ln x_1$

The data are from Gerrard et al. (ref 9). The straight lines have slopes near six, which shows that the solubility varies as about the (1/6) power of the hydrogen chloride partial pressure. This is not Henry's law behavior.

The slopes and intercepts of the four straight lines are given in the text. The hydrogen chloride partial pressures range from about 20 to 160 kPa.

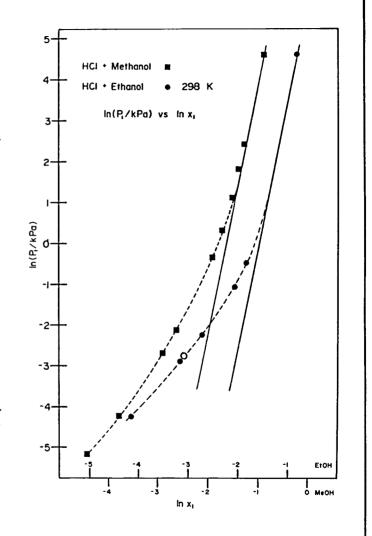
Figure 2. (→)

Hydrogen chloride + Methanol Hydrogen chloride + Ethanol

$$\ln (p_1/kPa) vs. \ln x_1$$

The data are from (ref 11), methanol, and (ref 2 and 6), ethanol.

A straight line of slope six is drawn through the solubility value at a hydrogen chloride partial pressure of 101.3 kPa (atmospheric pressure). The solubility in both alcohols appears to be approaching the line as the partial pressure increases. The open circle represents the value from (ref 6).





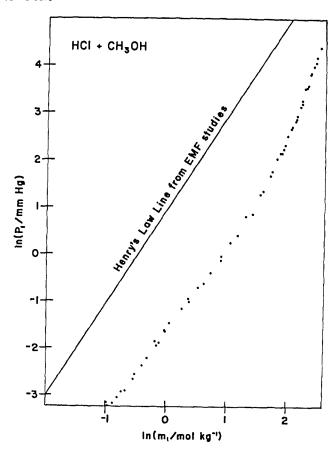


Figure 3. (†) Hydrogen chloride + Methanol (ref 11). $\ln (p_1/\text{mmHg}) \ vs. \ \ln (m_1/\text{mol kg}^{-1})$

The straight line (slope 2) is our estimate of the true Henry's law line. At the higher partial pressures of HCl (> 5 kPa) the experimental line approaches the slope of six observed for HCl + 1-butanol (Figure 1).

Figure 4. (next page,
$$\rightarrow$$
) Hydrogen chloride + 1-Alcohols, C₁ - C₇. ln x_1 $vs.$ 1000/(T/K)

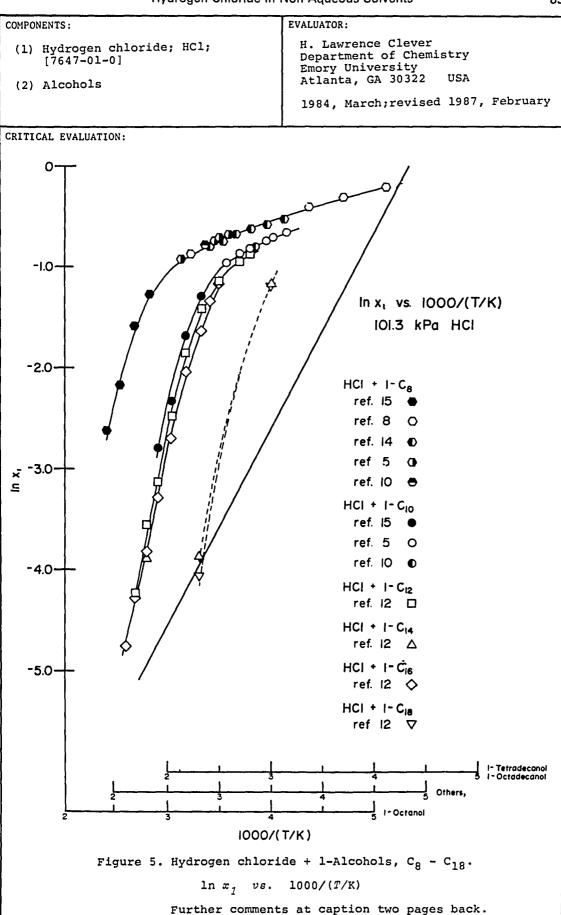
The ideal Raoult's law line to the right is drawn with respect to the 1-propanol abscissa. The lines were drawn from solubility values calculated from the linear regressions.

Figure 5. (second page, +) Hydrogen chloride + 1-Alcohols,
$$C_8$$
 - C_{18} .

$$\ln x_1 \quad vs. \quad 1000/(T/K)$$

A continuation of Fig. 4. The ideal Raoult's line to the right is drawn with respect to the 1-octanol abscissa. The solid lines were drawn from solubility values calculated from the linear regressions. The dotted lines (only two experimental values) were drawn to parallel the calculated lines.

EVALUATOR: COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA (2) Alcohols 1984, March; revised 1987, February CRITICAL EVALUATION: Ethanol ref ē ret. ref ref ē HCI + Normal Alcohols 'x uj Figure 4. Hydrogen chloride + l-Alcohols, $C_1 - C_7$. 1000/(T/K) $\ln x_1 vs.$



COMPONENTS:	EVALUATOR:
(1) Hydrogen chloride; HCl; [7647-01-0)	H. Lawrence Clever Department of Chemistry Emory University
(2) Alcohols	Atlanta, GA 30322 USA
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II. The solubility of hydrogen chloride in alcohols as a function of temperature at a hydrogen partial pressure of 101.3 kPa.

There are solubility data on 24 alcohols at a hydrogen chloride partial pressure of 101.3 kPa. Three systems have data at only one temperature, two systems at two temperatures, and for the other nineteen systems the data range from five to over twenty five temperatures. The temperature intervals studied range from 35 degrees for methanol to 220 degrees for 1-octanol.

Few of the papers give details of the HCl partial pressure measurement. In many of the experiments the gas is bubbled through the liquid and escapes against'atmospheric'pressure. The depth of the liquid (hydrostatic pressure contribution) and the actual atmospheric (barometer) pressure are not given. There could be an uncertainty in the pressure of several percent. If all of the HCl + alcohol systems show the same (1/6) power of partial pressure dependence of mole fraction as does the HCl + 1-butanol system discussed in section I the effect of pressure uncertainty is minimized. A three percent uncertainty in partial pressure would result in only a 0.5 percent uncertainty in the mole fraction solubility.

Most of the papers state the alcohol was dried and protected from water vapor during the experiment. However, none of the papers give a quantitative analysis of the alcohol water content. Jones $et\ al.$ (ref 2) studied the effect of water on the solubility of HCl in ethanol. Small amounts of water decrease the HCl solubility in ethanol. This effect is an unknown factor in the other alcohols.

The temperature dependent data have been fitted by the method of least squares to an equation of the type:

 $\ln x_1 = A_1 + A_2/(T/100 \text{ K}) + A_3 \ln (T/100 \text{ K}) + A_4(T/100 \text{ K}) + A_5(T/100 \text{ K})^2 + \cdots$

Most of the systems were well fitted by a three constant equation, but five systems required four constants (1-butanol, 1-hexanol, 1-decanol, 1-hexadecanol, and 2-butanol), and the 1-octanol systems required five constants. The linear regression equation, its standard error about the regression line in mole fraction, and the experimental temperature range are given for each system in Table 3. Table 2 contains smoothed values of the mole fraction solubility at ten degree intervals within the experimental temperature interval. A few values were extrapolated beyond the experimental temperature range. They are enclosed in ().

Figures 4 and 5 display the experimental data for the linear primary alcohols. The lines were drawn from values calculated from the linear regression equations. The straight line to the right is the Raoult's law ideal solubility line. The maximum deviation from Raoult's law behavior occurs near 335 K for all systems. It appears as if the experimental behavior will approach the Raoult's law line at very high temperatures. The normal boiling point of hydrogen chloride is 188.2 K. At this temperature the ideal mole fraction solubility reaches its limit of unit mole fraction hydrogen chloride.

It is reassuring to see the parallel nature of the $\ln x_1$ vs. 1000/(T/K) plots of Figures 4 and 5. It implies a consistency among the various workers in their measurement of the HCl solubility in alcohols. The data are classed tentative with a few exceptions noted in the following section on the individual systems. The values in the 273 to 313 K interval are believed to be reliable to within one-half or one percent. At the temperature extremes the uncertainty is probably greater, but probably no worse than three to five percent.

Starting at alcohol of carbon number 12 there appears to be a change in the solubility pattern. At 333 K the mole fraction solubility is about four percent less than in the lower molecular weight alcohols. All of the

solubility values for alcohols of carbon number 12, 14, 16, and 18 are from the paper of Fernandes and Sharma (ref 12). Whether the change indicates a systematic error in their measurement or a change in the solution property because of increasing fraction of hydrocarbon residue in the alcohol can not be determined. However, there is a possibility that the solubility data for these alcohols is less reliable than the values for the smaller carbon number alcohols.

The individual systems are discussed briefly below. There is additional information on the systems in Tables 2 and 3. Table 2 is arranged to make comparison of the smoothed solubility values for linear primary, branched primary, linear secondary, and branched secondary alcohols easy. The same arrangement is used in the discussion below and in Table 3. There are no HCl solubility data in tertiary alcohols. The tertiary alcohols normally react readily with HCl to form the chloride.

1. HCl + Methanol; [67-56-1]

Lobry de Bruyn (ref 1) reports two, Gerrard and Macklen (ref 5) six, Kohn (ref 3) one, and Chesterman (ref 4) one measurement. The 273.15 K measurement from (ref 1) and the single measurement from (ref 4) were not used in the linear regression. All other values were classed tentative.

2. HC1 + Ethanol; [64-17-5]

Lobry de Bruyn (ref 1) reports two, Kohn (ref 3) one, Chesterman (ref 4) two, and Gerrard and Macklen (ref 5) five measurements. The 305.15 K value from (ref 1) and the 288.15 K value from (ref 3) were not used in the linear regression. All other values were classed tentative.

3. HCl + 1-Propanol; [71-23-8]

Kohn (ref 3) reports two, Gerrard and Macklen (ref 5) six, and Cook (ref 13) five measurements. All values were classed as tentative and used in the linear regression.

4. HCl + 1-Butanol; [71-36-3]

Kohn (ref 3) reports three, Gerrard and Macklen (ref 5) seven, Gerrard $et\ al.$ (ref 8) six, Ionin $et\ al.$ (ref 10) one, and Fernandes (ref 15) one measurement. No values from (ref 3) were used. The 273.15 K value of (ref 8) and the 315.15 K value of (ref 15) were not used in the linear regression. All of the values used were classed as tentative.

5. HCl + 1-Pentanol; [71-41-0]

Kohn (ref 3) reports six, Gerrard and Macklen (ref 7) six, Gerrard et al (ref 8) thirteen, and Ionin et al. (ref 10) one measurement. The 334.15 K value from (ref 3) and all of the values from the other references were classed as tentative and used in the linear regression.

6. HC1 + 1-Hexanol; [111-27-3]

Gerrard and Macklen (ref 7) report six, and Fernandes (ref 15) three measurements. All were classed as tentative and used in the linear regression.

7. HCl + 1-Heptanol; [111-70-6]

Gerrard and Macklen (ref 7) report six, and Ionin $et\ al.$ (ref 10) one measurement. All values were classed as tentative and used in the linear regression.

8. HCl + 1-Octanol; [111-87-5]

Gerrard and Macklen (ref 5) report seven, Gerrard $et\ al.$ (ref 8) four, Ionin $et\ al.$ (ref 10) one, Ahmed $et\ al.$ (ref 14), and Fernandes (ref 15) four measurements. The values at 196.15 and 229.15 K from (ref 8), at 273.15 and 283.15 from (ref 14), and at 353.15 and 373.15 K from (ref 15) were omitted from the linear regression. All other values were classed as tentative.

9. HCl + 1-Nonanol; [143-08-8]

The single measurement of Ionin et al. (ref 10) was classed as tentative.

10. HCl + 1-Decanol; [112-30-1]

Gerrard and Macklen (ref 7) report six, Ionin et al. (ref 10) one, and Fernandes (ref 15) four measurments. All values were classed as tentative and used in the linear regression. 1-Decanol melts at 280.1 K, however, the saturated solutions are liquid well below the alcohol's normal m. p.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alcohols

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11. HCl + 1-Dodecanol; [112-53-8]

Fernandes and Sharma (ref 12) report the nine measurements on the system. They are classed as tentative and all were used in the linear regression. The authors report the solution at 453.15 K turned brown, however, the solubility value appears consistent with the other values. The 1-dodecanol melts at 297.0 K, but its solutions saturated with HCl are liquid to lower temperatures. Note the comment about these data at the top of the previous page.

HCl + 1-Tetradecanol; [112-72-1]

Fernandes and Sharma (ref 12) report the two measurements on the system. The values were classed as tentative.

HCl + 1-Hexadecanol; [36653-82-4]

Fernandes and Sharma (ref 12) report nine measurements. All values were classed tentative and used in the linear regression.

HC1 + 1-Octadecanol; [112-92-5]

Fernandes and Sharma (ref 12) report two measurements. The values were classed as tentative.

HC1 + 2-Methyl-1-propanol; [78-83-1]

Gerrard and Macklen (ref 5) report seven measurements. All values were classed as tentative and used in the linear regression.

HC1 + 2-Methyl-1-butanol; [137-32-6]

Gerrard and Macklen (ref 5) report seven measurements. All values were classed as tentative and used in the linear regression.

HC1 + 3-Methyl-1-butanol; [123-51-3]

Kohn (ref 3) reports two measurements at 278.15 K. The values were classed tentative, but may be less reliable than values from most other workers.

HC1 + 2,5,5-Trimethyl-1-hexanol; [3452-97-9]

Gerrard and Macklen (ref 5) report five measurements. All values were classed as tentative and used in the linear regression.

HC1 + 2-Propanol; [67-63-0]

Chesterman (ref 4) reports one, and Gerrard and Macklen (ref 5) five measurements. The single value from (ref 4) appears to be about four percent too small and was not used. The other values were classed as tentative and were used in the linear regression.

HCl + 2-Butanol; [78-92-2]

Gerrard and Macklen (ref 5) report six measurements from 281.25 to 312.95 K, and Gerrard et at. (ref 8) report seven measurements from 198.15 to 319.15 K. All values were classed as tentative and were used in the linear regression.

- 21. HCl + 3-Pentanol; [584-02-1]

22. HCl + 4-Heptanol; [589-55-9]

Gerrard and Macklen (ref 5) report five measurements for each system.

All values were classed as tentative and used in the linear regressions.

HC1 + 2-Octanol; [123-96-6]

Kohn(ref 3) reports one measurement at 279.15 K. The value was classed as tentative, but may be less reliable by 2 - 3 percent than values from other workers.

24. HCl + 4-Methyl-2-pentanol; [108-11-2]

Gerrard and Macklen (ref 7) report six measurements from 274.75 to 319.45 K, and Gerrard et al. (ref 8) report nine measurements from 201.15 and 311.15 K. The 307.45 K value from (ref 7) was not used. All other values were classed as tentative and used in the linear regression.

COMPONENTS:	EVALUATOR:
(1) Hydrogen chloride; HC1; [7647-01-0] (2) Alcohols	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA
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Table 2. Solubility of hydrogen chloride in normal alcohols. Tentative values of the mole fraction solubility at a hydrogen chloride partial pressure of 101.3 kPa as a function of temperature.

	Primar	y Normal	. Alco	hols					
	Methanol	Ethanol	l-Propanol	l-Butanol	l-Pentanol	1-Hexanol	l-Heptanol	1-Octanol	1-Nonanol
T/K									
193.15 203.15 213.15				(0.816) 0.767 0.724	(0.799) 0.765 0.729			(0.828) 0.776 0.724	
223.15 233.15 243.15				0.684 0.648 0.613	0.693 0.657 0.622			0.675 0.632 0.595	
253.15 263.15 273.15	- 0.490	_ 0.513	- 0.513	0.581 0.550 0.520	0.587 0.554 0.523	- (0.518)	- (0.516)	0.564 0.536 0.511	
283.15 293.15	0.463 0.434	0.488 0.462	0.488 0.463	0.492 0.464	0.493 0.464	0.493 0.467	0.494 0.469	0.488 0.464	-
298.15	0.419	0.448	0.449	0.451	0.450	0.454	0.456	0.452	0.449 ^a
303.15 313.15 323.15	0.404	0.434 0.407	0.436 0.410 -	0.437 0.412	0.437 0.412 0.388	0.441 0.414 0.387	0.443 0.415 0.387	0.439 0.412 0.383	-
333.15 343.15 353.15					0.366	0.359 0.330 0.301	0.360 - -	0.350 0.314 0.276	
363.15 373.15 383.15						0.272 0.244 0.217		0.237 0.198 0.160	
393.15 403.15 413.15						0.190		0.126 0.095 0.070	
423.15 433.15 443.15								-	
453.15 463.15 473.15									

a one experimental value.

Values in () were extrapolated outside the range of experimental measurement.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Alcohols EVALUATOR: H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA 1984, March, revised 1987, February

Table 2 (continued). Solubility of hydrogen chloride in alcohols. Tentative values of the mole fraction solubility of hydrogen chloride at a partial pressure of 101.3 kPa as a function of temperature.

	Primary	Normal	Alcoho	ols		Branche	d Prim	ary Alcohols
	l-Decanol	1-Dodecanol	l-Tetradecanol	l-Hexadecanol	l-Octadecanol	2-Methyl-1- propanol	2-Methyl-l- butanol	3-Methyl-l- butanol
T/K								
193.15 203.15 213.15			-					
223.15 233.15 243.15								
253.15 263.15 273.15	0.513					- (0.514)	- (0.526	-) 0.521 ^C
283.15 293.15	0.492 0.471	<u>-</u>				0.492 0.468	0.505 0.482	-
298.15	0.460 (0.424)		-		0.455	0.471	
303.15 313.15 323.15	0.420	0.421 0.399 0.364	- ((0.398) (0.365)	-	0.442 0.415	0.459 0.435 -	
333.15 343.15 353.15	0.309	0.321 0.275 0.228	0.313 ^b	0.315 0.260 0.207	0.309 ^b			
363.15 373.15 383.15	0.181	0.186 0.148 0.115		0.160 0.122 0.092				
393.15 403.15 413.15	0.081	0.089 0.067 0.050		0.069 0.051 0.039				
423.15 433.15 443.15	_	0.037 0.027 0.020	0.021b	0.029 0.022 0.017	0.018 ^b			
453.15 463.15 473.15		0.014		0.014 0.011 0.009				

b experimental values.

c estimated from two experimental values at a higher temperature.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Alcohols EVALUATOR: H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA 1984, March, revised 1987, February

Table 2 (continued). Solubility of hydrogen chloride in alcohols. Tentative values of the mole fraction solubility of hydrogen chloride at a partial pressure of 101.3 kPa as a function of temperature.

	- Par cra-	pressure of					temperature.
(cont.)	ont.) Linear and Branched Secondary Alcohols					
	2,5,5-Trimethyl- 1-hexanol	2-Propanol	2-Butanol	3-Pentanol	4-Heptanol	2-Octanol	4-Methyl- 2-pentanol
T/K							
193.15 203.15 213.15			0.779 0.732				(0.831) 0.793 0.755
223.15 233.15 243.15			0.691 0.656 0.624				0.717 0.680 0.645
253.15 263.15 273.15	- (0.517)	- (0.530)	0.594 0.566 0.539	- (0.535)	- (0.535)	- 0.535 ^d	0.610 0.578 0.547
283.15 293.15	0.495 0.470	0.508 0.484	0.512 0.486	0.514 0.491	0.513 0.490		0.517 0.489
298.15	0.457	0.472	0.473	0.479	0.478		0.476
303.15 313.15 323.15	0.444 0.418	0.460 0.435	0.460 0.435 (0.410)	0.467 0.443	0.466 0.443		0.463 0.438
333.15 343.15 353.15	- - -	- - -	-				
363.15 373.15 383.15							
293.15 403.15 413.15							
423.15 433.15 443.15							
453.15 463.15 473.15							

 $^{^{\}rm d}$ estimated from a single value at a higher temperature.

Values in () are extrapolated values from outside the range of the experimental measurements.

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Table 3. Hydrogen chloride in alcohols. Smoothing equation from linear regression, standard error about regression line (mole fraction), temperature range of experimental measurements.
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```
1-Hexadecanol
Methanol
                                             \ln x_1 = (387.1453 \pm 113.6435)
\ln x_1 = (18.1997 \pm 7.0628)
                                                  \frac{1}{-}(543.9591 \pm 163.0653)/(T/100K) - (275.4782 \pm 82.3463) \ln(T/100K)
      -(23.8284 ± 9.9260)/(T/100K)
      -(10.1400 \pm 3.4162) \ln(T/100K)
                                                  +(31.9656 \pm 10.3266)(T/100K)
\sigma = 0.0025
                                                  \sigma = 0.0063
    273.15 - 307.35 K
                                                       333.15 - 473.15 K
Ethanol
\ln x_1 = (13.6149 \pm 3.5862)
                                             1-Octadecanol
      -(17.7142 \pm 5.0459)/(T/100K)
                                              No equation, only two values.
                                             2-Methyl-1-propanol
      -(7.7589 \pm 1.7323) \ln(T/100K)
                                             \ln x_1 = (15.2839 \pm 1.1420)
\sigma = 0.0021
                                                   -(20.2632 \pm 1.6281)/(T/100K)
-(8.4901 \pm 0.5451) \ln (T/100K)
    273.15 - 313.25 K
1-Propanol
\ln x_1 = (12.4129 \pm 0.5637)
                                                  \sigma = 0.0006
      -(16.0956 \pm 0.7919)/(T/100K)
                                                       279.15 - 319.55 K
                                             2-Methyl-1-butanol
      -(7.1532 \pm 0.2727) \ln(T/100K)
                                             \ln x_1 = (10.1079 \pm 1.7033)
   = 0.0005
                                                   -(13.1798 \pm 2.4235)/(T/100K)
      267.65 -315.15 K
                                                   -(5.8961 \pm 0.8149) \ln(T/100K)
1-Butanol
                                                  \sigma = 0.0009
\ln x_1 = -(5.3500 \pm 1.800)
                                                       277.85 - 318.35 K
    +(8.4593 \pm 2.4336)/(T/100K)
                                             3-Methyl-1-butanol
    +(6.9795 \pm 1.9422) \ln(T/100K)
                                              No equation, only two values.
    -(1.9819 \pm 0.3824)(T/100K)
                                             2,5,5-Trimethyl-1-hexanol
   \sigma = 0.0015
                                             \ln x_1 = (13.2973 \pm 0.4197)
      195.15 - 318.15 K
                                                    -(17.4507 ± 0.5958)/(T/100K)
1-Pentanol
                                                   -(7.5306 \pm 0.2012) \ln(T/100K)
\ln x_1 = (4.9597 \pm 0.3413)
      -(5.4332 ± 0.4510)/(T/100K)
                                                  \sigma = 0.0001
                                                       280.05 - 313.65 K
      -3.6021 \pm 0.1737) \ln(T/100K)
    \sigma = 0.0033
                                             2-Propanol
                                             \ln x_1 = (11.5269 \pm 1.2174)
         201.15 = 334.15 K
                                                    -(15.0957 \pm 1.7321)/(T/100K)
l-Hexanol
                                                   -(6.6035 \pm 0.5822) \ln(T/100K)
\ln x_1 = -(45.5683 \pm 12.2455)
                                                  \sigma = 0.0005
    +(62.9042 \pm 16.8788)/(T/100K)
                                                       280.55 - 316.45 K
    +(46.3840 \pm 10.2143) \ln(T/100K)
                                             2-Butanol
    -(9.0526 \pm 1.5359)(T/100K)
                                             \ln x_1 = -(12.3518 \pm 7.7459)
    \sigma = 0.0014
                                                   +(17.7961 \pm 10.4797)/(T/100K)
         279.85 - 393.15
                                                   +(13.9946 \pm 8.2996) ln(T/100K)
1-Heptanol
                                                    -(3.2378 \pm 1.6256)(T/100K)
\ln x_1 = (16.6621 \pm 1.3802)
      -(22.1457 \pm 1.9973)/(T/100K)
                                                  \sigma = 0.0057
                                                       198.15 - 319.15 K
      -(9.1718 \pm 0.6496) ln(T/100K)
                                             3-Pentanol
    \sigma = 0.0013
                                             279.15 - 337.35 K
1-Octanol
\ln x_1 = (75.6012 \pm 28.4597)
                                                   -(6.1562 \pm 0.6476) \ln (T/100K)
      -(158.4921 ± 48.8758)/(T/100K)
                                                  \sigma = 0.0005
      -(200.3029 \pm 52.1084) ln(T/100K)
                                                       280.35 - 316.55 K
      +(82.3919 \pm 18.1865)(T/100K)
                                             4-Heptanol
                                             \ln x_1 = (9.9919 \pm 0.5128)
      -5.6328 ± 1.0389) (T/100K)
                                                    -(12.9965 \pm 0.7326)/(T/100K)
    \sigma = 0.0087
                                                    -(5.8317 \pm 0.2443) \ln(T/100K)
         196.15 - 413.15 K
                                                  \sigma = 0.0002
1-Nonanol
                                                       283.05 -318.45 K
No equation, only one experimental value.
                                              2-Octanol
1-Decanol
\ln x_1 = -(175.8767 \pm 68.5805)
                                              No equation, only a single value.
      +(239.8244 \pm 94.5801)/(T/100K)
                                              4-Methyl-2-pentanol

\ln x_1 = (4.0718 \pm 0.6401) \\
-(4.2973 \pm 0.8340)/(T/100K)

      +(170.1297 \pm 56.6925) ln(T/100K)
      -(30.5853 \pm 8.4252)(T/100K)
                                                   -(3.0877 \pm 0.3305) \ln(T/100K)
    \sigma = 0.0088
         273.15 - 413.15 K
                                                  \sigma = 0.0065
                                                       201.15 - 319.45 K
1-Dodecanol
\ln x_1 = (89.8907 \pm 7.6611)
      -(129.0024 ± 12.1823)/(T/100K)
      -(43.4629 \pm 3.3184) \ln(T/100K)
    \sigma = 0.0093
         303.15 - 453.15 K
1-Tetradecanol
 No equation, only two values.
```

- (1) Hydrogen Chloride; HCl; [7647-01-0]
- (2) Alcohols

EVALUATOR:

H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA

1984, March, revised 1987, February

CRITICAL EVALUATION:

- 1. Lobry de Bruyn, C. A. Z. Phys. Chem. 1892, 10, 782-9.
- Jones, W. J.; Lapworth, A.; Lingford, H. M. J. Chem. Soc. <u>1913</u>, 103, 252-63.
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- 4. Chesterman, D. R. J. Chem. Soc. 1935, 906-10.
- 5. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1956, 6, 241-4.
- 6. Fritz, J. J. J. Phys. Chem. 1956, 60, 1461.
- 7. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1959, 9, 85-8.
- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89-93.
- 9. Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. <u>1960</u>, 10, 115-21.
- Ionin, M. V.; Kurina, N. V.; Sudoplatova, A. E. Tr. po Khim. i Khim. Tekhnol. <u>1963</u>, (1), 47-8.
- 11. Schmid, H.; Maschka, A.; Sofer, H. Monatshefte 1964, 95, 348-58.
- 12. Fernandes, J. B.; Sharma, M. M. Indian Chem. Eng. 1965, 7, 38-40.
- 13. Cook, T. M. Thesis 1966, Gerrard, W., Adviser, University of London.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109-15.
- 15. Fernandes, J. B. J. Chem. Eng. Data 1972, 17, 377-9.
- 16. Gerrard, W. Solubility of Gases and Liquids, Plenum Press, New York, 1976, 275 pp.
- 17. Gerrard, W. Gas Solubilities, Pergamon Press, Oxford and New York, 1980, 497 pp.
- 18. Rupert, F. F. J. Am. Chem. Soc. <u>1909</u>, 31, 851-66; See also International Critical Tables <u>1928</u>, 3, 104.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Methanol; CH₄O; [67-56-1] VARIABLES: T/K = 273.15, 304.85 p = "barometric" ORIGINAL MEASUREMENTS: Lobry de Bruyn, C. A. Z. Phys. Chem. 1892, 10, 782 - 789. Rect. Trav. Chim. Pays-Bas 1892, 11, 112 - 157. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

Temperature		Parts HCl by	Mol Ratio	Mol Fraction	
t/°C	T/K	weight for 100 parts of methanol	n_1/n_2	x_1	
0	273.15	105	0.922	0.480	
31.7	304.85	75.1	0.659	0.397	

The compiler calculated the mole ratio and mole fraction values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was passed into a weighed amount of methanol in a bulb of 2 - 3 cm³ capacity until equilibrium was reached at the observed temperature and at a total pressure of about 760 - 770 mmHg (barometric). The bulb was sealed "à la lampe," and weighed. A titration was also mentioned, but the statement is vague.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Definite information not given.
- (2) Methanol. Simply stated that pure alcohol was used.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Kohn, G. (1) Hydrogen chloride; HCl; [7647-01-0] Ber. Dtschn. Chem. Ges. B. <u>1932</u>, 65, 589 - 595. (2) Methanol or Ethanol VARIABLES: PREPARED BY: T/K: 275.15 - 334.15 P/kPa: W. Gerrard 101 (atmospheric)

EXPERIMENTAL VALUES:

T/K	Alcohol wt/g	Hydrogen Chloride wt/g	Mol Ratio	Mol Fraction
Me	ethanol; C	H ₄ O; [67-5	6-1]	
276.15	19.9	21.4	0.944	0.486
Et	hanol; C ₂	н ₆ 0; [64-1	7-5]	
277.15 288.15	20.6 31.7	16.8 24.5	1.029 0.975	0.507 0.494

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: The hydrogen chloride was passed to the alcohol in a measuring cylinder in an ice-salt mixture. The temperature, "end temperature" was recorded, and the absorbed gas was weighed. The pressure was presumably atmospheric.	SOURCE AND PURITY OF MATERIALS: (1) Hydrogen chloride. Prepared from sodium chloride and sulfuric acid, and dried by sulfuric acid. (2) Alcohols. Kahlbaum specimens.
	ESTIMATED ERROR: $\delta wt/g = 0.1$
	REFERENCES:

COMPONENTS: (1) Hydrogen chloride; HCl; Chesterman, D. R. [7647-01-0] (2) Alcohols VARIABLES: T/K: 298.15 Total P/kPa: 101 (∿1 atm) ORIGINAL MEASUREMENTS: Chesterman, D. R. J. Chem. Soc. 1935, 906 - 910. W. Gerrard

EXPERIMENTAL VALUES:

T/K	Observed Pressure p/mmHg	Solubility g HCl g ⁻¹ Solution	Mol Fraction x1
Methano	1; CH ₄ O; [67-56-11	
298.15	750	0.44	0.41
Ethanol	; c ₂ H ₆ o; [64-17-5]	
298.15	752	0.39	0.45
2-Propa	nol; C ₃ H ₈ O	; [67-63-0]	
298.15	771	0.17	0.25

The mole fraction solubility values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The apparatus was that used for the conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess base which was back titrated with a standard acid solution.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅.
- (2) Methanol. Was stated to be the purest obtainable. Freed from acetone, dried with sodium, b.p./°C (759 mmHg) = 66.0.

Ethanol. Was stated to be the purest obtainable. Dried with calcium oxide, b.p./°C (752 mmHg) = 77.7.

2-Propanol. Was stated to be the purest obtainable. Dried over calcium, b.p./°C (745 mmHg) = 80.5.

	·
(2) Alcohols	
[/64/-01-0]	J. Appl. Chem. 1956, 6, 241-244
(1) Hydrogen chloride; HCl;	Gerrard, W.; Macklen, E.D.
COMPONENTS:	ORIGINAL MEASUREMENTS:

VARIABLES: T/K: See below

Total P/kPa : 101.325 (1 atm)

PREPARED BY: W. Gerrard

10041 1,7114 1 70 70 10 70 70 40 117				
EXPERIMENTAL VALUES:	T/K	Mole ratio	Mole* fraction *HCl	Smoothed** mole fraction *HCl
Methanol; CH ₄ O; [67-56-1]	273.15 275.25 280.35		0.483 0.469	0.487
	283.15 285.55 291.85	0.835 0.785	0.455 0.440	0.462
	293.15 300.75 303.15 307.35	0.700	0.412	0.435 0.405
Smoothing equation: ln x_{HCl} = Standard error in x_{HCl} a	313.15			0.374 50 ln(T/100)
Standard error in $\ddot{x}_{ m HCl}$	about the	e regression	line = 1.2	17×10^{-3}
Ethanol; C ₂ H ₆ O; [64-17-5]	273.15 276.15 283.15	1.021	0.505	0.513 0.487
	288.75 293.15		0.472	0.461
	297.55 303.15 307.15	0.816 0.732	0.449	0.434
	313.25 313.15		0.407	0.408

Smoothing equation: $\ln x_{HCl} = 11.631 - 14.943/(T/100) - 6.795 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 2.46 × 10⁻³

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an all-glass apparatus.

The all-glass absroption vessel (50 cm³) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Alcohols: high grade samples were distilled and attested.

ESTIMATED ERROR: $\delta T/K = \pm 0.1$ $\delta x_{HCl}/x_{HCl} = \pm 0.005 \text{ to } 0.01$

^{*} calculated by the compiler

^{**} smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]	ORIGINAL MEASU Gerrard, W.; M		
(2) Alcohols	J. Appl. Chem.	<u>1956</u> , 6, 241	-244
EXPERIMENTAL VALUES: T/K			othed** fraction
	x	HC1 x	нсі
1-Propanol; C ₃ H ₈ O; [71-23-8] 273.15 275.65		.507	0.513
281.65 281.15	0.969	.492	0.488
285.55 293.15		.482	0.463
298.75 303.15			0.436
307.35 313.15		.425	0.409
315.15 323.15		.404	0.383
Smoothing equation: $\ln x_{\text{HCl}} = 12.983$ Standard error in x_{HCl} about the	- 16.900/(T/100) regression line	$-7.428 \ln(T)$ = 2.67 × 10	(/100)
2-Propanol; C ₃ H ₈ O; [67-63-0] 273.15 280.55		.514	0.529
283.15 289.75			0.508
293.15 300.45	0.877	.467	0.484
303.15 306.45	0.824 0	.452	0.460
313.15 316.45	0.744	.427	0.435
Smoothing equation: $\ln x_{\text{HCl}} = 13.166$ Standard error in x_{HCl} about the		- 7.395 ln(T	0.409 7/100)
1-Butanol; C ₄ H ₁₀ O; [71-36-3] 273.15 277.15	1.023	.506	0.515
281.95 283.15 286.85		.494	0.491
291.05 291.15	0.887	.470	0.465
298.15 303.15		.453	0.439
308.95 313.15		.423	0.412
318.15 323.15	0.660 0	.398	0.385
Smoothing equation: $\ln x_{\text{HCl}} = 13.723$ Standard error in x_{HCl} about the	- 17.945/(T/100) regression line	$-7.779 \ln(T)$ = 7.31 × 10	(100)
2-Butanol; C ₄ H ₁₀ O; [78-92-2] 273.15 281.25		.516	0.533
283.15 283.35		.511	0.512
291.45 293.15	0.973	.493	0.489
298.65 303.15	0.909	.476	0.465
304.05 312.95 313.15		.463 .442	0.442
Smoothing equation: ln x _{HCl} = 10.431 Standard error in x _{HCl} about the * calculated by the compiler ** smoothing equation and smoothed v	- 13.623/(T/100) regression line alues were calcu	- 6.043 ln(T = 2.12 × 10	1/100) 3

COMPONENTS: (1) Hydrogen chloride; HCl;	2	ASUREMENTS: ; Macklen, E	.D.
[7647-01-0]		тет. <u>1956</u> , 6,	
(2) Alcohols		.o <u></u> , o,	
EXPERIMENTAL VALUES:			· · · · · · · · · · · · · · · · · · ·
T/K	Mole ratio		Smoothed**
	n HCl $^{/n}$ alcohol	fraction m	ole fraction
	ner arconor	xHC1	*HCl
		HC1	ncı
2 Wathul 4 managed 6 U 0 272 1	r		0 514
2-Methyl-1-propanol; C ₄ H ₁₀ O; 273.1 [78-83-1] 279.0		0.502	0.514
279.0		0.302	0.492
285.5		0.486	0.472
288.0		0.480	
292.2		0.470	
293.1			0.468
297.4		0.457	
303.1			0.442
306.4	5 0.766	0.434	
313.1			0.416
319.5	5 0.661	0.398	
323.1	5		0.389
			.
Smoothing equation: $\ln x_{HC1} = 15.284$ Standard error in x_{HC1} about th	- 20.263/(T/1 e regression l	00) - 8.490	ln(T/100)
Standard error in x_{HC1} about th	e regression l	line = $5.92 \times$	10 3
2 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7 7	-		0 535
3-Pentanol; C ₅ H ₁₂ O; 273.1 [584-02-1] 280.3		0 520	0.535
[584-02-1] 280.3 283.1		0.520	0.514
291.1		0.495	0.514
293.1		0.155	0.491
303.0		0.468	••••
303.1			0.467
306.1	5 0.853	0.460	
313.1			0.443
316.5		0.435	
323.1	5		0.419
	40.00011-14		. (=(400)
Smoothing equation: $\ln x_{HCl} = 10.674$ Standard error in x_{HCl} about the	- 13.968/(T/T	100) - 6.156	In(T/100)
Standard error in x _{HCl} about th	e regression 1	line = 5.39 x	10 "
2-Methyl-1-butanol; C _E H _{1,2} O; 273.1	5		0.526
2-Methyl-1-butanol; C ₅ H ₁₂ O; 273.1 [137-32-6] 277.8		0.516	0.520
283.1		0.510	0.505
284.9		0.501	
291.5		0.487	
293.1			0.482
296.8	5 0.899	0.473	
303.1			0.459
303.5		0.458	
312.9		0.435	0.436
313.1		0 424	0.436
318.3		0.424	0.412
323.1	ວ		0.412
Smoothing equation: $\ln x_{HC1} = 10.108$ Standard error in x_{HC1} about the	- 13.180/(T/1 e regression l	100) - 5.896 Line = 9.03 ×	ln(T/100) 10 ⁻³
* calculated by the compiler		.11 _ 4 _ 5 _ 3 _ 5	n t 01
** smoothing equation and smoothed	vaiues were ca	ятситатес ру	n.L. Clever

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]	ORIGINAL MEASUREMENTS: Gerrard, W.; Macklen, E.D.				
(2) Alcohols	J. Appl. Chem. <u>1956</u> , 6, 241-244				
EXPERIMENTAL VALUES:	Mole ratio Mole* Smoothed**				
	HCl ^{/n} alcohol fraction mole fraction				
	*HC1 *HC1				
4-Heptanol; C ₇ H ₁₆ O; 283.05 [589-55-9] 283.15	1.054 0.513				
[589-55-9]					
293.15	0.490				
294.45 303.15					
306.15	0.850 0.459				
313.15 318.45					
323.15	0.419				
Smoothing equation: $\ln x_{HC1} = 9.992$ - Standard error in x_{HC1} about the	12.996/(T/100) - 5.832 $ln(T/100)$ regression line = 1.80 × 10 ⁻⁴				
1-Octanol; C ₈ H ₁₈ O; [111-87-5] 273.15	0.516				
278.45 283.15					
285.65 289.65					
- 293.15	0.469				
299.15 303.15					
304.05	0.788 0.441				
311.15 313.15	0.416				
319.75 323.15					
Smoothing equation: $\ln x_{HC1} = 14.392$ Standard error in x_{HC1} about the					
3,5,5-Trimethyl-1-hexanol; 273.15 C ₉ H ₂₀ O; [3452-97-9] 280.05					
283.15 290.45					
293.15	0.470				
300.45 303.15	0.444				
308.25 313.15					
313.65	0.714 0.417				
323.15					
Smoothing equation: $\ln x_{HC1} = 13.297$ Standard error in x_{HC1} about the	- 17.451/($T/100$) - 7.531 $ln(T/100)$ regression line = 1.35 × 10 ⁻⁴				
<pre>** calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever</pre>					

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] Fritz, J. J. (2) Methanol; CH₄O; [67-56-1] J. Phys. Chem. 1956, 60, 1461. Ethanol; C₂H₆O; [64-17-5] PREPARED BY: T/K = 298.15 p₁/Pa = 0.11, 62 ORIGINAL MEASUREMENTS: Fritz, J. J. J. Phys. Chem. 1956, 60, 1461.

EXPERIMENTAL VALUES:

Temperature		Hydrogen Chloride Pressure		Molality Mol Ratio		Mol Fraction
t/ºC	T/K	p_1/mmHg		$m_1/\text{mol kg}^-$	n_1/n_2	x ₁
			· · · · · · · · · · · · · · · · · · ·	-		
М	lethanol					
25	298.15	8x10 ⁻⁴	1.1x10 ⁻⁶	0.56	0.0179	0.017
E	thanol					
25	298.15	0.46	6.1x10 ⁻⁴	1.00	0.0461	0.0440

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The vapor pressure of HCl was calculated from

 $\ln f_1 = (F/RT)(E_g^0 - E)$

where E is the voltage of the cell H_2 , Pt/HCl(alcohol)/AgCl, Ag, and E_g^0 is the standard potential of the cell for unit fugacity.

The E values were taken from Harned and Owen (ref 1), and the $E_{\mathcal{G}}^{0}$ value was taken from Aston and Gittler (ref 2).

The fugacity of HCl in hypothetical 1 molal standard state at 298.15 K is f_1^0/mmHg 3.18 in methanol and 38.5 in ethanol. The vapor pressure of HCl is then

$$f_1 = m_1^2 \Upsilon_{\pm}^2 f_1^0$$

assuming $f_1 = p_1$.

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

 $\delta m_1/m_1 = \pm 0.10$ (compiler)

- 1. Harned, H. S.; Owen, B. B.
 "Physical Chemistry of Electrolyte
 Solutions", Reinhold Pub. Co.,
 1950. p. 336.
- 1950, p. 336. 2. Aston, J. G.; Gittler, F. L. J. Am. Chem. Soc. 1955, 77, 3173.

The solution of HCl in methanol was prepared freshly each day, because of the slow conversion into chloromethane as reported by Carter and Butler (1). The molality of the solution for use in the vapor pressure measurements was determined by acid-alkali titration. Dry nitrogen was passed through the solution of the stated molality at 298.15 K slowly enough to give an effluent gas "saturated" with HCl and methanol. The effluent gas was passed into the first of two U-tubes to absorb the HCl in 0.5 N-NaOH, and most of the methanol, the increase in weight and a potentiometric titration (AgNO $_3$) giving the contents. The remaining methanol and entrained water vapor was collected in the second U-tube containing water-free magnesium chloride. The nitrogen was collected in a gasometer. The partial pressures, p_1 and p_2 were calculated by assuming the validity of Dalton's law.

The authors used the data of Oiwa (ref 2) to establish that Henry's constant in $f_1 = \mathrm{k} a_1$ is 2.58 mmHg.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: ESTIMATED ERROR: REFERENCES: 1. Carter, S. R.; Butler, J. A. V. J. Chem. Soc. 1924, 125, 963. 2. Oiwa, I. T. J. Phys. Chem. 1956, 60, 754.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Methanol; CH₄O; [67-56-1]

ORIGINAL MEASUREMENTS:

Schmid, H.; Maschka, A.; Sofer, H.

Monatshefte 1964, 95, 348 - 358.

EXPERIMENTAL VALUES:

<i>T</i> /K	Partial HCl p ₁ /mmHg	Pressures CH ₃ OH p ₂ /mmHg	Chloride	Mol Ratio n_1/n_2	Mol Fraction
298.15	0.0417 0.0389 0.0417 0.0473 0.0531 0.0538 0.0705 0.0772	124.6 125.1 125.1 124.0 123.2 124.3 126.6 124.6	0.375 0.379 0.416 0.446 0.478 0.507 0.580 0.598	0.0120	0.0119
	0.110 0.154 0.141 0.152 0.201 0.194 0.231 0.310 0.386 0.365 0.492 0.516	119.8 123.2 122.7 122.0 121.0 120.3 119.6 119.3 119.1 116.6 115.6	0.73 0.825 0.85 0.885 0.975 0.98 1.04 1.28 1.43 1.45 1.67	0.0234	0.0228
	0.671 0.961 0.903 1.27 1.49 2.21 2.34 3.63 4.01	113.2 111.8 110.7 107.8 105.4 102.7 101.2 97.2 94.4	2.06 2.45 2.46 2.85 3.23 3.67 4.12 4.6 4.85	0.0787	0.0730
	5.32 5.77 7.94 8.63 8.61 9.37	91.7 90.4 90.8 84.7 87.5 79.2	5.45 5.6 6.05 6.45 6.6 6.8	0.174	0.149
	10.2 12.4 14.8 15.2 17.4 17.8	79.6 82.9 78.5 77.2 77.5 73.4 70.4	6.9 7.25 7.75 7.85 8.25 8.3 8.4	0.221	0.181
	23.1 26.4 24.7 33.4 33.8 34.8 36.1	69.1 70.9 68.6 66.1 68.0 65.1 65.6	8.9 9.15 9.15 9.55 9.55 9.9	0.285	0.222
	45.8 47.6 54.5 58.9 65.4	55.1 60.9 55.4 51.3 51.2	10.5 10.55 11.15 11.45 11.7	0.336	0.251
	83.7	44.9	12.4	0.397	0.284

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Ethanol; C₂H₆O; [64-17-5] VARIABLES: T/K = 273.15, 305.15 p = "barometric" | CRIGINAL MEASUREMENTS: | Lobry de Bruyn, C. A. | Z. Phys. Chem. 1892, 10, 782 - 789. | Recl. Trav. Chim. Pays-Bas 1892, 11, 112 - 157. | PREPARED BY: | W. Gerrard

EXPERIMENTAL VALUES:

Temperature		Parts HCl by		Mol Fraction
t/°C	<i>T</i> /K	weight for 100 parts of ethanol ¹	ⁿ ₁ / ⁿ ₂	x 1
0	273.15	83	1.047	0.512
32	305.15	61.6	0.777	0.437

¹ Equivalent to g of gas per 100 g of solvent.

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was passed into a weighed amount of ethanol in a bulb of 2 - 3 cm³ capacity until equilibrium was reached at the observed temperature and at a total pressure of about 760 - 770 mmHg (barometric). The bulb was sealed "à la lampe," and weighed. A titration was also mentioned, but the statement is vague.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Definite information not given.
- (2) Ethanol. Simply stated that pure alcohol was used.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Ethanol; C₂H₆O; [64-17-5]

ORIGINAL MEASUREMENTS:

Jones, W. J.; Lapworth, A.; Lingford, H. M.

J. Chem. Soc. 1913, 103, 252-263.

VARIABLES:

$$T/K = 298.15$$

 $p_1/Pa = 14.4 - 625$
 $(0.108 - 4.69 \text{ mmHg})$

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Hydrogen Chloride	Hydrogen Chloride	Mole Ratio	Mol Fraction
pressure	c ₁ /mol dm ⁻³	n_1/n_2	x_1
0.108	0.275	0.0162	0.0159
• • - • -			0.0425
			0.0651
			0.1267
4.69	3.188	0.1965	0.1642
760.	10.45	0.82	0.45]1
	Chloride Pressure P ₁ /mmHg 0.108 0.417 0.811 2.63	Chloride Pressure p ₁ /mmHg Concentration c ₁ /mol dm ⁻³ 0.108 0.275 0.417 0.751 0.811 1.168 2.63 2.390 4.69 3.188	Chloride Chloride Pressure Concentration p_1/mmHg $c_1/\text{mol dm}^{-3}$ n_1/n_2 0.108 0.275 0.0162 0.417 0.751 0.0444 0.811 1.168 0.0696 2.63 2.390 0.1451 4.69 3.188 0.1965

¹ Calculated by the authors. The authors applied the Gibbs-Duhem equation to obtain the equation

 $\log(10 \ p_1/\text{mmHg}) = 1.284 \ \log X + 0.01106 \ X + 0.000115 \ X^2 - 0.256$ where X is $100(n_1/n_2)$, from the experimental data.

The authors also reported hydrogen chloride vapor pressures for ethanol + water mixtures up to 2.5 moles of water per ${\rm dm}^3$. The data for the aqueous ethanol solutions are not included in this volume.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A solution of dry ethanol + hydrogen chloride was prepared and placed in the middle of a three bubbler train.

The first bubbler contained pure ethanol, the second the solution of known composition, and the third contained water.

Hydrogen gas, prepared from zinc and dilute hydrochloric acid, suitably purified and dried, was passed through the system. The volume of hydrogen gas was measured. The HCl transferred from the alcohol solution to the water was titrated against standard barium hydroxide.

The HCl pressure over the ethanol + hydrogen chloride solution of known concentration was calculated from the hydrogen volume, amount of hydrogen chloride, and the vapor pressure of pure ethanol.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Source not given. Stated to be carefully dried.
- (2) Ethanol. Commercial absolute alcohol was distilled from calcium turnings. The ethanol density was $\rho_{\star}^{2,5}/g$ cm⁻³ = 0.78493.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ $\delta p_1/mHg = \pm 0.03$ $\delta x_1/x_1 = \pm 0.025$ (Compiler)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0]	Kohn, G. Ber. Dtschn. Chem. Ges. B. 1932,
(2) 1-Propanol	65, 589 - 595.
or	
1-Butanol	
VARIABLES: T/K: 275.15 - 334.15 P/kPa: 101 (atmospheric)	PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

T/K	Alcohol wt/g	Hydrogen Chloride wt/g		Mol Fraction
1-	Propanol;	с ₃ н ₈ 0; [[71-23-8]	
276.15	31.2	19.3	1.018	0.505
277.15	25.2	15.5	1.012	0.503
1-	Butanol:	С ₄ Н ₁₀ О; [71-36-31	
_		4-10-7		
278.15	30.2	14.3	0.961	0.490
279.15	30.0	15.6	1.056	0.513
279.15	30.9	16.1	1.058	0.514

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen chloride was passed to the alcohol in a measuring cylinder in an ice-salt mixture. The temperature, "end temperature", was recorded, and the absorbed gas was weighed. The pressure was presumably atmospheric.

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Prepared from sodium chloride and sulfuric acid, and dried by sulfuric acid.
- (2) Alcohols. Kahlbaum specimens.

ESTIMATED ERROR:

 $\delta wt/g = 0.1$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. 1-Propanol; C₃H₈O; [71-23-8]

ORIGINAL MEASUREMENTS:

Cook, T. M.

Thesis, 1966 University of London

VARIABLES:

T/K: 267.65 - 304.15 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction XHCl
267.65	1.110	0.526
273.15	1.052	0.513
281.65	0.971	0.493
288.55	0.901	0.474
304.15	0.767	0.434

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln X_{HC1} = 11.672 - 15.066/(T/100) - 6.790 \ln (T/100)$

Standard Error About Regression Line = 7.11×10^{-4}

T/K	Mol Fraction XHCl
263.15	0.536
273.15	0.513
283.15	0.489
293.15	0.463
303.15	0.434
313.15	0.411

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data were cited by Gerrard (1).

Hydrogen chloride was passed into a bubbler tube containing a weighed amount of solvent at the specified temperature until the increase in weight was constant at the barometric pressure (2).

For temperatures below 273 K a weighed amount (excess) of pyridine was quantitatively injected into the absorption vessel at the temperature of the thermostat. The tube was then weighed at room temperature.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Sample of best quality was self prepared, and was passed through concentrated sulfuric acid and calcium chloride.
- 2. 1-Propanol. Purified and attested.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.005$

- Gerrard, W.
 J. Chim. Phys. <u>1964</u>, 61, 73;
 Solubility of Gases in Liquids,
 Plenum Press, New York, <u>1976</u>.
- 2. Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109.

COMPONENT	s	:
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- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanols

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89-93.

VARIABLES:

T/K: See below Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

EXPERIMENTAL VALUES:	т/к п	Mole ratio HCl ^{/n} alkanol	Mole* fraction ^X HCl	Smoothed** mole fraction *HCl
1-Butanol; C ₄ H ₁₀ O; [71-36-3]	193.15 195.15 203.15	4.127	0.805	0.812 0.769
	213.15 223.15 233.15	2.176	0.685	0.728 0.688 0.650
	243.15 253.15 263.15		0.614	0.613 0.579 0.546
	273.15 283.15 293.15 303.15	-	0.516	0.516 0.487 0.460 0.435
	304.15 313.15 318.15	0.740	0.436 0.398	0.412
	323.15			0.390

Smoothing equation: $\ln x_{HCl} = 3.548 - 3.592/(T/100) - 2.881 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 3.04×10^{-3}

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determination at temperatures below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler was attached to a flask containing one dm³ of water, and allowed to warm slowly to room temperature (12 hours). The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method. A low temperature, Teddington-type YM thermostat was used for temperatures below 273 K, the control being to ±2 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: good specimen from a commercial cylinder was dried.
- (2) Alkanols : carefully purified, and purity rigourously attested.

ESTIMATED ERROR:

 $\delta T/K = \pm 2$ below 273 K $\delta x_{HCl}/x_{HCl} = \pm 0.005$ to 0.015

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.	
(2) Alkanols	J. Appl. Chem. <u>1959</u> , 9, 89-93.	
EXPERIMENTAL VALUES:		
T/K	Mole ratio Mole* Smoothed fraction mole fract	
	HCl ^{/n} alkanol fraction mole fract *HCl *HCl *HCl	.1011
2-Butanol; C ₄ H ₁₀ O; [78-92-2] 193.15 198.15	0.824 4.124 0.805	
203.15	0.779	•
213.15	2.719 0.731 0.736	
223.15		
233.15		
243.15		
253.15 263.15	0.592 0.562	
273.15		
283.15	0.508	
293.15		
303.15		
313.15)
319.15 323.15	0.738 0.425 0.420	`
323,13	0.420	'
Smoothing equation: $\ln x_{HCl} = 2.062 - 8$ Standard error in x_{HCl} about the	1.776/(T/100) - 2.029 $ln(T/100)$ regression line = 4.10 × 10 ⁻³	
1-Pentanol; C ₅ H ₁₂ O; [71-41-0] 193.15 201.15	0.798 3.424 0.774	3
203.15	0.765	i
213.15	0.730	
223.15	0.694	ŀ
231.15 233.15	1.985 0.665 0.658	,
243.15		
245.65		•
253.15	0.588	}
253.65	1.397 0.583	
263.15	0.554	
273.15	0.522	
275.15 283.15	1.091 0.522 0.492	,
293.15	0.463	
294.15	0.867 0.464	
298.05	0.816 0.449	
300.15	0.803 0.445	
303.15	0.436	,
305.55	0.761 0.432	
306.55	0.742 0.426 0.716 0.417	
310.25 313.15	0.716 0.417	,
314.05	0.695 0.410	
319.05	0.641 0.391	
323.15	0.386	
Smoothing equation: ln x _{HCl} = 5.154 -	5.677/(T/100) - 3.707 ln(T/100) regression line - 3.72 x 10 ⁻³	

Standard error in x_{HC1}^{HC1} about the regression line = 3.72×10^{-3}

 $^{^{\}ast}$ calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS:	ORIGINAL MEA	ASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Wyvill, P. I	Mincer, A. M. A.;
(2) Alkanols	J. Appl. Che	em. <u>1959</u> , 9, 89-93.
(2)		, , , , , , , , , , , , , , , , , , , ,
EXPERIMENTAL VALUES:	/K Mole ratio	Mole* Smoothed**
	n HCl $^{/n}$ alkanol	fraction mole fraction
		xHCl xHCl
4-Methyl-2-pentanol; C ₆ H ₁₄ O; 20	1.15 4.232	0.809
[108-11-2]	3.15	0.791
	0.65 3.060	0.754
	3.15	0.756
	3.15 2.486	0.713 0.719
	3.15	0.683
	3.15	0.648
	4.15 1.852	0.649
	3.15 1.576	0.612 0.614 0.581
1	3.15 3.15 1.249	0.555 0.549
	3.15	0.519
	3.15	0.491
	4.15 0.955	0.488
	3.15	0.464
	5.65 0.826	0.452
	1.15 0.802	0.445
	3.15	0.438
Smoothing equation: $\ln x_{HC1} = 4.58$	34 - 4.964/(T/100)) - 3.350 ln(T/100) ine = 7.66 × 10 ⁻³
Standard error in *HCl about	the regression li	ine = 7.66×10^{-3}
	3.15	0.821
	5.15 4.184	0.807
	3.15	0.774
	3.15 2.681	0.728 0.729 0.687
22	3.15	0.664
	9.15 1.972	0.648
	3.15 3.15	0.612
	3.15	0.577
	3.15	0.545
	3.15	0.516
	3.15	0.488
	3.15	0.462
1	3.15	0.438
	0.15 0.731	0.422
	3.15	0.416
Smoothing equation: $\ln x_{HC1} = 2.68$	32 - 2.476/(T/100)	- 2.426 ln(T/100)

Standard error in \times_{HC1}^{AC1} about the regression line = 1.35 \times 10⁻³

^{*} calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115 - 121.

EXPERIMENTAL VALUES:

Variation of temperature and pressure at constant mole fraction.

Variation	n of temp	perature	and pr	es-
sure at	constant	mole fra	action	(cont.)

т/к	Pressure P ₁ /mmHg	Mol Fraction	Т/К	Pressure P ₁ /mmHg	Mol Fraction
3.65	174	0.405	235.15	170	0.512
9.75	230		240.65	211	
4.35	263		246.85	252	
7.95	307		254.65	338	
3.15	371		261.45	438	
8.55	448		266.95	542	
3.65	531		267.45	546	
8.15	617		273.15	709	
2.15	687		277.15	847	
5.95	754		281.05	962	
9.15	821		282.55	1008	
2.95	884		284.75	1077	
6.85	973		286.55	1131	
			288.15	1182	
3.15	321	0.451			
7.35	366		Variation	of pressu	re and mole
3.05	453				t temperature.
6.55	504				· · · · · · · · · · · · · · · · · · ·
0.55	575		T/K	Pressure	Mol Fraction
1.95	608			p ₁ /mmHg	x_1
5.15 0.75	673 805				
6.15	945		273.15	171	0.405
9.15	1031		ì	321	0.451
1.65	1124		}	321	0.454
5.35	1249		ļ	456	0.480
	1247			710	0.512
2.15	309	0.454		760	0.516
9.75	408		278.15	212	0.405
3.55	466			377	0.451
0.35	593			387	0.454
3.35	652			552	0.480
8.55	779			760	0.503
5.65	972			877	0.512
0.95	1116		283.15	257	0.405
			200120	451	0.451
7.15	261	0.480		461	0.454
9.15	281			659	0.480
2.75	305			760	0.491
7.45	368			1023	0.512
3.15	456 533		200 15		
7.35	533 555		288.15	309	0.405
8.25	555 708			531 540	0.451
5.15	708			548 750	0.454
0.15 3.35	841 928			759 783	0.478 0.480
J. J.	1079		1	1183	0.512
7.95	1019		1	1100	0.512
7.95 9.15	1115				

See next page for additional information.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115 - 121.

VARIABLES:

T/K: 235.15 - 326.85 22.66 - 170.79 p_1/kPa : (170 - 1281 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

See preceding page.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

To measure the total pressure, taken to be p_1 , a weighed amount of 1-butanol was put into a flask fitted with a capillary bubbler tube through which the gas was passed into the liquid at approximately room temperature. By suitable adjustments of taps the flask was attached to the tapped end of a U-tube manometer containing mercury, the other limb being open to the atmosphere; the pressure, p_1 , was measured to within 1 mmHg for the condition of equilibriumesTIMATED ERROR: at each recorded temperature.

From a plot of p_1 vs. T/K the value of T/K for p_1 = 1 atm was read; and the separately determined mole fraction for that T/K (1) was taken to be the x_1 value for the series.

Data for the five series were reported 1. Gerrard, W.; Mincer, A. M. A.; as on the preceding page. From the set of p_1 vs. T/K curves, data given in the second table above were obtained.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. The sample was a good specimen obtained from a cylinder, and dried.
- (2) 1-Butanol. The sample was purified by a standard technique, and the purity was rigorously attested.

 $\delta p_1/\text{mmHq} = \pm 1$

REFERENCES:

Wyvill, P. L. J. Appl. Chem. 1959, 9, 89.

- (1) Hydrogen chloride; HC1; [7647-01-0]
- (2) 1-Butanol; C₄H₁₀O; [71-36-3] 1-Pentanol; C₅H₁₂O; [71-41-0] 1-Hexanol; C₆H₁₄O; [111-27-3]

ORIGINAL MEASUREMENTS:

Ionin, M. V.; Kurina, N. V.; Sudoplatova, A. E.

Tr. po Khim. i Khim. Tekhnol. 1963, (1), 47 - 48.

VARIABLES:

T/K: 298.15

Total p/kPa: 101.3 (atmospheric)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

ction
3
5
3

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was absorbed at a pressure which was not stated, and was probably barometric. The density of the solution was determined by a pyknometer. The hydrogen chloride absorbed was determined by an alkali titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from sodium chloride and sulfuric acid. Dried by calcium chloride.
- (2) 1-Alkanols. Source not given. Dried by calcium hydride.

ESTIMATED ERROR:

¹ Pure solvent refractive index.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1-Butanol; C₄H₁₀O; [71-36-3] VARIABLES: T/K = 315.15 p₁/kPa = 101.325 (1 atm) PREPARED BY: EXPERIMENTAL VALUES:

Tempe	rature	Mol Ratio	Mol Fraction
t/°C	<i>T</i> /K	n ₁ /n ₂	<i>x</i> ₁
42	315.15	0.66	0.40

The mole fraction value was calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The value above was credited to unpublished work of J. B. Fernandes and M. M. Sharma, University of Bombay, 1966. It is assumed the method was a chemical titration. ESTIMATED ERROR: REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 (1) Hydrogen chloride; HCl; 7647-01-0 (2) 1-Pentanol or 3-Methyl-1-butanol 	Kohn, G. Ber. Dtschn. Chem. Ges. B. 1932, 65, 589 - 595.
VARIABLES: T/K: 275.15 - 334.15 P/kPa: 101 (atmospheric)	PREPARED BY: W. Gerrard

T/K	Alcohol	Hydrogen Chloride	Mol Ratio	Mol Fraction
	wt/g	wt/g	ⁿ 1/ ⁿ 2	<i>x</i> 1
		or 1-amyl	alcohol;	С ₅ н ₁₂ 0;
275.15	55.0	22.9	1.005	0.501
278.15	50.0	19.9	0.961	0.490
318.15	55.0¹	21.5	0.944	0.485
308.15	23.5 ²	9.5	0.976	0.494
308.15	23.6³	7.6	0.777	0.437
323.15	23.6 ³	6.5	0.665	0.399
334.15	23.6 ³	5.6	0.573	0.364
3 C	-Methyl-1 5 ^H 12 ^O ; [1:	-butanol o: 23-51-3]	r isoamyl	alcohol;
278.15	31.6	13.85	1.058	0.514
~ , 0	40.3	17.3	1.036	0.509

- 1 Presumably 55.0 from position in original table.
- ² Described as a liquid mixture with paraffin.
- 3 The three values described as "one experiment".

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen chloride was passed to the alcohol in a measuring cylinder in an ice-salt mixture. The temperature, "end temperature" was recorded, and the absorbed gas was weighed. The pressure was presumably atmospheric.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Prepared from sodium chloride and sulfuric acid, and dried by sulfuric acid.
- (2) Alcohols. Kahlbaum specimens. The 3-methyl-1-butanol was stated to be free from pyridine.

ESTIMATED ERROR:

 $\delta wt/g = 0.1$

The mole ratio and mole fraction values were calculated by the compiler.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0](2) Alkanols	Gerrard, W.; Macklen, E.D. J. Appl. Chem. 1959, 9, 85-88.
VARIABLES: T/K: See below Total P/kPa : 101.325 (1 atm)	PREPARED BY: W. Gerrard

		Mole ratio Cl ^{/n} alcohol		Smoothed** mole fraction *HC1
1-Pentanol; C ₅ H ₁₂ O;	273.15			0.516
[71-41-0]	276.25	1.038	0.509	0.400
	283.15 285.55	0.947	0.486	0.492
	293.15	0.547	0.400	0.467
	294.15	0.867	0.464	0.407
	302.15	0.795	0.443	
	303.15			0.440
	306.05	0.762	0.432	
	313.15 313.45	0.701	0.412	0.413
Smoothing equation: ln x _{HC}	cl = 14.160 -	18.568/(T/1	00) - 7.98	35 ln(T/100)
Smoothing equation: $\ln x_{HG}$ Standard error in x_{HG}	cl = 14.160 - cl about the	18.568/(T/1 regression l	00) - 7.98 ine = 2.68	35 ln(T/100) 3 × 10 ⁻⁴
				85 ln(T/100) 8 × 10 ⁻⁴
	279.85 283.15		0.501	0.493
	279.85 283.15 290.25			0.493
	279.85 283.15 290.25 293.15	1.004	0.501	
	279.85 283.15 290.25 293.15 295.85	1.004	0.501	0.493 0.468
	279.85 283.15 290.25 293.15 295.85 303.15	1.004 0.904 0.852	0.501 0.475 0.460	0.493
	279.85 283.15 290.25 293.15 295.85	1.004	0.501	0.493 0.468
	279.85 283.15 290.25 293.15 295.85 303.15 308.55 313.15 318.75	1.004 0.904 0.852	0.501 0.475 0.460	0.493 0.468 0.441 0.413
Smoothing equation: ln x _{H0} Standard error in x _{H0} 1-Hexanol; C ₆ H ₁₄ O; [111-27-3]	279.85 283.15 290.25 293.15 295.85 303.15 308.55 313.15	1.004 0.904 0.852 0.742	0.501 0.475 0.460 0.426	0.493 0.468 0.441

Smoothing equation: $\ln x_{HCl}$ = 16.882 - 22.445/(T/100) - 9.284 $\ln(\text{T/100})$ Standard error in x_{HCl} about the regression line = 9.78 \times 10⁻⁴

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Alcohols: purified, distilled, and attested by physical constants.

ESTIMATED ERROR: $\delta x_{HC1}/x_{HC1} = \pm 0.005 \text{ to } 0.01$

REFERENCES:

Gerrard, W.; Macklen, E.D.
 J. Appl. Chem. 1956, 6, 241.

	ORIGINAL MEASUREMENTS:
COMPONENTS:	
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Macklen, E.D.
(2) Alkanols	J. Appl. Chem. <u>1959</u> , 9, 85-88.
EXPERIMENTAL VALUES:	Mole ratio Mole* Smoothed** n HCl $^{/n}$ alcohol fraction mole fraction x HCl x HCl
4-Methyl-2-pentanol; C ₆ H ₁₄ O; 273.1 [108-11-2] 274.7	
283.1	5 0.513
287.0 293.1	5 0.489
294.2 300.3	
303.1 307.4	5 0.832 0.454
313.1 319.4	
323.1	
Smoothing equation: $\ln x_{HC1} = 11.406$ Standard error in x_{HC1} about the	- $14.915/(T/100)$ - $6.539 \ln(T/100)$ e regression line = 6.14×10^{-4}
1-Heptanol; C ₇ H ₁₆ O; 279.8 [111-70-6] 283.1	
292.4	5 0.887 0.470
293.1 295.8	5 0.855 0.461
303.1 308.1	5 0.745 0.427
313.1 318.7	5 0.666 0.400
323.1 333.1	5 0.360
337.3 343.1	
Smoothing equation: $\ln x_{\text{HCl}} = 15.96$ Standard error in x_{HCl} about th	$8 - 21.150/(T/100) - 8.843 \ln(T/100)$ e regression line = 8.16×10^{-4}
1-Decanol; C ₁₀ H ₂₂ O; 273.1	
[112-30-1] 10 22 273.8 283.1	5 0.496
283.9 290.2	
293.1 303.1	
303.4 312.5	5 0.796 0.443
313.1 323.1	5 0.417
325.5 333.1	5 0.623 0.384
Smoothing equation: $\ln x_{HCl} = 13.79$ Standard error in x_{HCl} about the	$4 - 18.096/(T/100) - 7.787 \ln(T/100)$ e regression line = 8.37×10^{-4}

^{*} calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Fernandes, J. B. [7647-01-0] J. Chem. Eng. Data 1972, 17, (2) 1-Hexanol; C₆H₁₄O; [111-27-3] 377-379. VARIABLES: PREPARED BY: 353.15 - 393.15 101.325 (1 atm) T/K: H. L. Clever p_1/kPa :

EXPERIMENTAL VALUES:	
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Temp	erature	Mol Ratio¹	Mol Fraction
t/°C	<i>T/</i> K	$\frac{n_1/n_2}{}$	x_1
80	353.15	0.434	0.303
100	373.15	0.320	0.242
120	393.15	0.236	0.191

¹ Vapor pressure correction applied.

The mole fraction solubility values were calculated by the compiler. Smoothed Data: For use between 353.15 and 393.15 K.

 $\ln x_1 = -5.7174 + 15.9947/(T/100 K)$

The standard error about the regression line is 3.63×10^{-3} .

T/K	Mol Fraction
	x ₁
353.15 363.15 373.15 383.15	0.305 0.269 0.239 0.214
393.15	0.192

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: No information. The data above were credited to unpublished work of J. B. Fernandes and M. M. Sharma, University of Bombay, 1966. It is assumed the method is the same as for the HBr + 1-hexanol system. See that data sheet for details. ESTIMATED ERROR: REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Heptanol; C7H₁₆O; [111-70-6] 1-Octanol; C₈H₁₈O; [111-87-5] 1-Nonanol; C₉H₂₀O; [143-08-8] 1-Decanol; C₁₀H₂₂O; [112-30-1]

ORIGINAL MEASUREMENTS:

Ionin, M. V.; Kurina, N. V.; Sudoplatova, A. E.

Tr. po Khim. i Khim. Tekhnol. 1963, (1), 47 - 48.

VARIABLES:

T/K: 298.15

101.3 (atmospheric) P/kPa:

PREPARED BY:

W. Gerrard

EXPERIMENTAL	VALUES:				
T/K	Refractive	Solution	Concentration	Mol Ratio	Mol Fraction
	Index1	Density	c ₁ /mol dm ⁻³	ⁿ 1 ^{/n} 2	x_1
	n _D ²⁹⁸	$\rho/g cm^{-3}$	1		
1	-Heptanol				
298.15	1.4241	0.89480	5.14	0.844	0.458
1	-Octanol				
298.15	1.4293	0.89250	4.62	0.831	0.454
1	-Nonanol				
298.15	1.4337	0.88760	4.16	0.815	0.449
1	-Decanol				
298.15	1.4373	0.88244	3.83	0.816	0.449

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was absorbed at a pressure which was not stated, and was probably barometric. The density of the solution was determined by a pyknometer. The hydrogen chloride absorbed was determined by an alkali titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from sodium chloride and sulfuric acid. Dried by calcium chloride.
- (2) 1-Alkanols. Source not given. Dried by calcium hydride.

ESTIMATED ERROR:

¹ Pure solvent refractive index.

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. 1-Octanol; C₈H₁₈O; [111-87-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	ⁿ HC1/ ⁿ C ₈ H ₁₈ O	X _{HC1}
243.15	1.447	0.591
253.15	1.273	0.560
263.15	1.146	0.534
273.15	1.024	0.506
283.15	0.890	0.471
293.15	0.810	0.448

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln x_1 = 7.562 - 9.084/(T/100K) - 4.901 \ln(T/100K)$

Standard error about regression line = 2.81×10^{-3}

T/K Mol Fraction

	X _{HC1}
243.15	0.589
253.15	0.561
263.15	0.532
273.15	0.502
283.15	0.474
293.15	0.446
273.15 283.15	0.502 0.474

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K, a chemical titration was performed.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- 1-Octanol. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T = 0.2$ $\delta X/X = 0.005$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) 1-Octanol; C₈H₁₈O; [111-87-5]

ORIGINAL MEASUREMENTS:

Fernandes, J. B.

J. Chem. Eng. Data 1972, 17, 377-379.

VARIABLES:

T/K: 353.15 - 413.15 p_1/k Pa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES: _

Temp	erature	Mol Ratio1	Mol Fraction
t/°C	T/K	n_1/n_2	x_{7}
30	303.15	0.7922	0.442
40	313.15	0.716 ²	0.417
80	353.15	0.389	0.280
100	373.15	0.26	0.206
120	393.15	0.129	0.114
140	413.15	0.0785	0.0728

¹ Vapor pressure correction applied.

The mole fraction solubility values were calculated by the compiler.

Smoothed Data: For use between 353.15 and 413.15 K.

 $\ln x_1 = 95.0476 - 138.7062/(T/100 \text{ K}) - 45.1964 \ln (T/100 \text{ K})$ The standard error about the regression line is 1.50×10^{-2} .

T/K	Mol Fraction		
	$x_{_{ extstyle 1}}$		
353.15	0.285		
363.15	0.238		
373.15	0.194		
383.15	0.155		
393.15	0.121		
403.15	0.094		
413.15	0.071		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data above were credited to unpublished work of J. B. Fernandes and M. M. Sharma, University of Bombay, 1966. It is assumed the method is the same as for the HBr + 1-octanol system. See that data sheet for details.

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

REFERENCES:

 Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. <u>1959</u>, 9, 89.

² Interpolated from values in ref. (1).

COMPONENTS: ORIGINAL MEASUREMENTS: Kohn, G. Hydrogen chloride; HCl; [7647-01-0] Ber. Dtschn. Chem. Ges. B. 1932, (2) 2-Octanol or s-octyl alcohol; C₈H₁₈O; [123-96-6] 65, 589 - 595. **VARIABLES:** PREPARED BY: T/K: 275.15 - 334.15 P/kPa: W. Gerrard 101 (atmospheric) EXPERIMENTAL VALUES:

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen chloride was passed to the alcohol in a measuring cylinder in an ice-salt mixture. The temperature, "end temperature", was recorded, and the absorbed gas was weighed. The pressure was presumably atmospheric.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Prepared from sodium chloride and sulfuric acid, and dried by sulfuric acid.
- (2) Alcohols. Kahlbaum specimens.

ESTIMATED ERROR:

 $\delta wt/g = 0.1$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Decanol; C₁₀H₂₂O; [112-30-1]

ORIGINAL MEASUREMENTS:

Fernandes, J. B.

J. Chem. Eng. Data 1972, 17, 377-379.

VARIABLES:

T/K: 353.15 - 413.15 p,/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temp	erature	Mol Ratio1	Mol Fraction
t/°C	<i>T</i> /K	$\frac{n_1/n_2}{}$	x_1
30	303.15	0.800²	0.444
40	313.15	0.7122	0.416
60	333.15	0.567²	0.362
80	353.15	0.385	0.278
100	373.15	0.232	0.188
120	393.15	0.109	0.098
140	413.15	0.0655	0.0615

¹ Vapor pressure correction applied.

The mole fraction solubility values were calculated by the compiler. Smoothed Data: For use between 333.15 and 413.15 K.

> $\ln x_1 = 103.1643 - 150.3336/(T/100 K) - 49.0594 \ln (T/100 K)$ The standard error about the regression line is 1.18×10^{-2} .

T/K	Mol Fraction x_1
333.15 343.15 353.15 363.15 373.15	0.368 0.321 0.271 0.223 0.178

T/K	Mol Fraction
	x
383.15	0.139
393.15	0.107
403.15	0.080
413.15	0.060

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data above were credited to unpublished work of J. B. Fernandes and M. M. Sharma, University of Bombay, 1966. It is assumed the method is the same as for the HBr + 1-decanol system. See that data sheet for the details.

SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

- 1. Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89.

² Interpolated from values in ref. (1).

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Dodecanol; C₁₂H₂₆O; [112-53-8]

ORIGINAL MEASUREMENTS:

Fernandes, J. B.; Sharma, M. M.

Indian Chem. Eng. 1965, 7, 38 - 40.

VARIABLES:

T/K: 303.15 - 453.15 HCl P/kPa: 101.325 (760 mmHg)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	ⁿ 1 ^{/n} 2	x_1
303.15	0.724	0.420
313.15	0.634	0.388
333.15	0.472	0.321
353.15	0.3234	0.244
373.15	0.1862	0.157
393.15	0.0921	0.0843
413.15	0.0460	0.0440
433.15	0.0296	0.0287
453.15	0.01728 ¹	0.01471

¹ Material turned brown.

Smoothed Data: $\ln x_1 = 89.891 - 129.002/(T/100K) - 43.463 \ln (T/100K)$

Standard error about the regression line = 9.30×10^{-3}

•	
T/K	Mol Fraction
	x_1
303.15	0.421
313.15	0.400
333.15	0.321
353.15	0.229
373.15	0.148
393.15	0.0886
413.15	0.0502
433.15	0.0272
453.15	0.0142

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was bubbled into the solvent for more than an hour. Approximately 1 cm³ of the solution was transferred to a weighed sample tube and the whole re-weighed. The contents were transferred to water, and the chloride content determined by the Volhard method.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared by the method of Sloan (1).
- (2) 1-Dodecanol. Dehydag Deutsche Hydrierwerke GMBH. Minimum purity 95 per cent (usually 98+ per cent). Used as received.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta x_1/x_1 = 0.05$

REFERENCES:

 Sloan, A. D. B. Chem. Ind. 1964, 574.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1-Tetradecanol; C₁₄H₃₀O; [112-72-1] (2) Components: Fernandes, J. B.; Sharma, M. M. Indian Chem. Eng. 1965, 7, 38 - 40.

1-Octadecanol; C₁₈H₃₈O; [112-92-5]

VARIABLES:

T/K: 333.15, 433.15 HC1 P/kPa: 101.325 (760 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
l-Te	tradecanol	
333.15 433.15	0.462 0.0211	0.313 0.0207
1-00	tadecanol	
333.15 433.15	0.448 0.0178	0.309 0.0175

The compiler calculated the mole fraction solubility values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was bubbled into the solvent for more than an hour. Approximately 1 cm³ of the solution was transferred to a weighed sample tube and the whole re-weighed. The contents were transferred to water, and the chloride content determined by the Volhard method.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared by the method of Sloan (1).
- (2) 1-Tetradecanol and 1-Octadecanol. Both alcohols supplied by Dehydag Deutsch Hydrierwerke GMBH. Minimum purity 95 per cent (usually 98+ per cent). Used as received.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta x_1/x_1 = 0.05$

REFERENCES:

 Sloan, A. D. B. Chem. Ind. 1964, 574.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Hexadecanol; $C_{16}^{H}_{34}^{O}$; [36653-82-4]

ORIGINAL MEASUREMENTS:

Fernandes, J. B.; Sharma, M. M.

Indian Chem. Eng. 1965, 7, 38 - 40.

VARIABLES:

T/K: 333.15 - 473.15 HCl P/kPa: 101.325 (760 mmHg)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	n_1/n_2	x_1
333.15	0.462	0.316
343.15	0.358	0.264
353.15	0.2445	0.196
373.15	0.1491	0.130
393.15	0.0727	0.0678
413.15	0.0391	0.0376
433.15	0.0227	0.0222
453.15	0.0141 ¹	0.0139
473.15	0.008761	0.00868

¹ The material turned brown.

 $\ln x_1 = 35.863 - 40.148/(T/100K) - 20.670 \ln (T/100K)$ Smoothed Data: Standard error about the regression line = 9.67×10^{-3}

T/K	Mol Fraction
	<i>x</i> 1
333.15	0.346
353.15	0.205
373.15	0.121
393.15	0.0709
413.15	0.0417
433.15	0.0246
453.15	0.0145
473.15	0.00867

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was bubbled into the solvent for more than an hour. Approximately 1 cm3 of the solution was transferred to a weighed sample tube and the whole re-weighed. The contents were transferred to water, and the chloride content determined by the Volhard method.

- SOURCE AND PURITY OF MATERIALS:
 (1) Hydrogen chloride. Self prepared by the method of Sloan (1).
- (2) 1-Hexadecanol. Dehydag Deutsche Hydrierwerke GMBH. Minimum 95 per cent purity (usually 98+ per cent). Used as received.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta x_1/x_1 = 0.05$

REFERENCES:

1. Sloan, A. D. B. Chem. Ind. 1964, 574.

COMPONENTS:	EVALUATOR:
1. Hydrogen Chloride; HCl; [7647-01-0]	Peter G. T. Fogg Department of Applied Chemistry and Life Sciences,
2. Halogenated Alkanols	Polytechnic of North London, Holloway, London, N7 8DB, U.K.
	January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Halogenated Alkanols

Gerrard and co-workers (1-3) measured solubilities in several halogenated alkanols over temperature ranges at a total pressure equal to barometric pressure. Under the conditions of the experiments the differences between these solubilities and values for a partial pressure of 101.3 kPa are likely to be less than experimental error.

The presence of a halogen atom in 2-chloroethanol, 2-bromoethanol, 1-chloro-2-propanol and 1-bromo-2-propanol lowers the mole fraction solubilities of HCl relative to those in the unsubstituted alcohols but these solubilities are nevertheless appreciably higher than reference values from the Raoult's law equation. There is little difference between mole fraction solubilities in these solvents in the overlapping temperature range.

The presence of two halogen atoms in 1,3-dibromo-2-propanol and in 2,3-dibromo-1-propanol causes a greater lowering of solubility. Mole fraction solubilities in 2,3-dibromo-1-propanol are about double those in 1,3-dibromo-2-propanol. Perhaps this is due to steric factors.

Mole fraction solubilities in 2,2,2-trifluoroethanol and in 2,2,2-trichloroethanol are close to each other and lower than in the dibromopropanols but, despite the presence of three halogen atoms, the solubilities lie above the reference line from the Raoult's law equation.

Measurements reported by Gerrard & Macklen (1) for solubility in 2-chloroethanol, and in 2,2,2-trichloroethanol differ to some extent from those reported by Gerrard, Mincer & Wyvill (2,3). The maximum difference between smoothed values of mole fraction solubilities in 2-chloroethanol from the two sources is about 7%. The maximum difference in the case of 2,2,2-trichloroethanol is about 10%. These differences are not sufficient to cast doubt on the overall pattern of measurements in these solvents. Data from other sources are not available for comparison.

Mole fraction solubilities at 293.15 K and a partial pressure of 101.3 kPa.

Solvent	*HCl	Source
(Reference value)	0.024	(Raoult's law equation)
Ethanol	0.462	(evaluated value)
1-Propanol	0.463	(evaluated value)
2-Chloroethanol	0.300	(2)
	0.295	(1)
2-Bromoethanol	0.330	(1)
1-Chloro-2-propanol	0.318	(1)
1-Bromo-2-propanol	0.329	(1)
1,3-Dibromo-2-propanol	0.088	(1)
2,3-Dibromo-1-propanol	0.184	(1)
2,2,2-Trifluoroethanol	0.0480	(1)
2,2,2-Trichloroethanol	0.0600	(3)
- , - ,	0.0669	(1)

- 1. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1959, 9, 85 88.
- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89 - 91.
- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115 - 121.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. 2-Chloroethanol; C₂H₅ClO;
 [107-07-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 199.15 - 322.65 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	T/K	Mol Ratio	Mol Fraction
		n HC1/ n C2 H 5C1O	X _{HC1}
	199.15	2.858	0.741
	211.15	2.110	0.678
	233.15	1.247	0.555
	253.15	0.883	0.469
	279.65	0.557	0.358
	292.65	0.439	0.305
	308.35	0.315	0.240
	322.65	0.210	0.174

Smoothed Data: $\ln x_1 = -66.3023 + 92.9619/(T/100K) + 80.1282 \ln (T/100K) -18.0080 (T/100K)$

Standard error about the regression line = 1.06×10^{-2}

T/K	Mole Fraction ^x 1	T/K	Mole Fraction x1	
193.15	0.813	263.15	0.434	
203.15	0.717	273.15	0.390	
213.15 223.15	0.651 0.600	283.15 293.15	0.346 0.300	
233.15 243.15	0.556 0.516	303.15 313.15	0.256 0.214	
253.15	0.475	323.15	0.175	

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed at temperatures above 273 K was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determinations below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method.

A low temperature, Teddington type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- 2-Chloroethanol. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 \text{ below 273 K} \\ \delta X_1/X_1 = 0.02$

Hydrogen Chloride in Non-Aqueous Solvents				
COMPONENTS:	ORIGINAL MEASUREMENTS:			
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Macklen, E.D.			
(2) Halogenated alcohols	J. Appl. Chem. <u>1959</u> , 9, 85-88.			
VARIABLES: T/K: See below Total P/kPa: 101.325 (1 atm)	PREPARED BY: W. Gerrard			
EXPERIMENTAL VALUES:	Mole ratio Mole* Smoothed**	<u> </u>		

			HC1	"HCI
2-Chloroethanol; C ₂ H ₅ Cl0;	273.15			0.364
[107-07-3]	277.65	0.548	0.354	••••
	283.15			0.335
	285.15	0.485	0.327	
	293.15			0.295
	293.85	0.410	0.291	
	298.45	0.371	0.271	
	303.15			0.251
!	308.05	0.302	0.232	
	313.15			0.207
	318.55	0.224	0.183	
	323.15			0.166
Standard error in xHCl		regression	line = 2.17	
2-Bromoethanol; C ₂ H ₅ BrO;	273.15			0.362
[540-51-2]	278.55	0.532	0.347	
	282.85	0.494	0.331	
	283.15			0.330
	288.75	0.443	0.307	
	293.15			0.290
	294.55	0.397	0.284	
	301.05	0.345	0.257	
	303.15	0 201	0 210	0.247
	310.05	0.281	0.219	0.205
	313.15 318.35	0.225	0.184	0.205
	323.15	0.225	0.104	0.166
	323.13			0.100

Smoothing equation: $\ln x_{\text{HCl}} = 67.476 - 90.597/(\text{T}/100) - 35.154 \ln(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 1.05 × 10⁻³

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

 $n_{\rm HCl}/n_{\rm alcohol}$ fraction mole fraction

Xucl

- Hydrogen chloride: selfprepared and dried.
- Halo-alcohols: purified, distilled, and attested by (2) physical constants.

ESTIMATED ERROR: $\delta x_{\rm HC1}/x_{\rm HC1} = \pm 0.01 \text{ to } 0.02$

REFERENCES:

1. Gerrard, W.; Macklen, E.D. J. Appl. Chem. 1956, 6, 241.

		1				
COMPONENTS:	ORIGINAL MEASUREMENTS:					
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Macklen, E.D.					
(2) Halogenated alcohols		J. Appl. Chem. <u>1959</u> ,		9, 85-88.		
EXPERIMENTAL VALUES:		İ				
BAT BATTISATAD VILLOUD.	T/K	Mole ratio HCl ^{/n} alcohol	Mole* fraction ^X HCl	Smoothed** mole fraction [*] HCl		
1-Chloro-2-propanol; C ₃ H ₇ ClO; [127-00-4]	273.15 283.15	0.654	0.395	0.393 0.359		
	284.45 292.45	0.467	0.351 0.318	0.240		
	293.15 301.65 303.15	0.390	0.281	0.318 0.273		
	308.65	0.336	0.251			
	313.15 320.75 323.15	0.241	0.194	0.228 0.186		
Smoothing equation: $\ln x_{HCl} = 65.506 - 87.945/(T/100) - 34.079 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 3.74×10^{-3}						
1-Bromo-2-propanol; C ₃ H ₇ BrO; [19686-73-8]	280.15 283.15 293.15	0.604	0.377	0.367 0.329		
·	295.85 297.65 302.95	0.465 0.451	0.317 0.311 0.289	3332		
	303.15 312.15		0.250	0.287		
	313.15 321.05	0.269	0.212	0.245		
	323.15			0.204		
Smoothing equation: $\ln x_{\text{HCl}} = 60.861 - 82.074/(\text{T}/100) - 31.589 \ln(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 1.09 × 10 ⁻³						
1,3-Dibromo-2-propanol;	273.15	0 145	0 127	0.128		
C ₃ H ₆ Br ₂ ; [96-21-9]	273.35 283.15 289.85 293.15 297.05 302.05	0.145	0.127	0.108		
		0.107	0.0967	0.0878		
		0.085 0.074	0.0783 0.0689			
	303.15			0.0686		
	309.35 313.15	0.064	0.0602	0.0519		
	318.25 323.15	0.046	0.0440	0.0381		
		- 114.858/(T/ regression l		889 ln(T/100) × 10 ⁻³		

^{*} calculated by the compiler
** smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen chloride; HCl; (1) Gerrard, W.; Macklen, E.D. [7647-01-0] J. Appl. Chem. 1959, 9, 85-88. (2) Halogenated alcohols EXPERIMENTAL VALUES: T/K Mole ratio Mole* Smoothed** ⁿHCl^{/n}alcohol fraction mole fraction xHC1 x HCl 280.15 0.331 0.249 2,3-Dibromo-1-propanol; C₃H₆Br₂O; [96-13-9] 283,15 0.232 291.15 0.235 0.190 293.15 0.184 298.65 0.161 0.192 303.15 0.143 0.140 304.85 0.163 313.05 0.121 0.108 313.15 0.110 322.05 0.095 0.0868 323.15 0.0837 Smoothing equation: $\ln x_{HC1} = 48.152 - 59.615/(T/100) - 27.439 \ln(T/100)$ Standard error in x_{HC1} about the regression line = 2.80 × 10⁻³ 0.0728 273.15 2,2,2-Trifluoroethanol; $C_2H_3F_3O$; [75-89-8] 0.070 0.0654 277.85 0.0587 283.15 284.25 0.060 0.0566 0.0480 293.15 294.65 0.051 0.0485 302.65 0.041 0.0394 0.0387 303.15 0.0333 313.15 313.65 0.034 0.0329 Smoothing equation: $\ln x_{\text{HCl}} = -8.741 + 16.720/(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 1.26 × 10⁻³ 0.0932 273.15 2,2,2-Trichloroethanol; 0.0926 $C_2H_3Cl_3O; [115-20-8]$ 273.55 0.102 0.0811 283.15 288.35 0.081 0.0749 293.15 0.0669 294.45 0.068 0.0637 302.65 0.0539 0.057 303.15 0.0528 0.0400 313.15 313.65 0.041 0.0394 Smoothing equation: $\ln x_{HCl} = 98.026 - 132.665/(T/100) - 51.580 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 1.26 × 10⁻³ * calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Gerrard, W.; Mincer, A. M. A.; [7647-01-0] Wyvill, P. L. (2) 2,2,2-Trichloroethanol; J. Appl. Chem. 1960, 10, 115-121. C2H3Cl3O; [115-20-8] VARIABLES: PREPARED BY: T/K: 273.15 - 303.15 W. Gerrard Total P/kPa: 101.325 (1 atm) (smoothed data calculated by H.L. Clever)

E	XPERIMENTAL VALUES: _			-
		т/к	Mol Ratio	Mol Fraction
		273.15 278.15 279.65 285.15 288.35 294.75 297.85 303.15	0.104 0.0890 0.0860 0.0761 0.0733 0.0604 0.0591	0.0942 0.0817 0.0792 0.0707 0.0683 0.0570 0.0558 0.0486

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -8.814 + 17.592/(T/100)$

Standard error about the regression line is 1.34×10^{-3}

т/к	Mol Fraction x_1
273.15	0.0931
283.15	0.0742
293.15	0.0600
303.15	0.0492

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 2,2,2-Trichloroethanol. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.02$$

COMPONENTS:	EVALUATOR:
(1) Hydrogen chloride; HCl; [7647-01-0] (2) Alkenols and Alkynols	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA
	1983, July

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Unsaturated Alcohols.

Cook (ref 1) measured the solubility of hydrogen chloride at a partial pressure of $101.325~\mathrm{kPa}$ (1 atm) over the 263 - $293~\mathrm{K}$ temperature interval in eleven unsaturated alcohols. Eight of the alcohols are alkenols and three are alkynols.

The hydrogen chloride is more soluble in the alkenols than in the alkynols of similar molecular weight and structure. The alkenols range from three to seven carbon atoms. The mole fraction solubility increases as the carbon chain length increases and it increases with chain branching. The largest solubility is observed in the branched chain four carbon alkenol.

The data were fitted to an equation of the type

$$\ln x_1 = A_1 + A_2/(T/100 \text{ K}) + A_3 \ln (T/100 \text{ K})$$

by the method of least squares. The equations and a table of smoothed mole fraction solubility data are included on each data sheet. The data are classed as tentative. Although an uncertainty of 0.5 percent is noted on the data sheets, the data are considered accurate to 2 to 3 percent because of uncertainties in the pressure measurement.

Table 1 gives smoothed solubility values in mole fraction (x_1) and mole ratio (n_1/n_2) at temperatures of 273.15 and 293.15 K along with the semi-structural formulas of the alcohols. The trends in the hydrogen chloride solubility with structure mentioned briefly above can be seen in the table.

Table 1. Tentative mole ratio and mole fraction solubilities of hydrogen chloride in unsaturated alcohols at a partial pressure of 101.325 kPa and temperatures of 273.15 and 293.15 K.

Solvent Name and Structure			Solubi	lity	
		273.15 K		293.15 К	
		$\frac{n_1/n_2}{n_1}$	x_1	n_{1}/n_{2}	x 1
ALKENOLS					
2-Propen-1-ol	CH2=CHCH2OH	0.887	0.470	0.689	0.408
2-Buten-1-ol	сн ₃ сн=снсн ₂ он	1.024	0.506	0.828	0.453
3-Buten-1-ol	сн ₂ =снсн ₂ сн ₂ он	0.972	0.493	0.786	0.440
2-Methyl-2-pro					
	CH ₂ =C(CH ₃)CH ₂ OH	1.364	0.577	1.169	0.539
4-Penten-1-ol	Сн ₂ =снсн ₂ сн ₂ сн ₂ он	1.045	0.511	0.848	0.459
3-Penten-1-ol	CH3CH=CHCH2CH2OH	1.033	0.508	0.838	0.456
3-Hexen-1-ol	снзснзсн=снснзснзон	1.041	0.510	0.848	0.459
3-Hepten-1-ol	CH3CH2CH2CH=CHCH2CH2OH	1.053	0.513		
ALKYNOLS					
2-Propyn-1-ol	сн≡ссн он	0.429	0.300	0.272	0.214
3-Butyn-1-ol	сн≡ссн ₂ сн ₂ он	0.706	0.414	0.592	0.372
3-Butyn-2-01	сн≡ссно́нсна	1.033	0.508	0.876	0.467

COMPONENTS: (1) Hydrogen chloride; HCl; Cook, T.M. [7647-01-0] (2) Alkenols and alkynols VARIABLES: T/K: 252.15 - 303.05 ORIGINAL MEASUREMENTS: Cook, T.M. Thesis, 1966 University of London PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:		Mole ratio	Mole* fraction *HCl	Smoothed** mole fraction *HCl
2-Propyn-1-ol, (propargyl alcohol);	263.15 263.35	0.513	0.339	0.338
C ₃ H ₄ O; [107-19-7]	268.65 273.15	0.463	0.316	0.300
	275.15 278.15	0.410 0.387	0.291 0.279	
	283.15 289.65	0.351 0.297	0.260 0.229	0.258
	292.65 293.15	0.276 0.273	0.216 0.214	0.214
	303.15	J. 2. 7. 3	0.213	0.174

Smoothing equation: $\ln x_{\rm HCl}$ = 62.588 - 81.788/(T/100) - 33.685 $\ln({\rm T}/100)$ Standard error in $x_{\rm HCl}$ about the regression line = 1.73 \times 10⁻³

* calculated by the compiler.

Total P/kPa : 101.325 (1 atm)

** smoothing equations and smoothed values were calculated by H.L. Clever.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data were cited by Gerrard (1).

Hydrogen chloride was passed into a bubbler tube containing a weighed amount of solvent at the specified temperature until the increase in weight was constant at the barometric pressure (2). For temperatures below 273 K a weighed amount (excess) of pyridine was quantitatively injected into the absorption vessel at the temperature of the thermostat. The tube was then weighed at room temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Hydrogen chloride: sample of best quality was self prepared and was passed through concentrated sulfuric acid and calcium chloride.

(2) Alcohols: 2-buten-1-ol self prepared. All alcohols fractionally distilled.

	B.Pt.(1 atm)/~	C Refractive Index	Density
2-propyn-1-ol	114		d^{2} = 0.9712
2-propen-2-ol	96.5	$n_D^{21} = 1.4133$ $n_D^{21} = 1.4404$	
3-butyn-1-ol	128.5-130	$n_D^{21} = 1.4404$	$d^{2} = 0.922$
3-butyn-2-ol	104-105.5	$n_0^{21} = 1.4236$	$d^{20} = 0.887$
2-buten-1-ol	120.5-121.5	$n_D^{21} = 1.4236$ $n_D^{25} = 1.4333$	$d^{15} = 0.8570$
(33-3	4 at 8.5 mmHg)	Ь	
3-buten-1-ol	112-113		$d^{1\frac{5}{4}} = 0.8382$ $d^{2\frac{0}{4}} = 0.846$
2-methyl-2-propen-1-	ol 113-114.5	$n_D^{20} = 1.4262$	$d^{2}_{4}^{0} = 0.846$
3-penten-1-ol	137-138.5	$n_D^{20} = 1.4262$ $n_D^{21} = 1.4376$	
4-penten-1-ol	134-138	8	
3-hexen-1-ol	155-157	$n_D^{20} = 1.4380$	$d^{2}_{4}^{0} = 0.849$
3-hepten-1-ol	173-173.5	$n_D^{20} = 1.4380$ $n_D^{23} = 1.4394$	
		U	

ESTIMATED ERROR:

 $\delta x_{\rm HC1}/x_{\rm HC1} = 0.005$

- 1. Gerrard, W. J. Chim. Phys. <u>1964</u>, 61, 73;
- Solubility of Gases in Liquids, Plenum Press, New York, 1976.
- 2. Ahmed, W.; Gerrard, W.; Maladkar, W.K. J. Appl. Chem. 1970, 20, 109.

Hydrogen Chloride in Non-Aqueous Solvents COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Cook, T.M. 17647-01-01 Thesis, 1966 (2) Alkenols and alkynols University of London EXPERIMENTAL VALUES: T/K Mole ratio Mole* Smoothed** $n_{HC1}/n_{a1coho1}$ fraction mole fraction xHC1 xHC1 2-Propen-1-ol 263.15 0.993 0.498 0.498 0.470 (ally1 alcohol); C3H6O; 273.15 0.835 [107-18-6] 278.15 0.455 283.15 0.440 288.15 0.423 0.733 289.45 0.729 0.422 291.35 0.712 0.416 293.15 0.408 296.15 0.652 0.395 303.05 0.606 0.377 0.375 303.15 Smoothing equation: $\ln x_{\rm HCl}$ = 19.291 - 24.988/(T/100) - 10.845 $\ln({\rm T/100})$ Standard error in $x_{\rm HCl}$ about the regression line = 2.36 × 10⁻³ 3-Butyn-1-ol; C₄H₆O; 262.45 0.791 0.442 [927-74-2] 263.15 0.440 0.414 273.15 273.65 0.705 0.413 280.45 0.659 0.397 0.644 283.15 0.392 0.391 0.386 285.75 0.628 293.15 0.372 Smoothing equation: $\ln x_{\text{HCl}} = -3.030 + 5.107/(\text{T}/100) + 0.277 \ln(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 4.21×10^{-4} 3-Butyn-2-ol; C₄H₆O; [2028-63-9] 263.15 0.519 268.90 1.057 0.514 273.15 0.508 0.499 0.977 278.65 0.965 0.491 283.15 0.490 283.15 284.45 0.950 0.487 293.15 0.467 Smoothing equation: $\ln x_{\rm HCl}$ = 24.510 - 33.231/(T/100) - 12.958 $\ln({\rm T}/100)$ Standard error in $x_{\rm HCl}$ about the regression line = 8.94 × 10⁻⁴ 273.15 2-Buten-1-ol, 0.506 (3-methylallyl alcohol); 1.007 0.502 276.65 C₄H₈O; [6117-91-5] 280.45 0.980 0.495 0.488 283.15 283.35 0.950 0.487

Smoothing equation: $\ln x_{\text{HCl}} = 66.565 - 91.027/(\text{T}/100) - 33.757 \ln(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 3.22×10^{-4}

0.938

0.851

0.484

0.460

0.453

284.55

291.35

293.15

^{*} calculated by the compiler.

^{**} smoothing equations and smoothed values were calculated by H.L. Clever.

ORIGINAL MEASUREMENTS:

COMPONENTS:	- [ORIGINAL ME	ASUREMENTS	•
<pre>(1) Hydrogen chloride; HCl; [7647-01-0]</pre>		Cook, T.M.		
(2) Alkenols and alkynols		Thesis, <u>196</u> University		
EXPERIMENTAL VALUES:		Mole ratio IC1 ^{/n} alcohol	Mole* fraction *HCl	Smoothed** mole fraction *HCl
[627-27-0] 4 8 27	33.15 70.15 73.15	1.005	0.501	0.518 0.493
27 27 28	74.45 77.55 32.75	0.960 0.923 0.882	0.490 0.480 0.469	
29 29	33.15 90.35 92.75 93.15	0.811 0.790	0.448 0.441	0.467
Smoothing equation: $\ln x_{\text{HCl}} = 10$ Standard error in x_{HCl} about the		- 13.408/(T/ession line =	'100) - 6.3 : 1.17 × 10	
2-Methyl-2-propen-1-ol; 26 C ₄ H ₈ O; [513-42-8] 27	3.15	1.40	0.583	0.594
27 28	73.15 77.65 83.15 83.65	1.31	0.567 0.558	0.577 0.558
29 29 29	3.15 4.05 5.65	1.16 1.15	0.537 0.535	0.539
	9.25 13.15	1.11	0.526	0.519
Smoothing equation: $\ln x_{HC1} = 6$. Standard error in x_{HC1} about the	298 - regre	8.152/(T/10 ession line =	00) - 3.845 1.31 × 10	ln(T/100)
[39161-19-8]	3.15 5.55 3.15	1.115	0.527	0.532 0.508
28 28	5.25 0.05 2.45	1.009 0.967 0.939	0.502 0.492 0.484	
28	3.15 5.55 3.15	0.910	0.476	0.482 0.456
Smoothing equation: $\ln x_{\text{HCl}} = 11$ Standard error in x_{HCl} about the	.093 regre	- 14.188/(T/ ssion line =	(100) - 6.5 : 1.23 × 10	44 ln(T/100)
[821-09-0] 25 26	2.15 3.15 3.15 3.15	1.426	0.588	0.584 0.545 0.511
27 27 28	5.45 8.75 9.95	1.018 0.979 0.968 0.949	0.504 0.495 0.492 0.487	
28	3.15 6.25 3.15	0.905	0.475	0.483 0.459
Smoothing equation: $\ln x_{\text{HCl}} = -4$ Standard error in x_{HCl} about the	.807 regre	+ 7.868/(T/1 ssion line =	00) + 1.25 3.58 × 10	0 ₋₄ ln(T/100)

^{*} calculated by the compiler.

** smoothing equations and smoothed values were calculated by H.L. Clever.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0]	Cook, T.M.
(2) Alkenols and alkynols	Thesis, 1966 University of London

		Mole ratio C1 ^{/n} alcohol	Mole* fraction *HCl	Smoothed** mole fraction [*] HCl
3-Hexen-1-ol; C ₆ H ₁₂ O; [2305-21-7]	263.15 263.55	1.154	0.536	0.537
	273.15	_		0.510
	281.45	0.953	0.488	
	283.15		0.485	0.484
	288.05		0.473	
	293.15	0.849	0.459	0.459
Smoothing equation: $\ln x_{HCl}$ Standard error in x_{HCl} about	= 5.733 the regre	- 6.804/(T/1 ssion line =	00) - 3.89 : 9.91 × 10	6 ln(T/100)
3-Hepten-1-ol; C ₇ H ₁₄ O;	263.15			0.538
[10606-47-0]	263.55	1.161	0.537	
	272.75	1.056	0.514	
	273.15			0.513
	281.85	0.963	0.491	
	282.75	0.956	0.489	i
	282.85	0.955	0.488	
	283.15			0.488

Smoothing equation: $\ln x_{\rm HCl}$ = 8.160 - 10.185/(T/100) - 5.074 $\ln({\rm T}/100)$ Standard error in $x_{\rm HCl}$ about the regression line = 3.76 \times 10⁻⁴

EXPERIMENTAL VALUES:

^{*} calculated by the compiler.
** smoothing equations and smoothed values were calculated by H.L. Clever.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Alkanediols

EVALUATOR:

H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA

1983, July

CRITICAL EVALUATION:

The solubility of hydrogen chloride in alkanediols.

Hydrogen chloride + 1,2-Ethanediol; C₂H₆O₂; [107-21-1]

Three laboratories have reported solubility data on the system. O'Brien, Kenny and Zeurcher (ref. 1) studied the HCl + CH2OHCH2OH system at 298.15 K and HCl partial pressure range of 0.081 to 43.0 kPa. Matuzak (ref. 2) reported one solubility value at 310.9 K and 99.1 kPa partial pressure. Gerrard and Macklen (ref. 3) reported the solubility at a partial pressure of 101.3 kPa and ten temperatures between 273.15 and 319.65 K. All of the data are classed as tentative although, as discussed below, there is evidence the O'Brien et al. solubility data may be too small.

The one value of Matuszak at 310.9 K, when corrected to 101.3 kPa pressure by Henry's law, agrees exactly with the 310.9 K solubility value calculated from the smoothed data equation obtained from Gerrard and Macklen's data. This tends to support the reliability of the results of both laboratories.

At 298.15 K a graph of $\ln p_1$ vs. either $\ln x_1$ or $\ln (n_1/n_2)$ shows a poor correlation between the results of O'Brien et al. and of Gerrard and Macklen. If the Gerrard and Macklen value at 101.3 kPa is correct then the O'Brien et al. solubility values appear to be in error by being too small. Selected values of the data of O'Brien et al. at partial pressures of 0.081, 0.253, 0.324 and 3.67 kPa (0.0008, 0.0025, 0.0032 and 0.0357 atm) could form a line that would correlate with Gerrard and Macklen's value, but the other nine values, which fall on a satisfactory straight line, are too small. There is not enough evidence to discredit the results of O'Brien et al. but their data should be used with caution until confirmed by additional experiments.

Hydrogen chloride + Alkanediols (Table 1)

Gerrard and Macklen (ref. 3) report the solubility of hydrogen chloride in six alkanediols, including the 1,2-ethanediol discussed above, at 101.3 kPa hydrogen chloride partial pressure over the temperature interval of about 273 to 323 K.

The data were fitted by the method of least squares to an equation of the type ${\ensuremath{\mathsf{T}}}$

$$\ln x_1 = A_1 + A_2/(T/100 \text{ K}) + A_3 \ln(T/100 \text{ K})$$

The equation and a table of smoothed mole fraction solubility data are included on each data sheet. Table 1 contains the smoothed solubility values in mole fraction (x_1) and mole ratio (n_1/n_2) at temperatures of 273.15, 293.15 and 323.15 K and a partial pressure of 101.3 kPa along with the name and formula of each alkanediol.

Although only a limited number of solvents were studied one can observe several trends between solubility and structure. For alkanediols, ${^{\rm C}_{\rm n}}{^{\rm H}_{\rm 2n+2}}{^{\rm O}_{\rm 2}}$, the solubility in l,n-alkanediols increases as n increases. Within the butanediols the solubility decreases as the hydroxy groups are spaced nearer together. Thus the solubility decreases in the order

1,4-Butanediol > 1,3-Butanediol > 2,3-Butanediol

COMPONENTS: (1) Hydrogen chloride; HC1; [7647-01-0] (2) Alkanediols EVALUATOR: H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA 1983, July

CRITICAL EVALUATION:

Table 1. Tentative mole ratio (n_1/n_2) and mole fraction (x_1) solubilities of hydrogen chloride in alkanediols at a partial pressure of 101.325 kPa and temperatures of 273.15, 293.15 and 323.15 K.

Solvent Name	Solubility of HCl in Alkanediols						
and Structure	273.	273.15 к		293.15 К		313.15 K	
	$\frac{n_{1}/n_{2}}{2}$	x_1	n_1/n_2	x 1	n_1/n_2	x_1	
1,2-Ethanediol CH ₂ OHCH ₂ OH							
[107-21-1]	1.037	0.509	0.815	0.449	0.637	0.389	
1,3-Propanedio1 CH ₂ OHCH ₂ CH ₂ OH [504-63-2]	1.132	0.531	0.873	0.466	0.689	0.408	
1,3-Butanediol CH ₂ OHCH ₂ CHOHCH ₃ [107-88-0]	1,597	0.615	1.217	0.549	0.942	0.485	
1,4-Butanedio1 CH ₂ OHCH ₂ CH ₂ CH ₂ OH [110-63-4]	1.674	0.626	1.353	0.575	1.088	0.52	
2,3-Butanediol CH ₃ CHOHCHOHCH ₃ [513-85-9]	1.288	0.563	0.961	0.490	0.745	0.42	
1,5-Pentanedio1 CH ₂ OHCH ₂ CH ₂ CH ₂ CH ₂ OH [111-29-5]			1.506	0.601	1.212	0.548	

- O'Brien, S. J.; Kenny, C. L.; Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.
- 2. Matuszak, M. P. U. S. Patent 2,520,947 Sept. 5, 1950.
- 3. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1960, 10, 57.

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen chloride; HCl; O'Brien, S. J.; Kenny, C. L.; [7647-01-0] Zeurcher, R. A. (2) 1,2-Ethanediol or ethylene J. Am. Chem. Soc. 1939, 61, glycol; C₂H₆O₂; [107-21-1] 2504 - 2507. VARIABLES: PREPARED BY: T/K: 298.15 W. Gerrard P/kPa: 0.081 - 42.96 (0.0008 - 0.424 atm)

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Mol Ratio	Mol Fraction
	p ₁ /atm	$m_1/mol kg^{-1}$	n ₁ /n ₂	x_1
298.15	0.0008	1.33	0.0372	0.0359
	0.0025	2.27	0.0636	0.0598
	0.0032	2.45	0.0686	0.0642
	0.0046	2.72	0.0762	0.0708
	0.0074	3.02	0.0846	0.0780
	0.0075	3.07	0.0860	0.0792
	0.0086	3.11	0.0871	0.0801
	0.0079	3.13	0.0877	0.0806
	0.0357	4.66	0.130	0.115
	0.135	6.57	0.184	0.155
	0.139	6.63	0.186	0.157
	0.172	6.92	0.194	0.162
	0.424	8.78	0.246	0.197
	(1.00			0.249) 1

 $^{^{1}}$ Value from the compiler's graphical extrapolation of the plot of the above x_{1} vs. p_{1} data.

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are almost identical to those of Saylor (1). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) 1,2-Ethanediol. Eastman Kodak Co. Used as received.

0.02

ESTIMATED ERROR: $\delta T/K =$

REFERENCES:

Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1,2-Ethanediol or ethylene glycol; C₂H₆O₂; [107-21-1] VARIABLES: T/K = 310.9 p/kPa = 99.06 (743 mmHg) ORIGINAL MEASUREMENTS: Matuszak, M. P. U. S. Patent 2,520,947 September 5, 1950 Chem. Abstr. 1950, 44, 11044g W. Gerrard

EXPERIMENTAL VALUES:

Tempe	rature	Pressure	HCl Absorbed ¹	Mol Ratio	Mol Fraction
t/ ⁰ F	T/K	p/mmHg	g component 2	n_1/n_2	x_{1}
100	310.9	743	37.0	0.631	0.387

The author's statement was "HCl absorbed, weight per cent of oxycompound."

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No information.	No information.
	,
	ESTIMATED ERROR:
	REFERENCES:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Diols

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E.D.

J. Appl. Chem. 1960, 10, 57-62.

(2) DIOIS

VARIABLES: T/K: See below

Total P/kPa : 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

	T/K	Mole ratio	Mole* fraction ^X HCl	Smoothed** mole fraction *HC1
1,2-Ethanediol, (ethylene	273.15 276.25		0.509 0.500	0.509
glycol); C ₂ H ₆ O ₂ ; [107-21-1]	283.15		0.500	0.479
	284.15		0.474	V.1.5
	292.95	0.816	0.449	
	293.15			0.449
	295.35		0.442	
	301.25		0.425	
	303.15			0.419
	308.55		0.403	
	311.15		0.396	
	313.15			0.389
	317.85		0.374	
	319.65		0.369	
	323.15			0.360

Smoothing equation: $\ln x_{\rm HC1}$ = 14.252 - 18.247/(T/100) - 8.208 $\ln(\text{T/100})$ Standard error in $x_{\rm HC1}$ about the regression line = 1.18 \times 10⁻³

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and procedure were described by Gerrard and Macklen (1). The amount of gas absorbed by a measured weight of solvent was determined by re-weighing the bubbler tube to constant weight. the measured total pressure was barometric, very nearly 101.325 kPa. The temperature control was within 0.1 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Diols: purified by known methods; purity attested by boiling point and refractive index; distilled into the absorption vessel just before use.

ESTIMATED ERROR:

 $\delta x_{HC1}/x_{HC1} = \pm 0.005 \text{ to } 0.025$

REFERENCES:

Gerrard, W.; Macklen, E.D.
 J. Appl. Chem. <u>1956</u>, 6, 241.

0.425

COMPONENTS:		ORIGINAL M	EASUREMENTS	:
(1) Hydrogen chloride; HCl; [7647-01-0]		Gerrard, W.	.; Macklen,	E.D.
(2) Diols		J. Appl. Ci	nem. <u>1960</u> ,	10, 57-62.
VARIABLES:		PREPARED BY	<i>Y</i> :	
T/K: See below Total P/kPa : 101.325 (1 atm)		W. Ge	errard	
EXPERIMENTAL VALUES:		I		
	T/K	Mole ratio ⁿ HCl ^{/n} diol	Mole* fraction ^x HCl	Smoothed** mole fraction *HCl
1,3-Propanediol, (propylene glycol); C ₃ H ₈ O ₂ ; [504-63-2]	273.15 277.65 280.35	1.068	0.532 0.516 0.509	0.531
	282.65 283.15 290.25		0.498 0.475	0.498
	293.15 297.45	0.833	0.454	0.466
	306.65 310.85	0.705	0.428 0.413	
	313.15	0.652	0.395	0.408
	303.15 323.15			0.436 0.381
Smoothing equation: $\ln x_{HCl} = $ Standard error in x_{HCl} at	7.204 - oout the	- 8.297/(T/10 e regression	00) - 4.776 line = 1.42	ln(T/100) 2 × 10 ⁻³
1,3-Butanediol, (1,3-butylene glycol); C ₄ H ₁₀ O ₂ ; [107-88-0]	273.15 279.65 281.25	1.453 1.430	0.592 0.588	0.615
	283.15 285.65	1.353	0.575	0.582
	293.15 293.35		0.550	0.549
	298.65 300.15	1.128	0.530 0.526	
	303.15 303.75	1.049	0.512	0.516
	307.65 310.35	1.013	0.503	
	313.15 318.15	0.884	0.469	0.485
	323.15 326.35	0.801	0.445	0.454
İ	333 15			0.425

Smoothing equation: $\ln x_{\rm HCl}$ = 9.533 - 11.646/(T/100) - 5.728 $\ln(\text{T/100})$ Standard error in $x_{\rm HCl}$ about the regression line = 1.39 \times 10⁻³

333.15

^{*} calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Macklen, E.D.		
(2) Diols	J. Appl. Chem. <u>1960</u> , 10, 57-62.		
EXPERIMENTAL VALUES:			
T/K	Mole ratio Mole* Smoothed** n HCl $^{/n}$ diol fraction mole fraction x HCl x HCl		
2,3-Butanediol, (2.3-butylene 273.15	0.563		
$[g1yco1]; C_AH_{10}O_2; [513-85-9] 275.05$	1.246 0.555		
276.85			
283.15			
284.15	1.088 0.521		
288.85 293.15			
294.55			
302.75			
303.15 308.25			
313.15			
314.45			
321.05 323.15			
Smoothing equation: $\ln x_{\text{HCl}} = 5.667$ Standard error in x_{HCl} about the	- $5.930/(T/100)$ - $4.051 \ln(T/100)$ e regression line = 1.74×10^{-3}		
1,4-Butanediol, 273.15			
(tetramethylene glycol); 280.55			
C ₄ H ₁₀ O ₂ ; [110-63-4] 283.55 283.15			
284.65	1.491 0.599		
288.25 290.35			
290.33			
293.35			
294.35 298.35			
303.15			
304.75			
312.55 313.15			
Smoothing equation: $\ln x_{\text{HCl}} = 10.370$ Standard error in x_{HCl} about the	- 13.365/(T/100) - 5.917 $ln(T/100)$ e regression line = 7.56 × 10 ⁻⁴		
1,5-Pentanediol, 283.15			
(pentamethylene glycol); 286.55			
C ₅ H ₁₂ O ₂ ; [111-29-5] 291.75 293.15			
298.95	1.421 0.587		
303.15			
312.35 313.15			
316.95	1.163 0.538		
322.35			
323.15 332.75			
333.15			
Smoothing equation: $\ln x_{HC1} = 2.064$ Standard error in x_{HC1} about the	- 1.545/(T/100) - 1.903 $ln(T/100)$ e regression line = 2.21 × 10^{-3}		
* calculated by the compiler			
** smoothing equation and smoothed values were calculated by H.L. Clever			

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Aromatic and alicyclic alcohols

FVALUATOR.

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January 1989

CRITICAL EVALUATION:

Solubility of Hydrogen Chloride in Aromatic and Alicyclic Alcohols

Gerrard & Macklen (1) measured solubilities in benzenemethanol, phenylethanol and phenyl-1-propanol over temperature ranges at a total pressure of 1.013 bar. The contribution of the vapor pressure of the solvent to the total pressure was negligible under the conditions of the measurements and data may be taken to correspond to solubilities at a partial pressure of 1.013 bar. Measurements are self-consistent and correspond to a small increase in mole fraction solubility with increase in carbon number. No other data for these systems are available for comparison.

Mole fraction solubilities at 293.15 K and a partial pressure of 1.013 bar.

Methanol	0.434	(evaluated value)
Ethanol	0.462	(evaluated value)
Propanol	0.463	(evaluated value)
Benzenemethanol	0.412	(smoothed data based upon
Phenylethanol	0.425	measurements by
Phenyl-1-propanol	0.446	Gerrard & Macklen)

Gerrard & Macklen (2) also measured solubilities in cyclohexanol and in 2-methylcyclohexanol at a total pressure equal to barometric pressure over the temperature ranges 280.95 K to 314.75 K and 277.85 K to 321.85 K respectively. Both sets of measurements are self-consistent with mole fraction solubilities at the same temperature very close to each other. The smoothed value at 293.15 K for cyclohexanol is 0.507 and that for 2-methylcyclohexanol in 0.510. Under the conditions of measurement mole fraction solubilities for a total pressure of 1.013 bar are likely to be close to those at a partial pressure of gas of 1.013 bar. The corresponding smoothed value for solubility in 1-hexanol from measurements by these authors is 0.468. The data for cyclohexanol and 2-methylcyclohexanol may be accepted on a tentative basis.

- 1. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1956, 6, 241 244.
- 2. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1959, 9, 85 88.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Macklen, E.D. J. Appl. Chem. 1959, 9, 85-88.
(2) Cyclic alkanols	
VARIABLES:	PREPARED BY:
T/K: See below Total P/kPa : 101.325 (1 atm)	W. Gerrard

EXPERIMENTAL VALUES:	T/K	Mole ratio HC1 ^{/n} alcohol	Mole* fraction *HCl	Smoothed** mole fraction *HC1
Cyclohexanol: C.H. O:	273.15			0.531
Cyclohexanol; C ₆ H ₁₂ O; [108-93-0]	280.95	1.051	0.512	
	283.15			0.507
	285.15	1.013	0.503	
	289.55	0.968	0.492	
	293.15			0.484
	299.75	0.881	0.468	
	303.15			0.460
	307.85	0.815	0.449	
	313.15			0.437
	314.75	0.768	0.434	
Smoothing equation: $\ln x_{HC}$ Standard error in x_{HC}	1 = 6.643 - 1 about the	8.239/(T/100 regression	0) - 4.239 line = 4.73	ln(T/100) x × 10 ⁻⁴
2-Methylcyclohexanol;	273.15			0.533
C ₇ H ₁₄ O; [583-59-5]	277.85		0.523	
7.140, (300 5) 01	283.15		*****	0.510
	285.05	1.026	0.506	
	293.15			0.487
	296.05	0.925	0.481	
	302.35	0.869	0.465	
	303.15			0.463
	312.55	0.792	0.442	
	313.15			0.439
	321.85	0.722	0.419	
	323.15			0.416

Smoothing equation: $\ln x_{HC1} = 9.687 - 12.541/(T/100) - 5.698 \ln(T/100)$ Standard error in x_{HC1} about the regression line = 6.72 × 10⁻⁴

- * calculated by the compiler
 ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Alcohols: purified, distilled, and attested by physical constants.

ESTIMATED ERROR: $\delta x_{HC1}/x_{HC1}$ $= \pm 0.01$

REFERENCES:

1. Gerrard, W.; Macklen, E.D. J. Appl. Chem. 1956, 6, 241.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzenemethanol or benzyl alcohol; C₇H₈O; [100-51-6]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1956, 6, 241-244.

VARIABLES:

T/K: 278.65 - 316.85 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: -

т/к	Mole Ratio nHCl/nC7H8O	Mole Fraction
278.65 285.25 293.05 300.55 307.75 316.85	0.875 0.793 0.720 0.657 0.597	0.467 0.422 0.419 0.396 0.374 0.344

The mole fraction solubility values were calculated by the compiler.

Smoothed Data: $\ln x_1 = -3.085 + 6.441/(T/100)$

Standard error about regression line = 9.91×10^{-3}

T/K	Mole Fraction
	<u> </u>
273.15	0.483
283.15	0.445
293.15	0.412
303.15	0.383
313.15	0.358
323.15	0.336

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an (1) Hydrogen chloride. Self preall-glass apparatus.

The all glass absorption vessel (50 cm3) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- pared and dried.
- (2) Benzenemethanol or benzyl alcohol. High-grade specimen was distilled and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

 $\delta x_1/x_1 = 0.01$

- Hydrogen chloride; HCl; [7647-01-0]
- (2) Phenylethanol; C₈H₁₀O; [1321-27-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1956, 6, 241-244.

VARIABLES:

T/K: 278.35 - 315.85 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

T/K Mole Ratio Mole Fraction nHCl/nC8H100 278.35 0.878 0.468 287.05 0.796 0.443 292.35 0.747 0.428 299.25 0.686 0.407 309.35 0.608 0.378 315.85 0.565 0.361			
287.05	т/к		
	287.05 292.35 299.25 309.35	0.796 0.747 0.686 0.608	0.443 0.428 0.407 0.378

The mole fraction solubility values were calculated by the compiler.

Smoothed Data: $\ln x_1 = 12.392 - 15.658/(T/100) - 7.351 \ln (T/100)$

Standard error about regression line = 6.09×10^{-4}

T/K	Mole Fraction x 1
273.15	0.483
283.15	0.454
293.15	0.425
303.15	0.396
313.15	0.368
323.15	0.341

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen chloride was generated in an (1) Hydrogen chloride. Self preall-glass apparatus.

The all glass absorption vessel (50 cm3) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- pared and dried.
- (2) Phenylethanol. High-grade specimen was distilled and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

 $\delta x_1/x_1 = 0.005$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Phenyl-1-propanol; C₉H₁₂O; [1335-12-2]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1956, 6, 241-244.

VARIABLES:

T/K: 280.15 - 317.75 T/K: 280.15 - 317.75 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

T/K	Mole Ratio nHCl/nC ₉ H ₁₂ O	Mole Fraction x l
280.15 286.55 293.55 300.55 303.85 310.25 317.75	0.922 0.860 0.801 0.740 0.714 0.659 0.601	0.480 0.462 0.445 0.425 0.417 0.397 0.375

The mole fraction solubility values were calculated by the compiler.

Smoothed Data: $\ln x_1 = 19.778 - 26.354/(T/100) - 10.781 \ln (T/100)$

Standard error about regression line = 1.03×10^{-3}

т/к	Mole Fraction
273.15	0.495
283.15	0.472
293.15	0.446
303.15	0.418
313.15	0.389
323.15	0.360

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an (1) Hydrogen chloride. all-glass apparatus.

The all glass absorption vessel (50 $\,\mathrm{cm}^3)$ comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

- SOURCE AND PURITY OF MATERIALS;
- Self prepared and dried.
- (2) Phenyl-1-propanol. High-grade specimen was distilled and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

 $\delta x_1/x_1 = 0.005$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Ethers and Miscellaneous Solvents Containing Carbon, Hydrogen and Oxygen.

EVALUATOR:

Peter G. T. Fogg
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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Ethers and Miscellaneous Solvents Containing Carbon, Hydrogen and Oxygen.

The solubility in a wide range of alkyl ethers has been measured by Gerrard and his co-workers (1-3) over the temperature range 197 K to 301 K at a total pressure equal to barometric pressure. The solubility in 1-methoxybutane has also been measured over a total pressure range of 7 kPa to 226 kPa at temperatures 233.45 K to 286.15 K.

Mole fraction solubilities are appreciably higher than values corresponding to the Raoult's law equation i.e.

mole fraction = partial pressure / vapor pressure of liquid HCl

The variations of mole fraction solubility with pressure at a constant temperature for 1-methoxybutane may be compared with the variations expected from the Margules equation i.e.

$$P_{total} = P_g^{\circ} x_g^{\circ} \exp(\alpha x_s^2) + P_s^{\circ} x_s^{\circ} \exp(\alpha x_g^2)$$

where 'g' refers to the gas and 's' refers to the solvent. P° and P° are the vapor pressures of pure liquefied gas and solvent respectively.

The value of α may be found by substitution in the equation of the mole fraction solubility for one value of the total pressure at a particular temperature. The equation may then be used to draw the variation of mole fraction solubility with pressure which follows from the equation. As may be seen from fig. 1 the experimental data for 1-methoxybutane approximate to the curve from the Margules equation but do not exactly coincide with it except at the data point used to calculate the value of α . The curve does not pass through the origin because the pure solvent has a small vapor pressure at this temperature. Both the experimental measurements and the theoretical curve indicate that, at total pressures of about 101.3 kPa, there is relatively small change in mole fraction solubility with change of pressure, whereas at very low total pressures the change is relatively large.

Solubilities in other dialkyl ethers have not been measured over pressure ranges but the evaluator considers that the Margules equation is likely to give an approximate prediction of behaviour which is valid for the comparison of one system with another.

At the higher temperatures of measurement the lower ethers are appreciably volatile. 1,1'-Oxybisethane has a vapor pressure of about 75 kPa at 299 K, the highest temperature of measurement of solubility in this ether. According to Kapoor et al. the mole fraction solubility of hydrogen chloride in this solvent at 299.55 K and a total pressure of 101.3 kPa is 0.357. It follows from the Margules equation applied to this system that a saturated solution under these conditions is likely to have a partial pressure of hydrogen chloride of 82.3 kPa with the partial pressure of 1,1'-oxybisethane reduced to 19.0 kPa. It also follows from the Margules equation that the mole fraction solubility for a partial pressure of hydrogen chloride of 101.3 kPa would be about 0.374 compared with the solubility of 0.357 for a total pressure of 101.3 kPa. This difference is small despite the very high volatility of the pure solvent.

At lower temperatures for this solvent and at this temperature for higher ethers the difference between mole fraction solubility at a total pressure of 101.3 kPa and mole fraction solubility at this partial pressure is likely to be much smaller. At 283.95 K the vapor pressure of pure 1,1'-oxybisethane is about 40 kPa and experimental value of the mole fraction solubility of hydrogen chloride at a total pressure of 101.3 kPa is 0.475. The partial pressure of 1,1'-oxybisethane over the saturated solution is likely to be about 2.2 kPa and the corresponding value of mole fraction solubility for a partial pressure of 101.3 kPa to be about 0.477.

The evaluator considers that, for the purpose of general comparison of these sets of data for dialkyl ethers at a total pressure of 101.3 kPa, either one with another or with data for other systems, the contribution of the vapor pressure of the ether to the total pressure may be disregarded. Solubilities at

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Ethers and Miscellaneous Solvents Containing Carbon, Hydrogen and Oxygen.

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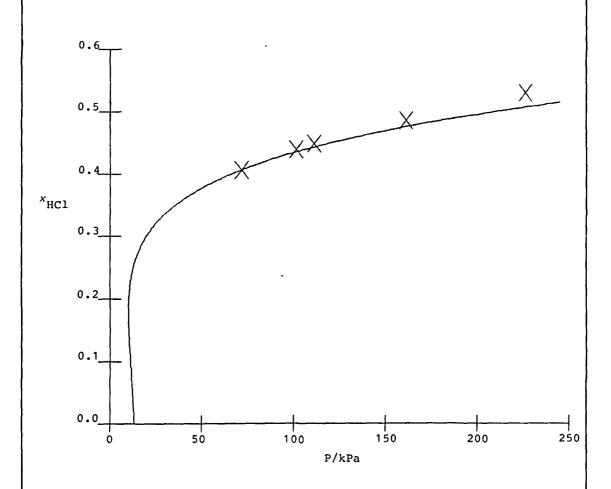


Figure 1

Experimental measurements of the variation with total pressure of the mole fraction solubility of hydrogen chloride in 1-methoxybutane (marked by crosses) and the variation from the Margules equation (shown as a curve).

Temperature = 286.15 K

(see ref. 3)

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a total pressure of 101.3 kPa may be considered to differ from solubilities at a partial pressure of 101.3 kPa by less than the experimental error in measurement.

The general pattern of data for a total pressure of 101.3 kPa is consistent but unusual. Over much of the temperature range the variation with temperature of mole fraction solubilities in the various ethers is almost linear. The solubility curves are very close to one another and there is very little change in pattern on going from the lower alkyl ethers with carbon number of four to higher ones with carbon number of 16. Mole fraction solubilities in 2-ethoxybutane are slightly higher than in the other alkyl ethers. At 273.15 the smoothed value given by Kapoor et al.(3) is 0.574 compared with the smoothed value of 0.537 for dissolution in 1-ethoxybutane.

Kapoor et al.(3) repeated some of the earlier measurements of the solubility in 1-methoxybutane, 1,1'-oxybispropane, 1,1'-oxybisbutane 1,1'-oxybispentane, and 1,1'-oxybis[3-methyl]-butane made with similar apparatus in the same laboratory by Gerrard & Macklen (1) or Ahmed, Gerrard & Maladkar (2). In all cases there is agreement within about 2%. Some measurements of solubility in alkyl ethers have been reported from other laboratories. Perkin's measurements (4) of solubility in 1,1'-oxybis[3-methyl]-butane over the temperature range 273.15 K to 298.15 K are close to the later measurements by Gerrard & Macklen and by Kapoor et al. The single measurement reported by Matuszak (5) at 297.6 K is significantly lower than solubilities reported by other authors and is rejected by the evaluator.

The evaluator recommends the following equation for solubilities in 1,1'-oxybis[3-methyl]-butane at a total pressure of 101.3 kPa for the temperature range 272.9 K to 307.45 K which is based upon experimental data obtained within this range:

 $\ln x_{HC1} = 299.563 - 11887.3/(T/K) - 45.7625 \ln(T/K)$

The standard deviation in values of $x_{\rm HCl}$ is 0.0081.

The data obtained by Kapoor $et\ al.$ should be used for solubilities at lower temperatures down to 194.65 K. These data are probably reliable but there are no other measurements at very low temperatures for comparison.

The solubility in 1,1'-oxybisethane at a total pressure equal to barometric pressure was also measured by Kapoor $et\ al.(3)$ over the temperature range 201.15 K to 299.55 K, by Schunke (6) over the range 263.95 K to 303.15 K, by Ionin & Shverina (7) and by Chesterman (8) at 298.15 K and also by Mirsaidov $et\ al.$ (9) at 273.15 K and 298.15 K. As explained above, the solubility in ethers is relatively insensitive to changes in pressure at pressures close to 101.3 kPa. Variation in barometric pressure from one set of data to another does not cause significant changes in solubility. Data presented by Kapoor $et\ al.$, by Schunke and by Chesterman agree fairly closely. The solubilities published by Mirsaidov $et\ al.$ are appreciably lower and the value given by Ionin & Shverina higher than values given by other authors. The following equation based upon measurements by Kapoor $et\ al.$, by Schunke and by Chesterman is recommended for solubilities in the range 260 K to 303 K:

 $\ln x_{HC1} = 75.090 - 2391.9/(T/K) - 11.940 \ln(T/K)$

The standard deviation in values of $x_{\rm HCl}$ is 0.0177.

Data published by Kapoor $et\ al.$ for lower temperatures down to 201.15 K are likely to be reliable. No other measurements down to this temperature are available for comparison.

Ionin & Shverina (7) measured the solubility in 1,1'-oxybisbutane at 298.15 K and a total pressure equal to barometric pressure. Their value of the fraction solubility is 0.447 which is high compared with the value of 0.39 from measurements by Kapoor et al.(3), and by Gerrard & Macklen (1) which are in

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satisfactory agreement where the two temperature ranges overlap. Ionin & Shverina also measured the solubility in 2,2'-oxybisbutane at 298.15 K. No other measurements of the solubility of hydrogen chloride in this solvent are available for comparison. In view of the uncertainty cast on their measurement of solubility in 1,1'-oxybisethane and in 1,1'-oxybisbutane published in the same paper the value for 2,2'-oxybisbutane should be treated with caution.

Gerrard & Macklen (1) measured the solubility of hydrogen chloride in (methoxymethyl)benzene, (ethoxymethyl)benzene, (butoxymethyl)benzene and 1,1'-[oxybis(methylene)]bisbenzene at total pressures equal to barometric pressure in the temperature range 273.15 K to 312.95 K. The measurements are self-consistent and likely to be reliable but no other measurements of solubility in these solvents are available for comparison. Mole fraction solubilities are appreciably higher than given by the Raoult's law equation but the presence of the benzene rings lowers solubility relative to that in dialkyl ethers as shown below:

Table 1 Mole fraction solubility of hydrochloric acid at 283.15 K, total pressure 101.325 kPa

Solvent	*HCl	Source
(Raoult's law equation) 1,1'-Oxybisethane (Methoxymethyl)benzene (Ethoxymethyl)benzene (Butoxymethyl)benzene 1,1'-[Oxybis(methylene)]bisbenzene	0.0305 0.478 0.421 0.419 0.407 0.352	evaluator's equation (1) (1) (1) (1)
Methoxybenzene Ethoxybenzene 1-Methoxy-2-methylbenzene 1,1'-Oxybisbenzene	0.144 0.149 0.112 0.049 (298.15 K	evaluator's equation evaluator's equation (1)) (11)
Tetrahydrofuran 1,4-D1oxane	0.581 0.517	(1)

Mole fraction solubility at barometric pressure is further reduced if the benzene ring is directly attached to the ether linkage. Unlike the ethers discussed above there is, in the case of alkyl aryl ethers and diaryl ethers, significant variation in mole fraction solubility with change in pressure at pressures close to 101.3 kPa. The assumption that mole fraction solubility varies linearly with pressure to about 101.3 kPa is probably a valid approximation for many purposes.

The solubility in methoxybenzene has been measured over a pressure and temperature range by O'Brien (10). Solubility at a total pressure of 101.3 kPa has also been measured over temperature ranges by Gerrard & Macklen and by Kapoor et al. Mole fraction solubilities at a partial pressure of 101.3 kPa by extrapolation of O'Brien's data are close to values from the other two sources, corrected where necessary for the small contribution of the solvent to the total vapor pressure. The evaluator recommends the following equation for mole fraction solubilities in the temperature range 277 K to 321.65 K based upon data from the three sources:

 $\ln x_{HC1} = -217.535 + 11508.4/(T/K) + 30.9874 \ln(T/K)$

The standard deviation in values of $x_{\rm HCl}$ is 0.0506.

Measurements made down to 195.65 K by Kapoor et al. are likely to be reliable but no other data for low temperatures are available for comparison.

O'Brien & King (11) measured Henry's constants for solubility in ethoxybenzene over the temperature range 283.15 K to 298.15 K. Gerrard and Macklen reported solubilities in this solvent at a total pressure of 101.3 kPa for the range 282.75 K to 322.95 K. The two sets of data are consistent to within 6%.

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The corresponding values of mole fraction solubilities fit the following equation:

 $\ln x_{HC1} = 67.4844 - 1288.90/(T/K) - 11.4837 \ln(T/K)$

The standard deviation for values of $x_{\rm HCl}$ is 0.0020.

O'Brien & King also measured Henry's constants for dissolution of hydrogen chloride in butoxybenzene at 293.15 k and 298.15 K. No other measurements for dissolution of the gas in this solvent are available for comparison. The corresponding mole fraction solubilities for a partial pressure of 101.3 kPa are close to those for dissolution in ethoxybenzene. There is no reason to doubt their reliability, within the limits of experimental error given by the author.

Solubility in 1-methoxy-2-methylbenzene at a total pressure of 101.3 kPa over the range 273.15 K to 316.45 K was measured by Gerrard & Macklen (1). The data indicate that the presence of the methyl group adjacent to the ether linkage reduces the mole fraction solubility relative to that in methoxy- and ethoxybenzene. There is no reason to doubt the reliability of the data but no other measurements on this system are available for comparison.

The solubility in 1,1'-oxybisbenzene was measured by O'Brien & King (11) at 298.15 K and 303.15 K and by Gerrard & Macklen (1) who reported solubilities at 101.3 kPa over the temperature range 273.15 K to 323.55 K. Matuszak (5) reported the solubility at a pressure of 99.6 kPa at 307.0 K. There is poor agreement between measurements by different authors as may be seen below:

Authors	T/K	$x_{ m HCl}$ at 101.3 kPa total pressure.
Gerrard & Macklen (1)	298.15	0.0593 (interpolated)
	303.15	0.0535
	307.0	0.0496
O'Brien & King (11)	298.15	0.0486
• • •	303.15	0.0461
Matuszak (5)	307.0	0.0290

The measurement by Matuszak can be rejected because it is so much smaller than values from the other sources. Gerrard's measurements are self consistent over a range of seven temperatures and may be more reliable than those published by O'Brien but further measurements on this system are needed for confirmation.

Chlorination of dialkyl ethers lowers the solubility of hydrogen chloride. Gerrard & Macklen (1) measured the solubility in 1,1'-oxybis[2-chloroethane] at a total pressure of 101.3 kPa from 273.15 K to 311.55 K. The contribution of the vapor pressure of the solvent to the total pressure may be disregarded over this temperature range. O'Brien (10) measured solubilities over pressure ranges below barometric pressure at 293.15 K to 313.15 K. Mole fraction solubilities are appreciably higher than values from the Raoult's law equation. Linear extrapolation of O'Brien's data to a partial pressure of 101.3 kPa gives mole fraction solubilities which are greater than values from Gerrard's measurements. At 293.15 K O'Brien's value is 0.149 compared with Gerrard's value of 0.132. At 313.15 K the values are 0.0927 and 0.0766 respectively. If the variation in mole fraction solubility with partial pressure of gas approximates to the Margules equation then the above differences are partly due to errors from the linear extrapolation of solubilities to a partial pressure of 101.3 kPa. Gerrard's data are likely to be the more reliable for a partial or total pressure of 101.3 kPa.

Gerrard & Macklen (1) also measured solubilities in oxybis[chloromethane], 1-chloro-1-(2-chloroethoxy)ethane and in 1,1'-oxybis[3-chloropropane] at a total pressure of 101.3 kPa over temperature ranges. The solubility in 1-chloro-1-(2-chloroethoxy)ethane is close to that in 1,1'-oxybis[2-chloroethoxy]. The effect of the chlorine in reducing solubility of hydrogen chloride is greatest in oxybis[chloromethane] and least in 1,1'-oxybis[3-chloropropane]. No other measurements of solubility in these three ethers are available for comparison but there is no reason to doubt their reliability.

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Solubility in 1,4-dioxane at a total pressure of 101.3 kPa over the temperature range 279.65 K to 312.85 K was also measured by Gerrard & Macklen. Solubilities are close to those in dialkyl ethers under the same conditions and are likely to be relatively insensitive to changes in partial pressure at pressures close to 101.3 kPa. A measurement by Matuszak at 305.4 K and a total pressure of 99.6 kPa is equivalent to a mole fraction solubility of 0.372 under these conditions. Correction of this measurement to a partial pressure of 101.3 kPa gives a value of 0.375, on the assumption that variation of pressure with composition may be approximately represented by the Margules equation. Interpolation of Gerrard's data to give a solubility at 307.4 k and correction to a partial pressure of 101.3 kPa gives a value of the mole fraction solubility of 0.401. Measurements of the solubility in other ethers reported by Matuszak are lower than solubilities reported by other workers and, in this case also, ought to be rejected in favour of the data reported by Gerrard & Macklen.

Gerrard & Macklen (1) also measured the solubility in tetrahydrofuran at a total pressure of 101.3 kPa over the range 278.15 K to 304.35 K. The measurements show that, under the conditions of the measurement the mole fraction solubility is higher than that in any other ether for which data are available. The measurements are likely to be reliable but data from other workers are not available for comparison.

Gerrard et al.(12) measured the solubility in 1,1,1-triethoxyethane at a total pressure equal to 101.3 kPa over the range 279.15 K to 314.35 K. The mole fraction solubility is 0.731 at 279.15 K but measurements show that there is a marked decrease over this temperature range with a value of 0.322 at 314.35 K. These authors also measured solubilities under similar conditions in 1,3-benzodioxole, 2,3-dihydro-1,4-benzodioxin, 3,4-dihydro-2H-1,2-benzodioxepin, 2-methyl-1,4-benzodioxan (12) and in phenol (13). All values of mole fraction solubilities fall above the reference line corresponding to the Raoult's law equation. No other data for these compounds are available for comparison.

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- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. <u>1959</u>, 9, 85 - 88.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Ethers

ORIGINAL MEASUREMENTS:

Kapoor, K.P.; Luckcock, R.G.; Sandbach, J.A.

J. Appl. Chem. Biotech. 1971, 21, 97-100.

VARIABLES:

T/K: see below

Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

	т/к	Mole ratio ⁿ HCl ^{/n} 2	Mole* fraction ^x HCl	Authors' da	ed *HCl** from equation
Methoxyethane, (ethyl methyl ether);		2.91 2.93	0.744 0.746		0.789
С ₃ н ₈ 0; [540-67-0]	243.15 251.65 253.15	1.806	0.644		0.685 0.638

Smoothing equation: $\ln x_{\rm HC1} = -2.154 + 4.317/({\rm T}/100)$ (for use between 233.15 K and 253.15 K) Standard error in $x_{\rm HC1}$ about the regression line = 9.98 × 10⁻³

* calculated by the compiler

** smoothing equation and mole fractions from the equation were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The bubbler-tube technique described by Gerrard, Mincer and Wyvill (1) was used. For temperatures between 303 K and 253 K and LBI thermostat containing liquid paraffin was used. For temperatures less than 253 K addition of small pieces of solid carbon dioxide and manual stirring enabled the temperature to be maintained within ±1 K. For 273.15 K a slurry of ice and water was used.

For temperatures below 273.15 K it was assumed that the loss of solvent by entrainment could be ignored. After saturation at a recorded temperature, the temperature was lowered by 10 K and pyridine was carefully added drop-wise to fix the hydrogen chloride as the pyridinium salt. After treatment with water, the chloride ion content was determined by the Volhard method or by use of an automatic titrimeter.

- SOURCE AND PURITY OF MATERIALS:
 (1) Hydrogen chloride: a good
 specimen was obtained from a
 cylinder, and dried.
- (2) 1,1'-oxybisethane, methoxybenzene, 1,1'-oxybisbutane, 1,1'-oxybis[3-methyl]-butane, 1,1'-oxybispentane, 1,1'-oxybishexane and 1,1'-oxybisoctane were commercial samples. 1,1'-oxybisheptane was prepared by the sulfuric acid method. Other ethers were prepared from an alcohol, sodium and an alkylhalide. All ethers were rigorously purified and attested.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5 (253-303 K)$ = $\pm 1 (< 253 K)$

 $\delta x_{\rm HC1}/x_{\rm HC1} = \pm 0.02$

REFERENCES:

 Gerrard, W.; Mincer, A.M.A.; Wyvill, P.L. J. Appl. Chem. 1959, 9, 89.

COMPONENTS: (1) Hydrogen chloride [7647-01-0] (2) Ethers	e; HCl;		ORIGINAL M Kapoor, K. Sandbach, J. Appl. C 21, 97-100	P.; Luckc J.A. Them. Biot	ock, R.G	
EXPERIMENTAL VALUES:	m/y	Molo	M-10*	Authors'	amontho	۰. **
	T/K	Mole ratio	Mole* fraction			from
I 		ⁿ HC1 ^{/n} 2	*HCl	ⁿ HC1 ^{/n} 2	xHC1	equation
1,1'-Oxybisethane	201.15	7.45	0.882			
(diethyl ether);	203.15			6.80	0.872	0.868
C ₄ H ₁₀ O; [60-29-7]	206.15 213.15	6.08	0.859			0.851
	213.15					0.812
	233.15			3.10	0.756	0.767
	234.15	3.01	0.751	-		
	243.15					0.711
	251.15	1.982	0.665			
	253.15	4 4 7 0		1.80	0.643	0.650
	259.65	1.470	0.595			
	262.15	1.365	0.577			0.589
	263.15 273.15	1.187	0.543	1.160	0.537	0.528
	277.65	1.018	0.504	1.100	0.557	0.520
	282.65	0.955	0.488			
	283.15		*	0.930	0.482	0.471
	283.65	0.898	0.473			
	283.95	0.903				
	286.95	0.874	0.466			
	290.55	0.776	0.437			
	299.55	0.556	0.357			
Smoothing equation:		(for us	se between	203.15 K	and 283.	T/100) 15 K)
Standard error in x _{HC}	cl about t	the regres	ssion line	= 1.50 ×	10 -	
1-Methoxypropane,	203.15			5.70	0.851	0.843
(methyl propyl	204.65	5.43	0.844	3.70	0.00	0.0.5
ether); C ₄ H ₁₀ O;	213.15		• • • • • • • • • • • • • • • • • • • •			0.808
[557-17-5]	215.65	3.91	0.796			
•	223.15					0.765
	233.15	2.55	0.718	2.45	0.710	0.715
	243.15			4.5	0 500	0.663
	253.15	1 225	0 570	1.45	0.592	0.610
	255.15 263.15	1.325	0.570			0.558
	273.15	1.069	0.517	1.085	0.520	0.508
	282.65	0.913	0.477			• • • • • • • • • • • • • • • • • • • •
	283.15	0.896	0.473			
	283.15			0.896	0.473	0.461
	283.35	0.891	0.471			
	297.35	0.609	0.378			
		4.2.4.00	45 202//m/		222 1-45	(400)

Smoothing equation: $\ln x_{\rm HCl} = 13.180 - 15.283/(T/100) - 8.222 \ln(T/100)$ (for use between 203.15 K and 283.15 K) Standard error in $x_{\rm HCl}$ about the regression line = 1.78 × 10⁻²

^{*} calculated by the compiler ** smoothing equation and mole fractions from the equation were calculated by H.L. Clever

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COMPONENTS:
                                               ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl;
                                               Kapoor, K.P.; Luckcock, R.G.;
                                               Sandbach, J.A.
J. Appl. Chem. Biotech. 1971,
     [7647-01-0]
(2) Ethers
                                               21, 97-100.
EXPERIMENTAL VALUES:
                                                            Authors' smoothed x_{HC1}
                            T/K
                                                 Mole*
                                        Mole
                                        ratio fraction
                                                                                 equation
                                      n_{HC1}/n_2
                                                   ^{x}HCl
                                                             ^{n}HC1^{/n}2
                                                                        ^{x}HCl
                           230.65
                                        3.07
                                                   0.754
1-Methoxypentane,
                           233.15
                                                              2.70
                                                                         0.730
                                                                                    0.734
(methyl pentyl
           C6H14O;
                           243.15
ether);
                                                                                    0.677
[628-80-8]
                           251.65
                                        1.617
                                                   0.618
                           253.15
                                                              1.55
                                                                         0.608
                                                                                    0.621
                           263.15
                                                                                    0.568
                           273.15
                                        1.049
                                                  0.512
                                                              1.060
                                                                         0.515
                                                                                    0.518
                           273.15
                                        1.070
                                                  0.517
                           283.15
                                                              0.910
                                                                         0.476
                                                                                    0.472
                                        0.920
                           283.35
                                                   0.479
                                        0.916
                                                   0.478
                           283.35
                                                   0.476
                                        0.908
                           283.55
                           298.65
                                        0.658
                                                   0.397
Smoothing equation: \ln x_{HCl} = 10.491 - 11.691/(T/100) - 6.835 \ln(T/100)
                                       (for use between 233.15 K and 283.15 K)
Standard error in x_{\rm HCl} about the regression line = 9.52 \times 10<sup>-3</sup>
                          198.15
                                                   0.860
2-Ethoxybutane,
                                        6.14
(2-buty1 ethy1
ether); C<sub>H</sub><sub>14</sub>O;
[2679-87-8]
                                                              5.45
                                                                         0.845
                           203.15
                                                                                    0.845
                                        4.81
                                                   0.828
                           209.15
                           213.15
                                                                                    0.832
                           219.15
                                        4.00
                                                   0.800
                           223.15
                                                                                    0.803
                           233.15
                                                              3.00
                                                                         0.750
                                                                                    0.763
                                                                                    0.716
                           243.15
                           253.15
                                                              2.00
                                                                         0.667
                                                                                    0.664
                           254.15
                                        1.96
                                                   0.662
                           263.15
                                                                                    0.611
                                                                        0.574
                           273.15
                                        1.35
                                                   0.574
                                                             1.35
                                                                                    0.558
                           283.15
                                                              1.05
                                                                         0.512
                                                                                    0.506
                           284.35
                                        1.00
                                                   0.500
                                                   0.442
                           294.15
                                        0.793
Smoothing equation: \ln x_{\rm HCl} = 16.485 - 19.715/(T/100) - 9.804 \ln(\text{T}/100) (for use between 203.15 K and 283.15 K) Standard error in x_{\rm HCl} about the regression line = 1.56 \times 10<sup>-2</sup>
                                                              6.30
                                                                         0.863
1,1'-Oxybispropane,
                           203.15
                                                                                    0.858
                                        6.00
                                                   0.857
(dipropyl ether);
                           204.15
                           213.15
                                                                                    0.837
C_6H_{14}O; [111-43-3]
                          213.65
                                                   0.829
                                        4.84
                           223.15
                                                                                    0.801
                           233.15
                                                              3.00
                                                                         0.750
                                                                                    0.753
                                                   0.770
                           233.65
                                        3.35
                                                                                    0.699
                           243.15
                           253.15
                                                              1.70
                                                                         0.630
                                                                                    0.642
                           253.65
                                        1.649
                                                   0.622
                                                                                    0.584
                           263.15
                                                  0.526
                                                              1.110
                                                                         0.526
                                                                                    0.527
                           273.15
                                        1.109
                                                  0.479
                           282.65
                                        0.918
                           282.95
                                        0.901
                                                   0.474
                                                              0.920
                                                                         0.479
                                                                                    0.473
                           283.15
                                        0.900
                           283.35
                                                   0.474
                           298.35
                                        0.653
                                                   0.395
Smoothing equation: \ln x_{HCl} = 17.491 - 20.745/(T/100) - 10.486 \ln(T/100)
Standard error in x_{HC1} about the regression line = 1.10 \times 10<sup>-2</sup>
```

^{*} calculated by the compiler
** amounting agustion and mole fractions from the

^{**} smoothing equation and mole fractions from the equation were calculated by H.L. Clever

```
ORIGINAL MEASUREMENTS:
COMPONENTS:
                                            Kapoor, K.P.; Luckcock, R.G.;
(1) Hydrogen chloride; HCl;
                                            Sandbach, J.A.
J. Appl. Chem. Biotech. 1971,
     [7647-01-0]
(2) Ethers
                                            21. 97-100.
EXPERIMENTAL VALUES:
                          T/K
                                     Mole
                                              Mole*
                                                        Authors' smoothed
                                                                             from
                                     ratio
                                             fraction
                                                               data
                                   n<sub>HC1</sub>/n<sub>2</sub>
                                                x
HCl
                                                         n_{HC1}/n_2
                                                                    x<sub>HC1</sub>
                                                                            equation
                                                          6.90
                                                                    0.873
                                                                              0.881
1-Methoxyhexane,
                         203.15
                                     6.68
                                                0.870
(hexyl methyl ether); 206.15
C7H160; [4747-07-3]
                         213.15
                                     4.64
                                                0.823
                                                                              0.831
                                                                              0.778
                         223.15
                         232.15
                                     2.93
                                                0.746
                                                          2.50
                         233.15
                                                                    0.714
                                                                              0.723
                         243.15
                                                                              0.668
                         251.95
                                     1.505
                                                0.601
                         253.15
                                                          1.50
                                                                    0 600
                                                                              0.615
                         263.15
                                                                              0.564
                         273.15
                                     1.060
                                                          1.060
                                               0.515
                                                                    0.515
                                                                              0.517
                         283.15
                                     0.918
                                                0.479
                                                          0.900
                                                                    0.474
                                                                              0.472
                                     0.900
                         283.75
                                               0.474
                                                0.453
                         289.95
                                     0.827
                         297.95
                                     0.667
                                                0.400
Smoothing equation: \ln x_{HC1} = 9.712 - 10.777/(T/100) - 6.396 \ln(T/100)
                                    (for use between 203.15 K and 283.15 K)
Standard error in x_{HC1} about the regression line = 1.36 × 10<sup>-2</sup>
                         203.15
1-Propoxybutane,
                                                          6.50
                                                                    0.867
                                                                              0.862
                                     6.17
                                                0.861
(buty1 propy1 ether); 203.65
C7H160; [3073-92-5]
                         213.15
                                                                              0.834
                                     4.80
                         213.65
                                                0.828
                         223.15
                                                                              0.796
                         233.15
                                                                    0.759
                                                                              0.750
                                                          3.15
                         234.15
                                     3.24
                                                0.764
                         243.15
                                                                              0.701
                         250.45
                                     1.820
                                                0.645
                         253.15
                                                          2.00
                                                                    0.667
                                                                              0.650
                                                                              0.598
                         263.15
                                                                              0.548
                         273.15
                                     1.199
                                               0.545
                                                          1.215
                                                                    0.549
                         273.15
                                     1.223
                                                0.550
                                                0.507
                         282.75
                                     1.030
                                     1.013
                         283.65
                                                0.503
                                                                    0.505
                         283.15
                                                          1.020
                                                                              0.500
                                     0.975
                         283.95
                                                0.494
                         294.35
                                     0.821
                                                0.451
                         297.75
                                     0.750
                                                0.429
Smoothing equation: \ln x_{HCl} = 13.255 - 15.510/(T/100) - 8.139 \ln(T/100)
                                    (for use between 203.15 K and 283.15 K)
Standard error in x_{HCl} about the regression line = 1.01 \times 10<sup>-2</sup>
                         200.15
                                     6.67
                                                0.870
1-Methoxyheptane,
                                                          6.20
                                                                    0.861
                                                                              0.862
(heptyl methyl
                         203.15
ether);
[629-32-3]
            C8H18O;
                                                                              0.818
                         213.15
                                                0.812
                         214.15
                                      4.31
                         223.15
                                                                              0.769
                                                                              0.717
                                                          2.45
                                                                    0.710
                         233.15
                                     2.76
                                                0.734
                         234.15
                                                                              0.665
                         243.15
                                                0.608
                         249.65
                                     1.554
                         253.15
                                                          1.45
                                                                    0.592
                                                                              0.613
                         263.15
                                                                              0.562
                                     1.041
                                               0.510
                         273.15
                                                          1.040
                                                                    0.510
                                                                              0.515
                                     0.905
                                                0.475
                                                          0.895
                                                                    0.472
                                                                              0.469
                         283.15
                         283.35
                                     0.899
                                                0.473
                         283.55
                                     0.890
                                                0.471
                         297.15
                                     0.686
                                                0.407
Smoothing equation: \ln x_{HCl} = 10.724 - 12.136/(T/100) - 6.912 \ln(T/100)
                                    (for use between 203.15 K and 283.15 K)
Standard error in x_{\rm HCl} about the regression line = 1.36 \times 10<sup>-2</sup>
                                     ** smoothing equation
  calculated by the compiler;
    and mole fractions from the equation were calculated by H.L. Clever
```

```
COMPONENTS:
                                            ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl;
                                            Kapoor, K.P.; Luckcock, R.G.;
                                            Sandbach, J.A.
     17647-01-01
                                            J. Appl. Chem. Biotech. 1971,
(2) Ethers
                                            21, 97-100.
EXPERIMENTAL VALUES:
                          T/K
                                     Mole
                                              Mole*
                                                        Authors' smoothed
                                                                            from*
                                     ratio
                                            fraction
                                                               data
                                   n_{\rm HCl}/n_2
                                                                           equation
                                               ^{x}HCl
                                                        n_{HC1}/n_2
                                                                   ^{x}HCl
1,1'-Oxybisbutane,
                         198.15
                                     7.28
                                               0.879
                                                         6.20
                                                                    0.861
                                                                              0.873
(dibutyl ether);
                         203.15
C8H18O; [142-96-1]
                                               0.856
                         205.65
                                     5.93
                         213.15
                                                                              0.844
                         223.15
                                                                              0.802
                         230.65
                                     3.35
                                               0.770
                         233.15
                                                         2.70
                                                                    0.730
                                                                              0.750
                                     3.09
                                               0.756
                         235.15
                                     3.06
                         235.65
                                               0.754
                         243.15
                                                                              0.693
                         252.95
                                     1.59
                                               0.614
                         253.15
                                                         1.60
                                                                   0.615
                                                                             0.634
                         263.15
                                                                              0.576
                                               0.512
                                                                             0.519
                         273.15
                                                                   0.513
                                     1.048
                                                         1.055
                         283.15
                                     0.841
                                               0.457
                                                         0.850
                                                                   0.459
                                                                              0.465
                         283.35
                                     0.848
                                               0.459
                         296.15
                                     0.693
                                               0.409
                         296.55
                                     0.674
                                               0.403
Smoothing equation: \ln x_{HCl} = 16.533 - 19.420/(T/100) - 10.032 \ln(T/100)
                                    (for use between 203.15 K and 283.15 K)
Standard error in x_{HC1} about the regression line = 1.36 \times 10<sup>-2</sup>
                         232.65
                                     2.67
                                               0.728
1-Methoxyoctane,
                                                         2.55
(methyl octyl ether); 233.15
                                                                   0.718
                                                                              0.726
                         243.15
                                                                              0.682
С<sub>9</sub>H<sub>20</sub>O; [929-56-6]
                                               0.682
                         243.45
                                     2.14
                         253.15
                                                         1.45
                                                                   0.592
                                                                             0.632
                         263.15
                                                                              0.579
                         273.15
                                     1.097
                                               0.523
                                                         1.080
                                                                   0.519
                                                                             0.525
                                     0.917
                         282.15
                                               0.478
                                               0.478
                         282.45
                                     0.915
                                               0.477
                         282.65
                                     0.913
                         283.15
                                                         0.905
                                                                   0.475
                                                                              0.473
                                               0.444
                         288.65
                                     0.797
Smoothing equation: \ln x_{HC1} = 16.533 - 19.420/(T/100) - 10.032 \ln(T/100)
                                    (for use between 233.15 K and 283.15 K)
Standard error in x_{HC1} about the regression line = 1.78 \times 10<sup>-3</sup>
                                               0.872
1,1'-Oxybispentane,
                         200.15
                                     6.80
                                               0.838
(dipentyl ether);
                        209.15
                                     5.19
C<sub>10</sub>H<sub>22</sub>O, [693-65-2]
                        213.15
                                     4.91
                                               0.831
                                                                              0.833
                                                                             0.793
                         223.15
                                               0.760
                         231.15
                                     3.17
                         233.15
                                                         2.80
                                                                   0.737
                                                                             0.744
                         243.15
                                                                              0.689
                         244.15
                                     2.05
                                               0.672
                                                         1.65
                                                                   0.623
                         253.15
                                                                             0.631
                                     1.529
                         255.65
                                               0.605
                         263.15
                                     1.377
                                               0.579
                                                                             0.574
                        273.15
                                                         1.105
                                                                   0.525
                                                                             0.518
                         273.95
                                     1.086
                                               0.521
                        283.15
                                                         0.900
                                                                   0.474
                                                                             0.464
                         283.55
                                     0.894
                                               0.472
                         283.75
                                     0.879
                                               0.468
                         298.05
                                     0.614
                                               0.380
Smoothing equation: \ln x_{HCl} = 16.682 - 19.668/(T/100) - 10.091 \ln(T/100)
Standard error in x_{\rm HCl} about the regression line = 9.95 × 10<sup>-3</sup>
                                    ** smoothing equation
 calculated by the compiler;
```

and mole fractions from the equation were calculated by H.L. Clever.

ORIGINAL MEASUREMENTS: COMPONENTS: Hydrogen chloride; HCl; Kapoor, K.P.; Luckcock, R.G.; [7647-01-0] Sandbach, J.A. (2) Ethers J. Appl. Chem. Biotech. 1971, 21, 97-100. EXPERIMENTAL VALUES: T/K Mole* Authors' smoothed Mole from1 ratio fraction data n_{HC1}/n_2 n_{HC1}/n_2 equation xHC1 xHC1 1,1'-0xybis-194.65 6.31 0.863 [3-methyl]butane, 196.15 6.06 0.858 (diisoamyl ether); 203.15 5.10 0.836 0.852 C₁₀H₂₂O; [544-01-4] 209.15 4.40 0.815 0.838 213.15 223.15 0.801 231.15 2.82 0.738 233.15 0.748 2.55 0.718 243.15 0.706 244.15 1.94 0.660 253.15 1.60 0.615 0.619 263.15 0.551 272.95 1.103 0.524 1.025 273.15 0.506 0.485 283.15 0.800 0.444 0.424 288.15 0.708 0.415 293.15 0.367 0.316 303.15 306.75 0.405 0.288 307.45 0.403 0.287 313.15 0.270 Smoothing equation: $\ln x_{HC1} = 23.711 - 28.359/(T/100) - 13.984 \ln(T/100)$ (for use between 203.15 K and 313.15 K) Standard error in x_{HC1} about the regression line = 2.72 \times 10⁻³ 8.87 0.899 197.65 1-Pentyloxyhexane, 0.872 6.80 0.881 (pentyl hexyl ether); 203.15 C₁₁H₂₄O; [32357-83-8] 210.65 0.840 5.25 0.852 213.15 0.809 223.15 3.68 0.786 229.65 231.15 3.52 0.779 233.15 3.00 0.750 0.755 0.696 243.15 253.15 1.65 0.623 0.634 1.507 0.601 253.65 0.572 263.15 273.15 1.080 0.519 0.513 274.15 0.514 1.057 283.15 0.890 0.471 0.457 0.875 0.467 283.65 0.465 283.95 0.870 296.95 0.620 0.383 299.65 0.571 0.363

Smoothing equation: $\ln x_{\rm HCl} = 17.865 - 21.023/(T/100) - 10.784 \ln(T/100)$ (for use between 203.15 K and 283.15 K) Standard error in $x_{\rm HCl}$ about the regression line = 1.78 \times 10⁻²

^{*} calculated by the compiler

^{**} smoothing equation and mole fractions from the equation were calculated by H.L. Clever.

```
ORIGINAL MEASUREMENTS:
 COMPONENTS:
                                               Kapoor, K.P.; Luckcock, R.G.;
 (1) Hydrogen chloride; HCl;
                                               Sandbach, J.A.
J. Appl. Chem. Biotech. 1971,
      [7647-01-0]
 (2) Ethers
                                               21, 97-100.
                                                            Authors' smoothed
                                                 Mole*
EXPERIMENTAL VALUES:
                            T/K
                                        Mole
                                                                                 fr8m1
                                        ratio
                                                fraction
                                                                   data
                                     n_{HC1}/n_{2}
                                                                                equation
                                                  XHC1
                                                            <sup>n</sup>HC1<sup>/n</sup>2
                                                                       xHC1
1,1'-Oxybishexane,
                           198.15
                                        8.37
                                                  0.893
                           203.15
(dihexyl ether);
                                                             6.60
                                                                        0.868
                                                                                  0.874
C<sub>12</sub>H<sub>26</sub>O; [112-58-3]
                           211.65
                                        5.07
                                                  0.835
                                                                                  0.847
                           213.15
                           223.15
                                                                                  0.805
                           233.15
                                        3.03
                                                  0.752
                                                             2.85
                                                                       0.740
                                                                                  0.752
                           240.15
                                        2.67
                                                  0.728
                           243.15
                                                                                  0.694
                           253.15
                                                             1.65
                                                                        0.623
                                                                                  0.634
                           254.65
                                        1.490
                                                  0.598
                                                  0.575
                                                                                  0.573
                           263.15
                                        1.353
                                        1.109
                           273.15
                                                  0.526
                                                             1.090
                                                                       0.522
                                                                                  0.515
                           283.15
                                                             0.895
                                                                       0.472
                                        0.877
                                                  0.467
                                                                                  0.459
                           289.55
                                        0.780
                                                  0.438
                           296.95
                                        0.632
                                                  0.387
                           301.15
                                        0.561
                                                  0.359
Smoothing equation: \ln x_{HC1} = 17.576 - 20.702/(T/100) - 10.610 \ln(T/100)
      Standard error in x_{\rm HCl} about the regression line = 1.53 \times 10<sup>-2</sup>
 1,1'-Oxybisheptane,
                           201.15
                                        7.32
                                                  0.880
                           203.15
                                                             6.80
                                                                       0.872
                                                                                  0.867
 (diheptyl ether);
C<sub>14</sub>H<sub>30</sub>O; [629-64-1]
                           212.65
                                        5.11
                                                  0.836
                                                                                  0.847
                           213.15
                                                                                  0.808
                           223.15
                                                  0.789
                           226.15
                                        3.75
                           233.15
                                                             3.10
                                                                        0.756
                                                                                  0.757
                                                                                  0.699
                           243.15
                           249.65
                                        1.830
                                                  0.647
                           253.15
                                                             1.70
                                                                       0.630
                                                                                  0.636
                           263.15
                                                                                  0.573
                                                                       0.524
                                                                                  0.512
                           273.15
                                        1.076
                                                  0.518
                                                             1.100
                                                  0.476
                                                             0.905
                                                                       0.475
                           283.15
                                        0.909
                                                                                  0.454
                           296.55
                                        0.605
                                                  0.377
                                                  0.368
                           297.65
                                        0.583
Smoothing equation: ln x_{HC1} =
                                     19.856 - 23.594 / (T/100) - 11.830 ln(T/100)
                                     (for use between 203.15 K and 283.15 K)
      Standard error in x_{\rm HCl} about the regression line = 1.47 \times 10<sup>-2</sup>
1-Heptyloxyoctane,
                           200.65
                                        6.94
                                                  0.874
                                                             6.60
                                                                                  0.865
 (heptyl octyl ether);
                           203.15
                                                                       0.868
C_{15}H_{32}O; [32357-84-9] 213.15
                                                  0.836
                                                                                  0.842
                                        5.10
                                                                                  0.802
                           223.15
                                                             3.00
                           233.15
                                        3.11
                                                  0.757
                                                                       0.750
                                                                                  0.751
                                                                                  0.693
                           243.15
                                                  0.632
                           251.15
                                        1.719
                           253.15
                                                             1.70
                                                                        0.630
                                                                                  0.633
                                                  0.587
                                        1.423
                           258.65
                                                                                  0.572
                           263.15
                                        1.094
                                                  0.522
                                                             1.100
                                                                       0.524
                                                                                  0.513
                           273.15
                           282.95
                                        0.914
                                                  0.478
                           283.15
                                                             0.900
                                                                       0.474
                                                                                  0.457
                                                  0.461
                           283.95
                                        0.854
                           297.55
                                                  0.377
                                        0.605
                                                  0.373
                           298.15
                                        0.594
Smoothing equation: \ln x_{HC1} =
                                     18.334 - 21.692/(T/100) - 11.006 \ln(T/100K)
                                    (for use between 203.15 K and 283.15 K)
                                    about the regression line = 1.23 \times 10^{-2}
** smoothing equation and mole
  Standard error in xHCl calculated by the compiler
   fractions from the equation were calculated by H.L. Clever.
```

COMPONENTS:			ORIGINAL M	IEASUREMEN	TS:	
(1) Hydrogen chlorid	o. HCl.		Kapoor, K.	D . Incko	oak P.C	
[7647-01-0]	e; nci;		Sandbach,	•	ock, R.G	· • ;
(2) Ethers		į	J. Appl. C 21, 97-100		ech. <u>197</u>	<u>'1</u> ,
EXPERIMENTAL VALUES:						
	T/K	Mole	Mole*	Authors'	smoothe	ed x _{ucl} **
		ratio		da - /-		ed xHC1**
		nHC1/n2	*HCl	ⁿ HC1 ^{/n} 2	xHC1	equation
1,1'-Oxybisoctane,	198.15	9.55	0.905			
(dioctyl ether);	200.15	7.48	0.882			
C ₁₆ H ₃₄ O; [629-82-3]	203.15			7.20	0.878	0.888
	213.15 223.15					0.859 0.815
	233.15			3.20	0.762	0.760
	242.15 243.15	2.46	0.711			0.699
	253.15			1.75	0.636	0.635
	257.15	1.525				:
	257.15 263.15	1.396	0.583			0.572
	272.15	1.111	0.526			
	273.15 283.15	0.878	0.468	1.080 0.878	0.519 0.468	0.511 0.453
	283.55	0.870		0.070	0.400	0.433
	299.55	0.548	0.354			
Smoothing equation:	$ln x_{vol} =$	18.591 -	21.892/(T/	100K) - 1	1.194ln(T/100K)
(for use between 203.15 K and 283.15 K) Standard error in x_{HCl} about the regression line = 1.69 \times 10 ⁻²						
Standard error in $x_{\rm H}$	Cl about t	ne regre	ession line	= 1.69 ×	10 -	
Methoxybenzene, (anisole); C ₇ H ₈ O;	195.65 203.15	4.50	0.818	2.80	0.737	0.762
[100-66-3]	211.65	1.79	0.642	2,00	0.707	
	213.15 223.15					0.677 0.580
	231.15	0.960	0.490			0.300
	233.15			0.90	0.474	0.485
	243.15 252.65	0.478	0.323			0.395
	253.15	••••	0,323	0.50	0.333	0.317
İ	263.15			0.25	0 200	0.250
	273.15 277.15	0.228	0.186	0.25	0.200	0.195
	283.15			0.16	0.138	0.151
	286.25 295.05	0.158 0.120				
	302.35	0.100				
Smoothing equation:	וחי –	33 800	38 701//m/	100) = 21	130 154	ም/100 ነ
1		(for	use betwee	n 203.15	K and 30	(2.35 K)
Standard error	in *HCl ab	out the	regression	line = 9.	11 × 10	• 3
I						

^{*} calculated by the compiler
** smoothing equation and mole fractions from the equation were calculated
by H.L. Clever.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1,1'-Oxybisethane or diethyl ether; C₄H₁₀O; [60-29-7] VARIABLES: T/K: 263.95 - 303.15 Total P/kPa: 97.1 - 98.7 (728 - 740 mmHg) ORIGINAL MEASUREMENTS: Schunke, J. Z. Phys. Chem. 1894, 14, 331 - 345. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

T/K	Hydrogen Chloride + Diethyl Ether (Wt1 + Wt2)/g	Hydrogen Chloride Wt ₁ /g	_	Mol Ratio	Mol Fraction
263.95	1.1770 1.7330 1.4565	0.43617 0.6570 0.56757	0.3705 0.3796 0.3752 0.3751 av.	. 1.219	0.549
273.55	2.3430 1.5170 2.00	0.8395 0.53472 0.7117	0.35407 0.35246 0.35585 0.3541 av.	1.115	0.527
287.95	1.9420 1.242 1.4370	0.5402 0.34675 0.39787	0.2781 0.2792 0.2768 0.2780 av.	. 0.782	0.439
303.15	2.5890 2.7895	0.5037 0.54385	0.1945 0.1949 0.1947 av.	. 0.491	0.329

The values of mole ratio and mole fraction were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed as a slow stream through 50 cm³ of ether in a wide-necked flask of 100 cm³ capacity. The prevailing pressure was barometric, 728 - 740 mmHg (97.1 - 98.7 kPa). (101.325 kPa = 760 mmHg)

The amount of hydrogen chloride absorbed was determined by an alkali titration.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Prepared from rock salt and sulfuric acid, and dried by sulfuric acid and calcium chloride.
- (2) Diethyl ether. Purified by a standard technique and dried over sodium. It had a specific gravity of 0.72396 at 285.15 K

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybisethane or diethyl ether; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Chesterman, D. R.

J. Chem. Soc. 1935, 906 - 910.

VARIABLES:

T/K: 298.15

Total P/kPa: 101 (∿1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Observed Pressure p/mmHg	Solubility g HCL g ⁻¹ Solution	Mol Fraction x1
298.15	760	0.22	0.36

The mole fraction value was calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus was that used for the conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with standard acid solution.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P205.
- (2) Diethyl ether. Was stated to be the purest obtainable. Freed from alcohol and acetone, and dried with sodium, b.p./°C (765 mmHg) = 35.5.

ESTIMATED E	KKOK:	

EXPERIMENTAL VALUES:

<i>T</i> /K	Hydrogen Chloride	Mol Ratio	Mol Fraction
	10 ² w ₁ /wt%	n_1/n_2	x ₁
273.15	26.5	0.732	0.423
298.15	17.0	0.416	0.294

The authors labeled the HCl content as HCl, %. The compiler assumed this was weight per cent to calculate the mole ratio and mole fraction.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the liquid until the concentration remained constant. The amount dissolved was determined by an alkali titration. The final pressure was presumably a total pressure equal to the atmospheric pressure.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Obtained from its concentrated aqueous solution by treatment with concentrated sulfuric acid.
- (2) 1,1'-Oxybisethane. Not stated.

ESTIMATED ERROR:

(1) Hydrogen chloride; HCl; [7647-01-0]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E.D.

J. Appl. Chem. 1960, 10, 57-62.

(2) Ethers

COMPONENTS:

VARIABLES:

T/K: See below

Total P/kPa : 101.325 (1 atm)

PREPARED BY:

W. Gerrard

		<u> </u>		
EXPERIMENTAL VALUES:		Mole ratio HC1 ^{/n} ether	Mole* fraction *HCl	
1-Methoxybutane, (butyl methyl ether); C ₅ H ₁₂ O; [628-28-4]		1.030 0.962 0.915	0.507 0.490 0.478	0.507
5.120, [020-20-4]	283.15 285.55		0.458 0.442 0.426	0.468
Smoothing equation: $\ln \frac{x}{\text{HCl}}$ Standard error in $\frac{x}{\text{HCl}}$	= 31.559 about the	- 41.243/(T/ regression		56 ln(T/100) × 10 ⁻⁴
1,1'-0xybis propane, (dipropyl ether); C ₆ H ₁₄ O; [111-43-3]	273.15 279.05 281.75		0.536 0.513 0.503	0.536
6-14-, 1	283.15 283.75 287.55 290.45	0.970	0.492 0.478 0.463	0.496
	293.15 297.15 303.15	0.757	0.431	0.450 0.402

Smoothing equation: $\ln x_{\rm HCl}$ = 39.791 - 52.612 /(T/100) - 21.052 $\ln({\rm T}/100)$ Standard error in $x_{\rm HCl}$ about the regression line = 1.16 \times 10⁻³

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and procedure were described by Gerrard and Macklen (1). The amount of gas absorbed by a measured weight of solvent was determined by re-weighing the bubbler tube to constant weight. the measured total pressure was barometric, very nearly 101.325 kPa. The temperature control was within 0.1 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Ethers: purified by known methods; purity attested by boiling point and refractive index; distilled into the absorption vessel just before use.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ $\delta x_{HC1}/x_{HC1} = \pm 0.005 \text{ to } 0.025$

REFERENCES:

 Gerrard, W.; Macklen, E.D. J. Appl. Chem. 1956, 6, 241.

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COMPONENTS:
                                                     ORIGINAL MEASUREMENTS:
                                                     Gerrard, W.; Macklen, E.D.
       Hydrogen chloride; HCl;
       [7647-01-0]
                                                     J. Appl. Chem. 1960, 10, 57-62.
(2)
       Ethers
EXPERIMENTAL VALUES:
                                                                                     Smoothed**
                                           T/K
                                                   Mole ratio
                                                                      Mole*
                                                 n_{\rm HCl}/n_{\rm ether}
                                                                     fraction mole fraction
                                                                      x
HCl
                                                                                        ^{x}HCl
                                                      1.061
                                                                      0.515
1,1'-Oxybisbutane,
                                          273.15
                                                                                        0.511
(dibutyl ether); C8H18O;
                                                                      0.493
                                          278.35
                                                      0.971
[142 - 96 - 1]
                                          281.25
                                                      0.922
                                                                      0.480
                                          283.15
                                                                                        0.475
                                          291.25
                                                      0.762
                                                                      0.432
                                          293.15
                                                                                        0.423
                                          297.65
                                                      0.663
                                                                      0.399
                                          303.15
                                                                                        0.364
                                          303.35
                                                      0.575
                                                                      0.365
                                          310.85
                                                      0.467
                                                                      0.318
                                          313.15
                                                                                        0.303
                                          313.75
                                                      0.423
                                                                      0.297
Smoothing equation: \ln x_{\rm HCl} = 75.759 - 102.235/(T/100) - 38.813 \ln(\text{T}/100) Standard error in x_{\rm HCl} about the regression line = 3.14 \times 10<sup>-3</sup>
1,1'-Oxybispentane, (dipentyl ether); C<sub>10</sub>H<sub>22</sub>O;
                                          273.15
                                                                                        0.516
                                          278.85
                                                      0.992
                                                                      0.498
[693-65-2]
                                          283.15
                                                                                        0.480
                                                      0.901
                                                                      0.474
                                          284.15
                                          290.35
                                                      0.799
                                                                      0.444
                                          293.15
                                                                                        0.430
                                          295.85
                                                      0.709
                                                                      0.415
                                          301.05
                                                      0.632
                                                                      0.387
                                          303.15
                                                                                        0.374
                                          304.95
                                                      0.575
                                                                      0.365
                                          308.85
                                                      0.515
                                                                      0.340
                                          313.15
                                                                                        0.317
Smoothing equation: \ln x_{HC1} = 65.285 - 87.839/(T/100) - 33.625 \ln(T/100)
Standard error in x_{HC1} about the regression line = 1.30 \times 10<sup>-3</sup>
1,1'-Oxybis [3-methyl butane], 273.15
                                                      0.994
                                                                      0.498
                                                                                        0.497
(disopentyl ether); C<sub>10</sub>H<sub>22</sub>O;
                                          278.65
                                                      0.881
                                                                      0.468
[544-01-4]
                                          282.75
                                                      0.818
                                                                      0.450
                                          283.15
                                                                                        0.447
                                          286.85
                                                      0.740
                                                                      0.425
                                          290.75
                                                      0.676
                                                                      0.403
                                          293.15
                                                                                        0.386
                                          297.15
                                                      0.559
                                                                      0.359
                                          303.15
                                                                                        0.321
Smoothing equation: \ln x_{HCl} = 79.232 - 105.846/(T/100) - 40.983 \ln(T/100) Standard error in x_{HCl} about the regression line = 2.45 \times 10^{-3}
                                         279.85
Methoxybenzene,
                                                      0.182
                                                                      0.154
                                        283.15
                                                                                        0.137
(methyl phenyl ether,
anisole); C<sub>7</sub>H<sub>8</sub>O; [100-66-3]
                                         290.35
                                                      0.124
                                                                      0.110
                                         293.15
                                                                                        0.101
                                         296.15
                                                      0.103
                                                                      0.0934
                                         303.15
                                                                                        0.0785
                                        304.35
                                                      0.082
                                                                      0.0758
                                         313.15
                                                                                        0.0647
                                         313.65
                                                      0.068
                                                                      0.0637
                                         321.65
                                                      0.061
                                                                      0.0575
                                         323.15
                                                                                        0.0561
Smoothing equation: \ln x_{HC1} = -89.382 + 135.432/(T/100) + 38.016 \ln(T/100)
Standard error in x_{HC1} about the regression line = 9.29 \times 10^{-4}
 * calculated by the compiler
     smoothing equation and smoothed values were calculated by H.L. Clever
```

ORIGINAL MEASUREMENTS: COMPONENTS: Hydrogen chloride; HCl; Gerrard, W.; Macklen, E.D. (1)[7647-01-0] J. Appl. Chem. 1960, 10, 57-62. (2) Ethers EXPERIMENTAL VALUES: T/K Mole ratio Smoothed** Mole* n_{HC1}/n_{ether} fraction mole fraction x HCl x_{HCl} 0.181 1-Methoxy-2-methylbenzene, 273.15 0.153 0.152 0.147 (methyl o-tolyl ether); 277.65 0.128 $C_8H_{10}O$; [578-58-5] 283.15 0.112 0.126 0.112 284.35 288.15 0.108 0.0975 293.15 0.0860 0.0792 296.15 0.086 302.75 0.076 0.0706 303.15 0.0691 308.75 0.064 0.0602 313.15 0.0577 316.45 0.059 0.0557 323.15 0.0498 Smoothing equation: $\ln x_{\rm HCl} = -56.671 + 87.230/(T/100) + 22.744 \ln(T/100)$ Standard error in $x_{\rm HCl}$ about the regression line = 2.70 × 10⁻³ (Methoxymethyl) benzene, 273.15 0.463 278.95 0.784 0.439 (benzyl methyl ether); $C_8H_{10}O$; [538-86-3] 280.65 0.766 0.434 283.15 0.421 0.712 0.416 284.85 284.65 0.696 0.410 0.608 291.75 0.378 293.15 0.371 297.35 0.537 0.349 302.35 0.474 0.322 303.15 0.318 Smoothing equation: $\ln x_{HCl} = 60.979 - 81.245/(T/100) - 31.851 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 2.64×10^{-3} 0.177 Ethoxybenzene, (phenyl ethyl 282.75 0.150 ether; phenetole); C8H10O; 0.149 283.15 [103-73-1] 290.55 0.142 0.124 293.15 0.115 298.15 0.112 0.101 0.0902 303.15 305.15 0.097 0.0884 0.079 0.0732 311.25 313.15 0.0718 322.95 0.062 0.0584 0.0580 323.15 Smoothing equation: $\ln x_{HC1} = -9.547 + 21.649/(T/100)$ Standard error in x_{HC1} about the regression line = 1.65 × 10⁻³

^{*} calculated by the compiler

^{**} smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS:	ORIGINAL ME	ASUREMENTS:
(1) Hydrogen chloride; HCl;	Gerrard, W.	; Macklen, E.D.
[7647-01-0]		em. 1960, 10, 57-62.
(2) Ethers	, ", ", ", ", ", ", ", ", ", ", ", ", ",	10, 3, 02.
EXPERIMENTAL VALUES: T/K	Mole ratio	Mole* Smoothed**
-,	n HCl $^{/n}$ ether	fraction mole fraction
		xHCl xHCl
(Ethoxymethyl) benzene, 282.	35 0.737	0.424
(benzyl ethyl ether); 283.	15	0.419
C ₉ H ₁₂ O; [539-30-0] 288. 289.		0.397 0.394
293.	15	0.376
300.		0.335
303. 304.		0.321
309.		0.285
313.		0.261
314. 319.		0.255 0.224
323.		0.204
Smoothing aquation: ln v = 105 9	18 _ 1/5 039//T	/100) 53 416 ln(m/100)
Smoothing equation: $\ln x_{\text{HCl}} = 105.9$ Standard error in x_{HCl} about to	he regression 1:	$\sin = 3.04 \times 10^{-3}$
HC1		
(Butoxymethyl) benzene, 273.	15 0.810	0.448 0.448
(benzyl butyl ether); 277.	25 0.764	0.433
$C_{11}H_{16}O$; [588-67-0] 282.		0.410
283. 287.		0.407
292.		0.357
293.		0.355
298. 303.		0.327
307.	75 0.379	0.275
310. 313.		0.258
Smoothing equation: $\ln x_{HC1} = 73.44$ Standard error in x_{HC1} about the	O - 98.334/(T/10	00) - 38.058 ln(T/100)
Standard error in x _{HCl} about to	ne regression 1:	ine = 9.24 × 10
1 1! Overhighengens 273	15 0 117	0.105 0.105
1,1'-Oxybisbenzene 273. (diphenyl ether); C ₁₂ H ₁₀ O; 280.		0.105 0.105 0.0859
[101-84-8] 283.	15	0.0824
290. 293.		0.0706 0.0659
293.		0.0610
303.	15	0.0535
307. 313.		0.0494
314	35 0.045	0.0431
323.		0.0357
323.		0.0367
Smoothing equation: $\ln x_{HC1} = -9.03$ Standard error in x_{HC1} about the	3 + 18.524/(T/10	00)
Standard error in xHCl about the	ne regression li	ine = 1.57 × 10 ⁻³
		i
* coloulated by the		
* calculated by the compiler ** smoothing equation and smoothed	values were cal	culated by H.L. Clever
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COMPONENTS:		ORIGINAL ME	EASUREMENTS	:
<pre>(1) Hydrogen chloride; HCl; [7647-01-0]</pre>		Gerrard, W.	; Macklen,	E.D.
		J. Appl. Ch	em. <u>1960</u> ,	10, 57-62.
(2) Ethers				
EXPERIMENTAL VALUES:	m / v			
	т/К n,	Mole ratio HCl ^{/n} ether	Mole* fraction	Smoothed** mole fraction
		HCI etner	*HCl	*HCl
1,1'-[Oxybis(methylene)]bis-	273.15	0.643	0.391	0.389
benzene, (dibenzyl ether); C ₁₄ H ₁₄ O; [103-50-4]	277.65 280.35	0.597 0.569	0.374 0.363	
14-14-7 (283.15			0.352
	284.65 287.35	0.526 0.500	0.345 0.333	
	292.95	0.446	0.308	
	293.15			0.309
	299.75	0.390	0.281	0 262
	303.15 305.95	0.338	0.253	0.263
	312.95	0.279	0.218	
	313.15			0.219
Smoothing equation: $\ln x_{HC1} = 6$ Standard error in x_{HC1} above.	61.356 out the	- 81.792/(T/1 regression l	00) - 32.1 ine = 2.01	99 ln(T/100) × 10 ⁻³
Tetrahydrofuran; C ₄ H ₈ O;	273.15			0.624
[109-99-9]	278.15	1.545	0.607	
	279.35 283.05	1.505 1.382	0.601 0.580	
	283.15	1,502	0.500	0.581
	288.15	1.226	0.551	
	290.55 293.15	1.145	0.534	0.515
	293.15	0.949	0.487	0.515
	302.35	0.793	0.442	
•	303.15	0 745	0 437	0.436
	304.35	0.745	0.427	
Smoothing equation: $\ln x_{\text{HCl}} = 9$ Standard error in x_{HCl} above	91.037 - out the	- 123.087/(T/ regression l	100) - 46. ine = 1.05	223 ln(T/100) × 10 ⁻³
1,4-Dioxane; C ₄ H ₈ O ₂ ;	273.15			0.548
[123-91-1]	279.65	1.134	0.531	•
	283.15 284.85	1.031	0.508	0.517
	289.85	0.944	0.486	
	293.15			0.470
	296.65	0.819	0.450	
	302.35 303.15	0.721	0.419	0.414
	308.35	0.625	0.385	- • - • -
	312.85	0.549	0.354	0 254
	313.15			0.354
Smoothing equation: $\ln x_{HCl} = 0$ Standard error in x_{HCl} about	57.100 - out the	- 90.850/(T/1 regression l	00) - 34.2 ine = 1.92	76 ln(T/100) × 10 ⁻³

^{*} calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

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COMPONENTS:
                                                    ORIGINAL MEASUREMENTS:
       Hydrogen chloride; HCl;
                                                    Gerrard, W.; Macklen, E.D.
       [7647-01-0]
                                                    J. Appl. Chem. 1960, 10, 57-62.
(2) Ethers
EXPERIMENTAL VALUES:
                                           T/K
                                                   Mole ratio
                                                                     Mole*
                                                                                    Smoothed**
                                                                    fraction mole fraction
                                                <sup>n</sup>HCl<sup>/n</sup>ether
                                                                     xHC1
                                                                                       x<sub>HCl</sub>
                                        273.15
                                                     0.072
                                                                     0.0672
                                                                                       0.0669
Oxybis [chloromethane],
                                        277.35
                                                                     0.0557
(dichloromethyl ether):
                                                     0.059
C_2H_4Cl_2O: [542-88-1]
                                        283.15
                                                                                       0.0460
                                                     0.044
0.038
                                        286.55
                                                                     0.0421
                                        292.15
                                                                     0.0366
                                        293.15
                                                                                       0.0360
Smoothing equation: \ln x_{HCl} = -187.524 + 268.433/(T/100) + 86.128 \ln(T/100)
Standard error in x_{HCl} about the regression line = 6.93 × 10<sup>-4</sup>
                                         273.15
                                                                                        0.242
1-Chloro-1-(2-chloroethoxy)
ethane, (\alpha \beta - dichloroethy1) 279.85
ether); C_4H_8Cl_2O; [1462-34-6] 283.15
                                                     0.247
                                                                     0.198
                                                                                        0.180
                                                     0.206
                                         284.85
                                                                     0.171
                                                     0.201
                                                                     0.167
                                         285.75
                                                                     0.143
                                         291.45
                                                     0.167
                                                                                        0.135
                                         293.15
                                                     0.145
                                         295.55
                                                                     0.127
                                         298.05
                                                     0.134
                                                                     0.118
                                         303.15
                                                                                        0.103
                                         309.65
                                                    0.093
                                                                     0.0851
                                         313.15
                                                                                        0.0783
                                         318.15
                                                     0.074
                                                                     0.0689
                                         323.15
                                                                                        0.0601
Smoothing equation: \ln x_{HCl} = 10.599 - 5.264/(T/100) - 10.044 \ln(T/100)
Standard error in x_{HCl} about the regression line = 6.67 \times 10<sup>-4</sup>
1,1'-Oxybis [2-chloroethane], 273.15
                                                     0.297
                                                                     0.229
                                                                                      0.228
(ββ'-dichloroethyl ether);
                                                                                      0.174
                                        283.15
                                                     0.202
                                                                     0.168
C<sub>4</sub>H<sub>8</sub>Cl<sub>2</sub>O; [111-44-4]
                                        284.15
                                        288.85
                                                     0.175
                                                                     0.149
                                                                                      0.132
                                        293.15
                                        297.65
                                                     0.133
                                                                     0.117
                                        303.15
                                                     0.114
                                                                     0.102
                                                                                      0.101
                                        306.45
                                                     0.100
                                                                     0.0909
                                        311.55
                                                     0.087
                                                                     0.0800
                                                                                      0.0766
                                        313.15
Smoothing equation: \ln x_{HCl} = 23.200 - 23.438/(T/100) - 16.018 \ln(T/100)
Standard error in x_{HCl} about the regression line = 1.09 × 10<sup>-3</sup>
1,1'-Oxybis [3-chloropropane], 273.15
                                                     0.391
                                                                     0.281
                                                                                        0.285
(YY'-dichloropropyl ether);
                                                                                        0.213
                                         283.15
C<sub>6</sub>H<sub>12</sub>Cl<sub>2</sub>O; [629-36-7]
                                         283.55
                                                     0.269
                                                                     0.212
                                         290.85
                                                     0.213
                                                                     0.176
                                                                                        0.159
                                         293.15
                                         298.15
                                                     0.162
                                                                     0.139
                                         303.15
                                                                                        0.119
                                         303.45
                                                     0.131
                                                                     0.116
                                                                                        0.0895
                                         313.15
                                         314.15
                                                     0.090
                                                                     0.0826
                                         323.15
                                                     0.075
                                                                     0.0698
                                                                                        0.0634
Smoothing equation: \ln x_{HC1} = 21.558 - 20.124/(T/100) - 15.370 \ln(T/100)
Standard error in x_{HC1} about the regression line = 4.64 \times 10^{-3}
   calculated by the compiler
 ** smoothing equation and smoothed values were calculated by H.L. Clever
```

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-methoxybutane or butyl methyl ether; C₅H₁₂O; [628-28-4]

ORIGINAL MEASUREMENTS:

Kapoor, K. P.; Luckcock, R. G.; Sandbach, J. A.

J. Appl. Chem. Biotech. <u>1971</u>, 21, 97 - 100.

VARIABLES:

T/K: 203.15 - 296.55 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALU	FC			_
EXPERIMENTAL VALUE	T/K	Mol Ratio	Mol Fraction	
		n ₁ /n ₂	x_1	
	203.15	5.98	0.857	
	214.15	4.11	0.804	
	246.15	1.706	0.630	The mole fraction
	251.15	1.523	0.604	solubility values
	256.65	1.312	0.567	were calculated
	273.15	1.075	0.518	by the compiler.
	282.95	0.908	0.476	by the compiler.
	283.15	0.895	0.472	
	283.15	0.907	0.476	
	296.15	0.685	0.407	
	296.55	0.688	0.408	_

Smoothed Data: For use between 203.15 and 293.15 K.

 $\ln x_1 = 8.308 - 9.080/(T/100K) - 5.635 \ln (T/100K)$ Standard error about the regression line is 9.71 x 10⁻³

T/K	Author's S	moothed Data	Compiler's Eqn.
	Mol Ratio	Mol Fraction	Mol Fraction
	ⁿ 1 ^{/n} 2	x_1	x_1
203.15	6.00	0.857	0.856
213.15			0.805
223.15			0.753
233.15	2.45	0.710	0.700
243.15			0.649
253.15	1.45	0.592	0.599
263.15			0.552
273.15	1.075	0.518	0.507
283.15	0.907	0.476	0.466
293.15			0.427

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The bubbler-tube technique described by Gerrard, Mincer, and Wyvill (1) was used. For temperatures between 303 and 253 an LBI thermostat containing liquid paraffin was used. For temperatures less than 253 K addition of small pieces of solid carbon dioxide and manual stirring enabled the temperature to be maintained within ±1 K. For 273.15 K a slurry of ice and water in a vacuum flask was used.

For temperatures below 273.15 K it was assumed that the loss of solvent by entrainment could be ignored. After saturation at a recorded temperature, the temperature was lowered by 10 K and pyridine was carefully added drop-wise to fix the hydrogen chloride as the pyridinium salt. After treatment with water, the chloride ion content was determined by the Volhard method or by use of an automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. A good specimen was obtained from a cylinder, and dried.
- (2) Butyl methyl ether. Prepared from 1-butanol, sodium, and iodomethane. The ether was rigorously purified and attested.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5 253 - 303 K$ = $\pm 1 < 253 K$ $\delta x_1/x_1 = 0.02$

REFERENCES:

 Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. <u>1959</u>, 9, 89.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Methoxybutane or butyl methyl ether; $C_5H_{12}O$; [628-28-4]

ORIGINAL MEASUREMENTS:

Kapoor, K. P.; Luckcock, R. G.; Sandbach, J. A.

J. Appl. Chem. Biotech. <u>1971</u>, 21, 97 - 100.

EXPERIMENTAL VALUES:

Variation of temperature and pressure at constant mole fraction.

ure	at	constant mo	le fraction.
	r/ĸ	Pressure P ₁ /mmHg	Mol Fraction
	2.95		0.405
	9.25 9.65		
	9.95		
	5.45		
	3.15 9.95		
	5.25		
293	3.25	724	
299	9.95	940	
	3.45		0.450
	5.45 5.45		
	3.75		
	L.15		•
	5.45 3.15		
	1.25		
	35		
222	2.35	83	0.490
	35		
	9.35 9.15	180.5 275	
	7.85	399.2	
	.05	526	
	2.15 L.55	695.5	
	3.55	974 1363	
217	7.75	103.2	0.536
225	3.35	143	
	.35	194.5	
	2.15 3.65	323.5 511.5	
	.45	665.5	
267	7.45	844.5	
	2.05 95	1003 1409	
~ 0 1		1403	

Variation of pressure and mole fraction at constant temperature.

т/к	Pressure P ₁ /mmHg	Mol Fraction
233.45	53.7	0.411
	84	0.455
	133	0.494
	206.5 760	0.539 0.688
	760	0.688
243.85	88.7	0.411
	142	0.455
	217	0.494
	343	0.538
	760	0.635
256.35	150	0.410
	250.5	0.454
	372.5	0.492
	565	0.537
	760	0.574
270.25	273.5	0.409 *
	444.5	0.452
	656	0.491
	760	0.508
	944	0.535
286.15	537	0.407
	760	0.440
	833	0.450
	1210	0.487
	1698	0.531

Continued on next page. Variation of mole fraction solubility with temperature at one atm HCl pressure.

(1) Hydrogen chloride; HCl; [7647-01-0]

(2) 1,1'-0xybisalkanes; $C_4H_{10}O$, $C_6H_{14}O$, and $C_8H_{18}O$

ORIGINAL MEASUREMENTS:

Ionin, M. V.; Shverina, V. G.

Zh. Obshch. Khim. 1965, 35, 209-211.

J. Gen. Chem. USSR (Engl. Transl.) 1965, 35, 211 - 212.

VARIABLES:

COMPONENTS:

T/K: 298.15

Total P/kPa: 101.3 (atmospheric)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Refractive	Solution	Mol Ratio	Mol Fraction
	Index ¹ Density n_D^{298} ρ/g cm ⁻³		n ₁ /n ₂	<i>x</i> ₁
1,1'-0x	ybisethane o	r diethyle	ther; C ₄ H ₁₀	0; [60-29-7]
298.15	1.3523	0.8133	0.802	0.445
2,2'-0x [108-20	ybispropane	or di-isop	ropyl ether	; C ₆ H ₁₄ O;
298.15	1.3660	0.8086	0.799	0.444
1,1'-0x [142-96	ybisbutane c	or dibutyl	ether; C ₈ H ₁	.80;
298.15	1.3966	0.8253	0.808	0.447

¹ Pure solvent refractive index.

The mole ratio values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The ether was saturated with hydrogen chloride at 298.2 K and atmospheric pressure, not specified. An aliquot of the solution was diluted with water, and titrated with alkali.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from "chemically pure" sodium chloride and sulfuric acid; and was dried by sulfuric acid and anhydrous calcium chloride.
- (2) 1,1'-Oxybisalkanes. The ethyl and 2-propyl ethers were "pure" grade materials, freed from peroxy compounds, dried with sodium and distilled. The butyl ether was self prepared.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Ethoxybutane or butyl ethyl ether; C₆H₁₄O; [628-81-9]

ORIGINAL MEASUREMENTS:

Kapoor, K. P.; Luckcock, R. G.; Sandbach, J. A.

J. Appl. Chem. Biotech. 1971, 21, 97 - 100.

EXPERIMENTAL VALUES:

Variation of temperature and pressure at constant mole fraction.

sure at	constant	mole fraction.
т/к	Pressure p ₁ /mmHg	
234.65 243.05 251.05 258.15 265.95 273.15 279.35 286.25 293.05 299.25	31.0 54.2 91 132.5 205.7 301 408.5 562.5 743.2 977	0.430
233.85 242.35 250.15 258.15 265.05 273.15 280.55 286.55	56.2 94.2 144 229.5 326 482 668.5 860	0.484
231.65 236.15 244.15 251.65 256.45 265.15 273.15 281.95	87 115 184.5 261.3 334 510 735	0.535
233.05 239.15 247.45 255.15 262.15 268.15 273.15	195 266.7 400 565.7 757.8 957 1156	0.597

Variation of pressure and mole fraction at constant temperature.

т/к	Pressure p ₁ /mmHg	Mol Fraction
233.45	26.1 51.9 92.0 189.2 760	0.441 0.490 0.539 0.602 0.732
243.85	56.6 102.5 175 336 760	0.440 0.490 0.539 0.601 0.685
256.35	123 206.5 334 696 760	0.439 0.489 0.538 0.599 0.626
270.25	257 419 638 760 1038	0.437 0.487 0.536 0.555 0.596
285.65	551 760 963 1036	0.433 0.470 0.480 0.532

Continued on next page. Variation of mole fraction with temperature at one atm pressure.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Butyl ethyl ether; C₆H₁₄O; [628-81-9] ORIGINAL MEASUREMENTS:

Kapoor, K. P.; Luckcock, R. G.; Sandbach, J. A.

J. Appl. Chem. Biotech. 1971, 21, 97 - 100.

VARIABLES:

T/K: 205.15 - 297.15 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	T/K	Mol Ratio	Mol Fraction	_
ł		n ₁ /n ₂	x_1	
1	205.15	5.75	0.852	
	213.15	4.31	0.812	The mole fraction
	217.65	4.24	0.809	solubility values
	232.15	2.95	0.747	were calculated
	245.95	2.17	0.685	by the compiler.
	246.75	2.15	0.683	
	273.15	1.161	0.537	
{	281.45	1.000	0.500	
	282.15	0.996	0.499	
!	285.65	0.919	0.479	
	297.15	0.716	0.417	_

Smoothed Data: For use between 203.15 and 283.15 K.

 $\ln x_1 = 15.722 - 18.665/(\mathrm{T/100K}) - 9.460 \ln (\mathrm{T/100K})$ The standard error about the regression line is 6.90 x 10⁻³

T/K	Author's S	moothed Data	Compiler's Eqn.
	Mol Ratio	Mol Fraction	Mol Fraction
	ⁿ 1 ^{/n} 2	x_1	x_1
203.15	6.15	0.860	0.845
213.15			0.823
223.15			0.790
233.15	2.93	0.746	0.747
243.15			0.698
253.15	1.90	0.655	0.646
263.15			0.592
273.15	1.150	0.535	0.539
283.15	0.965	0.491	0.489

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:
The bubbler-tube technique described by Gerrard, Mincer, and Wyvill (1) was used. For temperatures between 303 and 253 an LBI thermostat containing liquid paraffin was used. For temperatures less than 253 K addition of small pieces of solid carbon dioxide and manual stirring enabled the temperature to be maintained with in + 1 K. For 273.15 K a slurry of ice and water in a vacuum flask was used.

For temperatures below 273.15 K it was assumed that the loss of solvent by entrainment could be ignored. After saturation at a recorded temperature, the temperature was lowered by 10 K and pyridine was carefully added drop-wise to fix the hydrogen chloride as the pyridinium salt. After treatment with water, the chloride ion content was determined by the Volhard method or by use of an automatic titrimeter.

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. A good specimen was obtained from a cylinder, and dried.
- (2) Butyl ethyl ether. Prepared from alcohol, sodium, and alkyl bromide. The ether was rigorously purified and attested.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.5 253-303 K$ = $\pm 1 < 253 K$

 $\delta x_1/x_1 = 0.01$

REFERENCES:

 Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89.

- (1) Hydrogen chloride; HCl; [76,47-01-0]
- (2) 1,1'-Oxybis[3-methylbutane] or diisoamyl ether; C₁₀H₂₂O; [544-01-4]

ORIGINAL MEASUREMENTS:

Perkin, W. H.

J. Chem. Soc. 1894, 65, 20 - 28.

VARIABLES:

T/K: 273.15 - 298.15

p/kPa: 101.3 (atmospheric?)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Tempo t/C	erature T/K			Mol Ratio	Mol Fraction
		Weighing	Titration	11/112	x_1
0	273.15	18.61	18.70	1.00	0.500
5	278.15	16.78	17.04	0.892	0.472
9	282.15	16.28	16.26	0.843	0.458
13	286.15	15.05	15.40	0.791	0.442
15	288.15	14.59	14.91	0,761	0.432
25	298.15	11.27	11.58	0.569	0.362

The author considered the titration values more accurate than the weighing values.

The mole ratio and mole fraction values were calculated from the titration weight per cents by the compiler.

Smoothed Data: $\ln x_1 = 98.038 - 132.498/(T/100K) - 49.990 \ln(T/100K)$

Standard error about the regression line is 5.70×10^{-3} .

T/K	Mol Fraction
	<u>x</u> 1
273.15	0.496
283.15	0.456
293.15	0.397

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the liquid until bubbles passed through unabsorbed. The amount of gas absorbed was weighed; and also determined by transferring a weighed quantity of solution to a stoppered bottle containing water and titrating with alkali.

The author states that the difference in the two values is due to evaporization of solvent during the bubbling process.

The pressure was not specified, but appears to have been atmospheric.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. No information.
- (2) 1,1'-Oxybis[3-methylbutane].
 Kahlbaum.

ESTIMATED ERROR:

Hydrogen Chloride in Non-Aqueous Solvents						
COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]	ORIGINAL MEASUREMENTS: Matuszak, M. P.					
(2) 1,1'-Oxybis[3-methyl butane] or dissoamyl ether; C ₁₀ H ₂₂ O; [544-01-4]						
VARIABLES: T/K = 297.6 p/kPa = 99.59 (747 mmHg)	PREPARED BY: W. Gerrard					
EXPERIMENTAL VALUES:						
t/or m/k n/mmkg g HCl	bsorbed Mol Ratio Mol Fraction per 100 ponent 2 n_1/n_2 x_1					
76 297.6 747 10	.0 0.435 0.303					
1 The author's statement was "oxycompound." The mole ratio and mole fraction val	HCl absorbed, weight per cent of ues were calculated by the compiler.					
	INFORMATION CONTROL OF MATERIALS					
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:					
No information.	No information. ESTIMATED ERROR: REFERENCES:					

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. 1,1'-Oxybisoctane or Dioctyl ether; C₁₆H₃₄O; [629-82-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol	Fraction
	n HC1/ n C ₁₆ H ₃₄ O		X _{HC1}
253.15	1.70		0.630
263.15	1.35		0.574
273.15	1.06		0.515
283.15	0.88		0.468
293.15	0.685		0.407

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = 24.890 - 30.734/(T/100) - 14.226 \ln (T/100)$

Standard error about regression line = 4.85×10^{-3}

T/K	Mol	Fraction
		X _{HC1}
253.15 263.15 273.15 283.15 293.15		0.629 0.575 0.519 0.463 0.409

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K, a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- Gerrard W.
 J. Appl. Chem. Biotechnol. 1972,
 22, 623 650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Methoxybenzene or anisole; C₇H₈O; [100-66-3]

ORIGINAL MEASUREMENTS: O'Brien, S. J.

J. Am. Chem. Soc. 1942, 64, 951 - 953.

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Henry's	Mol Ratio	Mol Fraction
	p ₁ /mmHg	$m_1/mol kg^{-1}$	Constant k ¹	ⁿ 1 ^{/n} 2	<i>x</i> ₁
293.15	30.3	0.0378	1.05	0.0041	0.0041
	66.7	0.0926	0.95	0.0100	0.0099
	70.7	0.100	0.93	0.0108	0.0107
	82.7	0.109	0.99	0.0118	0.0116
	(760		0.97 av.	0.111	0.100)2
303.15	52.7	0.059	1.18	0.00637	0.00633
	66	0.073	1.21	0.00788	0.00782
	85	0.092	1.22	0.00994	0.00984
	168	0.180	1.23	0.0194	0.0191
	181	0.200	1.19	0.0216	0.0211
	408	0.448	1.20	0.0484	0.0461
	(760		1.21 av.	0.0892	0.0819)2
308.15	45.9	0.0449	1.34	0.00485	0.00483
	72.0	0.0720	1.31	0.00778	0.00772
	77.8	0.0764	1.34	0.00825	0.00762
	250	0.250	1.31	0.0270	0.0263
	264	0.253	1.37	0.0273	0.0266
	410	0.400	1.35	0.0432	0.0414
	(760		1.34 av.	0.0806	0.0746)2
313.15	61.8	0.0463	1.56	0.00500	0.00498
	82.3	0.0735	1.48	0.00793	0.00787
	98.8	0.0887	1.46	0.00958	0.00949
	106	0.0929	1.61	0.0100	0.0099
	216	0.179	1.59	0.0193	0.0190
	(760		1.54 av.	0.0701	0.0655) ²

 $^{^{1}}$ k/atm mol⁻¹ kg = $(p_{1}/atm)/(m_{1}/mol kg^{-1})$

Note: The molality, m_1 , is essentially a *mole ratio* form. If linear for this, *not* linear for mole fraction, except in the limit of infinite dilution.

 $^{^2}$ Value calculated by the compiler from the average value of Henry's constant, assuming a linear function of $p_{\it 1}$ vs. $\it m_{\it 1}$, as the original author appeared to imply.

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen chloride; HCl; O'Brien, S. J. [7647-01-0] J. Am. Chem. Soc. 1942,64, 951 - 953. (2) Methoxybenzene or anisole; C_7H_8O ; [100-66-3] **VARIABLES:** PREPARED BY: T/K: 293.15 - 313.15 W. Gerrard 4.04 - 54.66 P/kPa: (30.3 - 410 mmHg)

EXPERIMENTAL VALUES:

See preceeding page.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Anisole. Eastman Kodak Co. Dried and distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- O'Brien, S. J.; Kenny, C. L.
 Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Ethoxybenzene or ethyl phenyl ether or phenetole; C₈H₁₀O; [103-73-1] VARIABLES: T/K: 283.15 - 298.15 P/kPa: 101.325 (1 atm) O'Brien, S. J.; King, C. V. J. Am. Chem. Soc. 1949, 71, 3632 - 3634. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's Constant ¹	Mol Ratio	Mol Fraction
	Constant'	n ₁ /n ₂	x ₁
283.15	0.70 ± 0.03	0.178 0.174 ²	0.151 0.148 ²
293.15	0.90 ± 0.01	0.136 0.136 ²	0.120 0.119 ²
298.15	1.02 ± 0.04	0.120	0.107

 $^{^{1}}$ k/atm mol⁻¹ kg = (p₁/atm)/(m₁/mol kg⁻¹)

All of the mole ratio values were calculated by the compiler.

The experimental measurements were probably carried out at pressures below one-half atm partial pressure of HCl. The Henry's constant values are the mean of from 2 to 6 values followed by the average deviation of the mean.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al.(2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution is added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Not stated. Probably prepared from potassium chloride and sulfuric acid as in previous work (2).
- (2) Ethoxybenzene. Eastman Kodak Co. Dried and distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

REFERENCES:

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

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² Values as recalculated by the compiler.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Butoxybenzene or butyl phenyl ether; C₁₀H₁₄O; [1126-79-0]

ORIGINAL MEASUREMENTS:
O'Brien, S. J.; King, C. V.

J. Am. Chem. Soc. 1949, 71, 3632 - 3634.

VARIABLES:

ጥ/Κ: 293.15, 298.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's Constant ¹ k	Mol Ratio	Mol Fraction
293.15	1.21 ± 0.05	0.124	0.110
298.15	1.37 ± 0.04	$0.111 \\ 0.109^{2}$	0.100 0.0987 ²

 $^{^{1}}$ k/atm mol⁻¹ kg = (p₁/atm)/(m₁/mol kg⁻¹)

All of the mole ratio values were calculated by the compiler.

The experimental measurements were probably carried out at pressures below one-half atm partial pressure of HCl. The Henry's constant values are the mean of from 2 to 6 values followed by the average deviation of the mean.

From the slope of log x_1 vs. 1/T. The enthalpy of solution is -3.78 kcal mol^{-1} (-15.82 kJ mol^{-1}).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et at. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution is added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The HCl in the The tap is closed. upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated. Probably prepared from potassium chloride and sulfuric acid as in previous work (2).
- Eastman Kodak Co. (2) Butoxybenzene. Dried and distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Values as recalculated by the compiler.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'-Oxybisbenzene or diphenyl ether; $C_{12}H_{10}O$; [101-84-8]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; King, C. V.

J. Am. Chem. Soc. 1949, 71, 3632 - 3634.

VARIABLES:

T/K: 298.15, 303.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

•				
T/K	Henry's Constant ¹	Mol Ratio	Mol Fraction	
	Constant k	n _{1/n2}	x_1	
298.15	3.33 ± 0.07	0.0520 0.0511 ²	0.0494 0.0486 ²	
303.15	3.52 <u>+</u> 0.01	0.0462 0.0482 ²	0.0442 0.0461 ²	

 $^{^{1}}$ k/atm mol⁻¹ kg = (p₁/atm)/(m₁/mol kg⁻¹)

All of the mole ratio values were calculated by the compiler.

The experimental measurements were probably carried out at pressures below one-half atm partial pressure of HCl. The Henry's constant values are the mean of from 2 to 6 values followed by the average deviation of the mean.

From the slope of $\log x_1$ vs. 1/T. The enthalpy of solution is -3.80 kcal mol⁻¹ (-15.90 kJ mol⁻¹).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution is added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated. Probably prepared from potassium chloride and sulfuric acid as in previous work (2).
- (2) 1,1'-Oxybisbenzene. Eastman Kodak Co. Dried and distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

² Values as recalculated by the compiler.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1,1'-Oxybisbenzene or diphenyl ether; Cl2Hl0O; [101-84-8] VARIABLES: T/K = 307.0 p/kPa = 99.95 (747 mmHg) EXPERIMENTAL VALUES: Temperature Pressure HCl Absorbed¹ Mol Ratio Mol Fraction g HCl per 100 g component 2 n ₁ /n ₂ x ₁ 93 307.0 747 0.63 0.0294 0.0286 ¹ The author's statement was "HCl absorbed, weight per cent of oxycompound." The mole ratio and mole fraction values were calculated by the compiler Method/APPARATUS/PROCEDURE: No information. No information. No information.	186 Hydrogen Chlorid	le in Non-Aqueous Solvents
Temperature Pressure HCl Absorbed¹ Mol Ratio Mol Fraction t/°F T/K p/mmHg g HCl per 100 g component 2 n ₁ /n ₂ x ₁ 93 307.0 747 0.63 0.0294 0.0286 ¹ The author's statement was "HCl absorbed, weight per cent of oxycompound." The mole ratio and mole fraction values were calculated by the compiler AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1,1'-Oxybisbenzene or dipheny ether; C ₁₂ H ₁₀ O; [101-84-8] VARIABLES: T/K = 307.0	Matuszak, M. P. U. S. Patent 2,520,947 September 5, 1950 Chem. Abstr. 1950, 44, 11044g PREPARED BY:
The author's statement was "HCl absorbed, weight per cent of oxycompound." The mole ratio and mole fraction values were calculated by the compiler AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:		1 Through 11 Well Battle Well Battle
The author's statement was "HCl absorbed, weight per cent of oxycompound." The mole ratio and mole fraction values were calculated by the compiler . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	+/or T/k n/mmHg g l	HCl per 100 " /" "
Oxycompound." The mole ratio and mole fraction values were calculated by the compiler . AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	93 307.0 747	0.63 0.0294 0.0286
METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:	•	
	IIXUA	LIARY INFORMATION
No information. No information.	METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
	No information.	No information.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1'Oxybis[2-chloroethane];
 C₄H₈Cl₂O; [111-44-4]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.

J. Am. Chem. Soc. 1942, 64, 951 - 953.

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Henry's	Mol Ratio	Mol Fraction
	P ₁ /mmHg	m ₁ /mol kg ⁻¹	Constant k1	ⁿ 1 ^{/n} 2	<i>x</i> ₁
293.15	23.7	0.0419	0.75	0.0060	0.0060
	53	0.090	0.78	0.0129	0.0127
	103	0.168	0.81	0.0240	0.0235
	109	0.182	0.79	0.0260	0.0254
	116	0.198	0.78	0.0283	0.0275
	122	0.202	0.80	0.0289	0.0281
	186	0.305	0.80	0.0436	0.0418
	287	0.481	0.79	0.0688	0.0644
	533	0.794	0.88	0.114	0.102
	(760		0.82 av.	0.174	0.149)2
298.15	6.6	0.0091	0.95	0.00130	0.00130
	38.1	0.0572	0.88	0.00818	0.00811
	54.3	0.0758	0.94	0.01084	0.01073
	68.3	0.103	0.87	0.0147	0.0145
	84	0.126	0.88	0.0180	0.0177
	94	0.140	0.88	0.0200	0.0196
	124	0.165	0.99	0.0236	0.0231
	124	0.175	0.94	0.0250	0.0244
	215	0.308	0.92	0.0440	0.0422
	365	0.502	0.96	0.0718	0.0670
	363	0.518	0.92	0.0741	0.0690
	378	0.538	0.93	0.0769	0.0714
	413	0.555	0.98	0.0794	0.0735
	401	0.556	0.95	0.0795	0.0737
	418	0.571	0.96	0.0817	0.0755
	(760		0.94 av.	0.152	0.132)2
303.15	17.2	0.0224	1.00	0.00320	0.00319
	25.6	0.0292	1.15	0.00418	0.00416
	260	0.343	1.00	0.0490	0.0468
	283	0.366	1.02	0.0523	0.0497
	(760		1.03 av.	0.139	0.122)2
313.15	70.9	0.0711	1.31	0.0102	0.0101
	160	0.165	1.28	0.0236	0.0231
	177	0.166	1.41	0.0237	0.0232
	307	0.265	1.52	0.0379	0.0365
	307	0.291	1.37	0.0416	0.0400
	(760		1.40 av.	0.1021	0.0927)2

 $^{^{1}}$ k/atm mol⁻¹ kg = $(p_{1}/atm)/(m_{1}/mol kg^{-1})$

The compiler calculated the values of mole ratio and mole fraction.

Another name for the solvent is 2,2'-dichloroethyl ether.

Note: Henry's constant. The molality is essentially of a *mole ratio* form. If linear for this, *not* linear for mole fraction, except in the limit of infinite dilution.

² Value calculated by the compiler from the average value of Henry's constant, assuming a linear function of p_1 vs. m_1 , as the original author appeared to imply.

COMPONENTS: ORIGINAL MEASUREMENTS: O'Brien, S. J. Hydrogen chloride; HCl; [7647-01-0] J. Am. Chem. Soc. 1942, 64, (2) 1,1'Oxybis[2-chloroethane]; 951 - 953. C4H8Cl2O; [111-44-4] VARIABLES: T/K: PREPARED BY: 293.15 - 313.15 W. Gerrard P/kPa: 0.88 - 71.06(6.6 - 533 mmHg)

EXPERIMENTAL VALUES:

See preceeding page

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of (1) Hydrogen chloride. Prepared from Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

- SOURCE AND PURITY OF MATERIALS:
- chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) 1,1'-Oxybis[2-chloroethane]. Eastman Kodak Co. Dried and distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 1,4-Dioxane; C₄H₈O₂; [123-91-1] VARIABLES: T/K = 305.4 p/kPa = 99.59 (747 mmHg) ORIGINAL MEASUREMENTS: Matuszak, M. P. U. S. Patent 2,520,947 September 5, 1950 Chem. Abstr. 1950, 44, 11044g W. Gerrard

EXPERIMENTAL VALUES:

Tempe	erature	Pressure	HCl Absorbed1	Mol Ratio	Mol Fraction
t/°F	<i>T</i> /K	p/mmHg	g HCl per 100 g component 2	n_{1}/n_{2}	x_1
90	305.4	747	24.5	0.592	0.372

 $^{^{\}rm 1}$ The author's statement was "HCl absorbed, weight per cent of oxycompound."

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No information.	No information.
	ESTIMATED ERROR:
	REFERENCES:
	REFERENCES:
	§

COMPONENTS: ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; (1) Hydrogen chloride; HCl; [7647-01-0] Wyvill, P. L. (2) 1,1,1-Triethoxyethane; $C_8H_{18}O_3$; J. Appl. Chem. 1960, 10, 115-121. [78 - 39 - 7]VARIABLES: PREPARED BY: T/K: 279.15 - 314.35 W. Gerrard Total P/kPa: 101.325 (1 atm) (smoothed data calculated by H.L. Clever) ΕX

T/K	Mol Ratio THC1 C8H18O3	Mol Fraction ^x l
279.15	2.720	0.731
284.35	2.366	0.703
290.65	1.956	0.662
296.75	1.501	0.600
304.75	1.053	0.513
307.35	0.915	0.478
314.35	0.477*	0.323
314.35	0.475*	0.322

^{*}A third mole ratio value of 0.441 was probably quoted in error.

The compiler calculated the mole fraction values.

 $\ln x_1 = 307.395 - 427.249/(T/100) - 150.683 \ln (T/100)$ Smoothed Data: Standard error about the regression line is 2.62×10^{-2}

T/K	Mol Fraction x 1
283.15	0.720
293.15	0.663
303.15	0.518
313.15	0.351

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1,1,1-Triethoxyethane. Carefully purified, and purity rigorously attested.

Solvent name is ethyl orthoacetate in paper, IUPAC name is triethyl ESTIMATED ERROR: orthoacetate.

$$\delta x_1/x_1 = 0.012$$

COMPONENTS: (1) Hydrogen chloride; HCl; Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. (2) 1,3-Benzodioxole; C₇H₆O₂; J. Appl. Chem. 1960, 10, 115 - 121. VARIABLES: T/K: 273.15 - 304.85 Total P/kPa: 101.325 PREPARED BY: W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mole Ratio	Mol Fraction
	ⁿ HC1/nC7H6O2	<i>x</i> 1
273.15	0.130	0.115
278.95	0.112	0.101
283.75	0.0909	0.0833
293.35	0.0735	0.0685
304.85	0.0571	0.0540

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -9.511 + 20.056/(T/100 \text{ K})$

The standard error about the regression line is 2.73×10^{-3} .

T/K	Mol Fraction x_1
273.15	0.114
283.15	0.0882
293.15	0.0693
303.15	0.0553

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

Other names for the solvent are o-phenylene methylene ether and 1,2-(methylenedioxy)benzene.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1,3-Benzodioxole. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.025$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2,3-Dihydro-1,4-benzodioxin; C₈H₈O₂; [493-09-4]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 275.95 - 303.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
275.95	0.225	0.184
284.45	0.178	0.151
294.85	0.137	0.120
303.15	0.111	0.100

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 6.173 - 1.814/(T/100) - 7.102 \ln (T/100)$

Standard error about regression line is 2.85×10^{-4}

T/K	Mol Fraction
•	$\frac{x_1}{x_1}$
273.15	0.196
283.15	0.156
293.15	0.124
303.15	0.100

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 2,3-Dihydro-1,4-benzodioxin.
 Carefully purified, and purity rigorously attested.

Solvent name is o-phenylene dimethylene ether in paper, IUPAC name is 1,4-benzodioxan.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

(1) Hydrogen chloride; HCl; [7647-01-0]

(2) 3,4-Dihydro-2H-1,2-benzodioxepin; J. Appl. Chem. 1960, 10, 115-121. $C_9H_{10}O_2$; [7216-18-4]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

VARIABLES:

T/K: 273.15 - 305.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl ^{/n} C ₉ H ₁₀ O ₂	Mol Fraction
273.15	0.255	0.203
281.05	0.197	0.165
286.35	0.172	0.147
294.35	0.142	0.124
305.15	0.108	0.0975

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -8.519 + 18.903/(T/100)$

Standard error about regression line is 1.19×10^{-3}

T/K	Mol Fraction
273.15	0.202
283.15	0.158
293.15	0.126
303.15	0.102
313.15	0.0835

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 3,4-Dihydro-2H-1,2-benzodioxepin. Carefully purified, and purity rigorously attested.

Solvent name is o-phenyl trimethylene ether in the paper.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.01$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2-Methyl-1,4-benzodioxan; C₉H₁₀O₂; [5966-54-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 273.15 - 303.45 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC9H10O2	Mol Fraction x1
273.15	0.438	0.305
274.95	0.414	0.293
280.85	0.336	0.251
281.85	0.319	0.242
284.35	0.293	0.227
287.15	0.273	0.214
294.55	0.209	0.173
303.45	0.152	0.132

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 55.372 - 67.933/(T/100) - 31.537 \ln (T/100)$

Standard error about the regression line is 1.77×10^{-3}

T/K	Mol Fraction x1
273.15	0.305
283.15	0.236
293.15	0.179
303.15	0.134

AUXILIARY INFORMATION

METHOD 'APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa)

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 2-Methyl-1,4-benzodioxan. Carefully purified, and purity rigorously attested.

Solvent name is o-phenylene monomethyl dimethylene ether in paper.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Phenol; C₆H₆O; [108-95-2]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1959, 9, 85 - 88.

VARIABLES:

T/K: 313.55 - 335.85 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	nHC1/nC6H60	xHC1
313.55	0.039	0.0375
315.15	0.035	0.0338
321.35	0.028	0.0272
329.35	0.024	0.0234
335.85	0.023	0.0225

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = -510.007 + 767.213/(T/100) + 229.285 \ln (T/100)$

Standard error about regression line = 5.32×10^{-4}

T/K	Mol Fraction
	xHCl
313.15 323.15 333.15	0.0377 0.0260 0.0226

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Self prepared and dried.
- (2) Phenol. Purified, distilled, and attested by physical constants.

ESTIMATED ERROR:

 $\delta x/x = 0.02$

REFERENCES:

 Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1956, 6, 241.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Aliphatic Carboxylic Acids

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
Polytechnic of North London,
Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Aliphatic Carboxylic Acids.

The solubility in acetic acid has been measured at barometric pressure over various temperature ranges by Cupr (1), by Gerrard & Macklen (2), by Ahmed et al.(3), by Kitvinenko & Kapova (4), and by Kumar & Gehlawat (5). Mole fraction solubilities for a partial pressure of 101.3 kPa derived from data provided by the last four groups may be fitted to the equation:

 $\ln x_{HC1} = 70.224 - 1056.9/(T/K) - 12.092 \ln(T/K)$

The standard deviation in values of $x_{\rm HC1}$ is 0.0095.

This equation is based upon data for 253.15 K to 353.15 K. The data, published by Cupr, for 298.15 K, but not that for 273.15 K, are in accord with this smoothing equation.

Rodebush & Ewart (6) measured solubilities of hydrogen chloride in acetic acid at 298 K over a pressure range of 1.25 kPa to 12.4 kPa. The data are consistent with data for higher pressures published by other authors.

Gerrard & co-workers (2,3) also measured solubilities over temperature ranges in formic acid, propanoic acid, butanoic acid, hexanoic acid, 2-methyl propanoic acid and 3-methyl butanoic acid. The total pressure was equal to barometric. At 298.15 K there is a general tendency for mole fraction solubilities corrected to a partial pressure of 101.3 kPa to increase with chain length in the case of straight chain acids. Branching tends to lower the solubility. These measurements appear to be self consistent but there are no data by other authors for comparison.

Gerrard & Macklen (2) measured solubilities in chloroacetic acid and trichloroacetic acid over temperature ranges of about 320 K to 340 K at a total pressure of 101.3 kPa. The contribution of these solvents to the total pressure is small in this temperature range and the measured solubilities may be equated with solubilities at a partial pressure of 101.3 kPa. The presence of chlorine lowers the solubilities relative to that in acetic acid itself in this temperature range but the difference in solubilities in the two chlorinated solvents is very small.

Mole fraction solubilities at 323.15 K and a partial pressure of hydrogen chloride of 101.3 kPa.

Acetic acid 0.054 (from recommended equation) Chloroacetic acid 0.0280 (Gerrard & Macklen - interpolated) Trichloroacetic acid 0.0288

- 1. Cupr, V. Recl. Trav. Chim. Pays-Bas 1928, 47, 55 72.
- 2. Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1956, 6, 241 244.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109 - 115.
- Kitvinenko, V. I.; Kapova, Z. K. Izv. Akad. Nauk. Kaz. SSR, Ser. Khim. 1972, 22, 75 - 77.
- Kumar, S.; Gehlawat, J. K. J. Chem. Tech. Biotechnol. <u>1979</u>, 29, 353 - 360.
- 6. Rodebush, W. H.; Ewart, R. H. J. Am. Chem. Soc. 1932, 54, 419 423.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Aliphatic carboxylic acids

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E.D.

J. Appl. Chem. 1956, 6, 241-244

VARIABLES:

T/K: See below Total P/kPa : 101.325 (1 atm) PREPARED BY:

W. Gerrard

EXP	EKIME	NTAL	ANTORS:	

EXPERIMENTAL VALUES:	•	Mole ratio Cl ^{/n} acid	Mole* fraction ^X HCl	Smoothed** mole fraction *HCl
Formic acid; CH ₂ O ₂ ;	273.15		0.0750	0.0838
[64-18-6]	281.25 283.15	0.082	0.0758	0.0728
	288.65	0.069	0.0645	
	293.15 295.65	0.060	0.0566	0.0598
	303.15	0.000	0.0300	0.0468
	303.65	0.049	0.0467	0.0351
	313.15 316.05	0.033	0.0319	0.0351
	323.15		-	0.0254

Smoothing equation: $\ln x_{HCl} = 104.052 - 141.039/(T/100) - 54.632 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 1.09 × 10⁻³

Acetic acid; C ₂ H ₄ O ₂ ;	283.15			0.155
[64-19-7]	284.15	0.189	0.159	
	289.15	0.165	0.142	
	293.15			0.136
	300.15	0.121	0.108	
	303.15			0.100
	312.65	0.074	0.0689	
	313.15			0.0632
	323.15			0.0350
	323.25	0.035	0.0338	

Smoothing equation: $\ln x_{HCl} = 329.714 - 458.556/(T/100) - 162.979 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 5.96×10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an all-glass apparatus.

The all-glass absorption vessel (50 cm³) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Acids: high grade specimens were distilled and attested.

ESTIMATED ERROR:

 $\delta T/K =$ ±0.1

±0.01 to 0.02 $\delta x_{\text{HCl}}/x_{\text{HCl}} =$

^{*} calculated by the compiler

^{**} smoothing equation and smoothed values were calculated by H.L. Clever.

198	Hydrogen Chlo	ride in N	Ion-Aqueous S	olvents	
	NENTS: Hydrogen chloride; HCl; 7647-01-0]		1	EASUREMENTS .; Macklen,	
1	Aliphatic carboxylic acids	3	J. Appl. C	hem. <u>1956</u> ,	6, 241-244
EXPER	MENTAL VALUES:	т/к ^п і	Mole ratio	Mole* fraction *HC1	Smoothed** mole fraction *HCl
[79-05	noic acid; C ₃ H ₆ O ₂ ; 0-4] sing equation: ln * _{HCl} = 6 standard error in * _{HCl} abo	273.15 278.05 280.15 283.15 290.15 293.15 296.45 303.15 308.15 313.15 315.45 323.15 324.15	0.170 0.160 0.139 0.126 0.098 0.084 0.068	0.145 0.138 0.122 0.112 0.0892 0.0775 0.0637 100) - 34.0 line = 1.45	0.150 0.135 0.117 0.0986 0.0811 0.0652 17 ln(T/100) × 10 ⁻³
Butanc [107-9	oic acid; C ₄ H ₈ O ₂ ; 2-6	282.75 283.15 291.05 293.15 294.45 303.15 306.25 313.15 316.95 323.15	0.206 0.166 0.152 0.105 0.085	0.1710 0.1420 0.1320 0.0950 0.0783	0.172 0.133 0.105 0.0841 0.0683
Smooth	ling equation: $\ln x_{HC1} = -\frac{1}{2}$ tandard error in x_{HC1} abo	9.216 a ut the	- 21.107/(T/ regression	100) line = 3.01	× 10 ⁻³
2-Meth C ₄ H ₈ O ₂	ylpropanoic acid; ; [79-31-2]	291.35 293.15 298.65 303.15 303.95 313.15 320.45 323.15	0.138 0.119 0.101 0.068	0.1210 0.1060 0.0917 0.0637	0.117 0.0945 0.0754 0.0596
Smooth	ing equation: $\ln x_{HCl} = 4$ tandard error in x_{HCl} abo	0.660 - ut the	- 51.184/(T/ regression	100) - 23.56 line = 2.18	55 ln(T/100) × 10 ⁻³
3-Meth C ₅ H ₁₀ O	2; [503-74-2]	273.15 278.95 283.15 287.55 293.15 301.15 303.15 306.95 313.15 318.15 323.15	0.200 0.154 0.108 0.093 0.069	0.1670 0.1330 0.0975 0.0851 0.0645	0.191 0.150 0.118 0.0925 0.0729 0.0575
, care	ing equation: $\ln x_{HCl} = 1$ Standard error in x_{HCl} ulated by the compiler othing equation and smoot				

EXPERIMENTAL VALUES:

T/K	Acetic Acid	Hydrogen Chloride	Mol Ratio	Mol Fraction
	w_1 /wt %	g per 100 g solvent	n_{1}/n_{2}	<i>x</i> ₁
273.15	89.49 100.0	31.392 25.0 ¹	0.4111	0.2921
298.15	99.45 100.0	8.349 7.60	0.125	0.111

The author reported the solubility of hydrogen chloride at a total pressure of one atm (101.325 kPa) in various solutions of aqueous acetic acid.

The compiler used the author's data to estimate the solubility of HCl in 100 % acetic acid. The mole ratio and mole fraction values were calculated from the estimated values. The compiler prepared his own plot of g HCl per 100 g solvent vs. weight % acetic acid for the estimate.

The values at 273.15 K are for a hypothetical pure liquid acetic acid, since acetic acid is normaly a solid at this temperature. The melting point of acetic acid is 289.75 K (16.604 °C).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of the initial solution of acetic acid was determined by titration with carbonate free sodium hydroxide solution with phenolphalein as indicator.

Hydrogen chloride was absorbed in the liquid in a U-tube absorber. Samples were removed for the estimation of HCl content by titration with silver nitrate.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. The gas was prepared from sodium chloride and sulfuric acid.
- (2) Acetic acid. Merck and Co.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Rodebush, W. H.; Ewart, R. H. [7647-01-0] (2) Acetic acid; C₂H₄O₂; J. Am. Chem. Soc. 1932, 54, [64-19-7] 419 - 423. VARIABLES: PREPARED BY: T/K = 298.00 $p_1/kPa = 1.29 - 12.40$ W. Gerrard (9.7 - 93.0 mmHg)

EXPERIMENTAL	VALUES:			
ı	Temp	erature	Hydrogen Chloride Partial Pressure	Mol Fraction
	t/°C	<i>T/</i> K	p ₁ /mmHg	<i>x</i> ₁
	24.85	298.00	9.7	0.00242
1			9.4	0.00206
			15.0	0.00349
			17.3	0.00406
			28.6	0.00632
			31.6	0.00695
			46.9	0.0105
			50.9	0.0110
			52.8	0.0115
			58.8	0.0137
			93.0	0.0208

The following approximate results were also given:

- a 5 wt % solution had p_1 = 470 mmHg (x_1 = 0.0798, by compiler), and a 3 wt % solution had p_1 = 300 mmHg (x_1 = 0.0484, by compiler).

NOTE: The data recorded in the table should not be extrapolated linearly beyond 100 mmHg.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A dynamic method was used to determine the vapor pressure of the hydrogen chloride over the solution of acetic acid. A known volume of air was drawn through the solution, and the contents were determined by chemical titrations. Allowance for the pressure due to acetic acid appears to have been 15.6 mmHg, the vapor pressure of pure acetic acid at 25 °C.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from c. p. sodium chloride and c. p. 95 % sulfuric acid.
- (2) Acetic acid. Strictly c. p. acetic acid (99.5 %) was distilled, and the middle portion was frozen to give acid (99.7 %).

ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Acetic acid; C₂H₄O₂; [64-19-7]

ORIGINAL MEASUREMENTS:

Kumar, S.; Gehlawat, J. K.

J. Chem. Tech. Biotechnol. 1979, 29, 353 - 360.

VARIABLES:

T/K: 303 - 333

Total P/kPa: 101

PREPARED BY:

W. Gerrard H. L. Clever

EXPERIMENTAL VALUES:

-,	Estimato ICl Pre		Hydrogen Chloride Concentration	Estimated Mol Ratio	Estimated Mol Fraction
F	/kPa	p_1/atm	$c_1/\text{mol dm}^{-3}$	n_1/n_2	x_1
	-				
303	99	0.98	1.96	0.113	0.102
313	97	0.96	1.37	0.080	0.074
323	93.5	0.926	0.88	0.052	0.0495
333	89.2	0.883	0.57	0.034	0.033

The compiler calculated the hydrogen chloride partial pressure, mole ratio and mole fraction values. The partial pressure was calculated by subtracting the vapor pressure of acetic acid from 101 kPa (1 atm). The mole ratio and mole fraction values were calculated with the assumption that the solution density was equal to the density of pure acetic acid.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was bubbled through the solvent at atmospheric pressure. The increase of weight on the take up of HCl by the acetic acid was determined

- SOURCE AND PURITY OF MATERIALS:
 - (1) Hydrogen chloride. Analytical grade.
- HCl by the acetic acid was determined. (2) Acetic acid. Analytical grade.

ESTIMATED ERROR:

 $\delta c/c = 0.15$ (authors)

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. Acetic Acid; C₂H₄O₂;
 [64-19-7]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. <u>1970</u>, 20, 109 - 115

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	n HC1/ n C $_{2}$ H $_{4}$ O $_{2}$	X _{HC1}
253.15 263.15 273.15 283.15 293.15	0.65 0.46 0.29 0.21 0.15	0.394 0.315 0.225 0.174 0.130

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = 34.487 - 38.426/(T/100) - 21.778 \ln (T/100)$

Standard error about regression line 8.82×10^{-3}

T/K	Mol Fraction
	x _{HCl}
253.15 263.15	0.398 0.305
273.15	0.231
283.15 293.15	0.174 0.130
298.15	0.112

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1, 2).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- Acetic Acid. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.025$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. <u>1972</u>, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Acetic acid; C₂H₄O₂; [64-19-7]

ORIGINAL MEASUREMENTS:

Kitvinenko, V. I.; Kapova, Z. K.

Izv. Akad. Nauk. Kaz. SSR, Ser. Khim. 1972, 22, 75 - 77.

VARIABLES:

T/K = 293.15 - 353.15p/kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Hydrogen Chloride	Mol Fraction 1	Mol Fraction ²
	ω ₁ /wt %	x_1	x_1
293.15	8.21	0.128	0.130
313.15	4.75	0.0760	0.0793
333.15 353.15	2.83 1.29	0.0458 0.0211	0.0515 0.0285

¹ The mole fraction values were calculated by the compiler assuming the weight per cent solubility values were for a total pressure of one atm.

The solubility of hydrogen chloride in aqueous acetic acid is also reported in the paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

It was stated that the apparatus of Cupr (1) was used.

The concentration of HCl was determined as weight % at successive intervals of time until a constant value was obtained.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. The gas was prepared from sodium chloride and sulfuric acid. Dried by sulfuric acid.
- (2) Acetic acid. Stated to be of 99.8 per cent purity.

ESTIMATED ERROR:

REFERENCES:

1. Cupr, V.

**Recl. Trav. Chim. Pays-Bas 1928,
47, 55.

 $^{^2}$ The mole fraction values were calculated by the compiler for a hydrogen chloride partial pressure of one atm. The acetic acid vapor pressure was calculated as $p_2=p_2^0\,(1\,-\,x_1)$ where $p_2^{}$ is the pure liquid acetic acid vapor pressure.

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. Hexanoic Acid; C₆H₁₂O₂;
 [142-62-1]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. <u>1970</u>, 20, 109 - 115.

VARIABLES:

T/K: 213.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

nHCl/nC6H12O2 EXPERIMENTAL VALUES: Mol Fraction T/K X_{HC1} 1.68 0.627 213.15 0.569 1.32 223.15 233.15 1.04 0.510 243.15 0.75 0.429 0.346 253.15 0.53 0.38 0.275 263.15 0.213 0.27 273.15 283.15 0.20 0.167 293.15 0.19 0.160

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $1n \times_{HC1} = 28.986 - 33.458/(T/100) - 18.135 1n (T/100)$ Standard error about regression line = 1.73 x 10⁻²

T/K	Mol Fraction
	X _{HC1}
213.15	0.647
223.15	0.569
233.15	0.489
243.15	0.412
253.15	0.342
263.15	0.280
273.15	0.226
283.15	0.182
293.15	0.145

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K, a chemical titration was performed.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- Hexanoic Acid. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.03$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chloroacetic acid; C₂H₃O₂Cl; [79-11-8]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1956, 6, 241-244.

VARIABLES:

T/K: 322.15 - 338.65 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: __

T/K	Mole Ratio nHCl/nC2H3O2Cl	Mole Fraction x1
322.15	0.030	0.0291
328.45	0.023	0.0225
338.65	0.015	0.0148

The mole fraction solubility values were calculated by the compiler.

Smoothed Data: $\ln x_1 = -17.436 + 44.786/(T/100)$

Standard error about regression line = 1.71×10^{-4}

T/K	Mole Fraction x_1
313.15	0.0435
323.15	0.0280
333.15	0.0184
343.15	0.0125

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an all-glass apparatus.

The all glass absorption vessel (50 cm³) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Self prepared and dried.
- (2) Chloroacetic acid. High-grade specimen was distilled and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

 $\delta x_1/x_1 = 0.01$

- Hydrogen chloride; HCl; [7647-01-0]
- (2) Trichloroacetic acid; C2HCl3O2; [76-03-9]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1956, 6, 241-244.

VARIABLES:

T/K: 323.65 - 339.85 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mole Ratio nHC1/nC2HC13O2	Mole Fraction x 1
323.65	0.029	0.0282
329.55	0.023	0.0225
335.35	0.018	0.0177
339.85	0.015	0.0148

The mole fraction solubility values were calculated by the compiler.

Smoothed Data: $\ln x_1 = 85.160 - 110.324/(T/100) - 46.522 \ln (T/100)$

Standard error about regression line = 1.09×10^{-4}

T/K	Mole Fraction
	<u>x</u> 1
323.15	0.0288
333.15	0.0194
343.15	0.0129

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

all-glass apparatus.

The all glass absorption vessel (50 cm3) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas $\,$ absorbed was determined by weighing.

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride was generated in an (1) Hydrogen chloride. Self prepared and dried.
 - (2) Trichloroacetic acid. Highgrade specimen was distilled and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

 $\delta x_1/x_1 = 0.005$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Esters of Carboxylic Acids and of Carbonic Acid

EVALUATOR:

Peter G. T. Fogg
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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Esters of Carboxylic Acids and of Carbonic Acid.

Gerrard & Macklen (1) have measured the solubility of hydrogen chloride in various alkanoic esters over temperature ranges at a total pressure equal to barometric pressure. Mole fraction solubilities are high relative to reference values given by the Raoult's law equation (0.0214 at 298.15 K). If the variation of mole fraction solubilities approximates to the Margules equation then mole fraction solubilities at a partial pressure of 101.3 kPa will be close to mole fraction solubilities at a total pressure of 101.3 kPa even though pure solvents have appreciable vapor pressures at the temperatures of measurement.

Table 1. Mole fraction solubilities of hydrogen chloride in alkyl esters of carboxylic acids at 298.15 K and total pressure of 1.013 bar.

Ester &	Gerrard Macklen·(1)	Ionen & Shverina (2)	Chesterman (3)	Cook (4)
ethyl formate	0.170			
methyl acetate	0.302	0.250	0.63	
ethyl acetate	0.314	0.240	0.39	
1-methylethyl acetate	0.343	0.240		
propyl acetate	0.328	0.243		
2-methylpropyl acetate	0.338			
1-methylpropyl acetate	0.343			
butyl acetate	0.331	0.244		
pentyl acetate	0.333			
octyl acetate	0.334			
phenyl acetate	0.190			
benzyl acetate	0.243			
ethyl benzeneacetate	0.261			
ethyl propanoate	0.315			
ethyl butanoate	0.324			
propyl butanoate				0.293

Gerrard's measurements indicate that mole fraction solubilities in straight chain alkyl acetates increase with chain length. The solubility in propyl butanoate from an extrapolation of measurements by Cook does not fit into the pattern. Solubilities in non-linear alkyl acetates are greater than in linear acetates having the same carbon number. Solubility also increases with carbon number in the series ethyl formate to ethyl butanoate. Mole fraction solubility in phenyl acetate is less than in methyl acetate but is greater in benzyl acetate and ethyl benzeneacetate.

Solubilities at 298.15 K and a total pressure of 1.013 bar were also reported by Ionen & Shverina (2) for methyl, ethyl, propyl, 1-methylethyl and butyl acetates. The values of mole fraction solubilities are appreciably less than those reported by Gerrard. Mole fraction solubilities in methyl acetate and ethyl acetate from data published by Chesterman (3) for the same conditions are, on the contrary, appreciably greater than Gerrard's values.

The measurements reported by Gerrard & Macklen extend over a much wider range of temperatures than those reported by other workers. Their data are self consistent for each compound. Nevertheless, in view of the discrepancies between data from different sources, further measurements on these systems are required.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Esters of Carboxylic Acids and of Carbonic Acid

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

Gerrard and co-workers (1,5) have also measured solubilities in various chlorinated esters and in the ethyl ester of bromoacetic acid over temperature ranges at a total pressure of 1.013 bar. The presence of halogen lowers the mole fraction solubility of hydrogen chloride. be seen in Table 2, solubilities in the various chlorinated derivatives of ethyl acetate are less than in ethyl acetate itself. The greater the number of chlorine atoms the lower the solubility. Solubilities in derivatives of chlorinated acetic acid are less than in derivatives of 2-chlorinated Solubility in the ethyl ester of bromoacetic acid is less than ethanols. in the ethyl ester of chloroacetic acid. Solubility in the ethyl ester of 3-chloropropionic acid is less than in ethyl propionate. Solubility in the ethyl and in the 1-propyl ester of chloroformic acid is less than in ethyl formate. In general the data for this class of compounds is self-consistent and likely to be reliable although later measurements of the solubility in ethyl and propyl chloroformate (5) are not in agreement with earlier measurements (1) in the same laboratory.

Table 2 Mole fraction solubilities of hydrogen chloride in chlorinated esters at 298.15 K and total pressure of 1.013 bar.

Ester	* _{HCl} at 298.15 к	Reference
(ethyl formate)	0.170	(1)
ethyl chloroformate	0.0526	(1)
	0.0666	(5)
1-propyl chloroformate	0.0582	(1)
	0.0794	(5)
hexyl chloroformate	0.0943	(5)
butyl chloroformate	0.0822	(5)
(ethyl acetate)	0.314	(1)
ethyl chloroacetate	0.157	(6)
ethyl bromoacetate	0.172	(1)
ethyl dichloroacetate	0.172	(1)
1 -		
ethyl trichloroacetate	0.0653	(1)
2-chloroethyl acetate	0.209	(1)
2,2,2-trichloroethyl acetate	0.153	(1)
(phenyl acetate)	0.190	(1)
phenyl chloroacetate	0.150	(5)
ethyl propanoate	0.315	(1)
ethyl 3-chloropropanoate	0.227	(6)
1		(0)

Gerrard et al.(5) measured solubilities in four esters of carbonic acid at a total pressure of 1.013 bar over temperature ranges. Solubilities are high relative to the reference line corresponding to the Raoult's law equation. Under the conditions of the experiments the mole fraction solubility at a total pressure of 1.013 bar will differ from the mole fraction solubility at a partial pressure by less than 2%. Mole fraction solubilities in the different esters are close to each other in the overlap of the temperature ranges. Solubility of hydrogen chloride in ethyl 2-chloroethyl carbonate was also measured by these authors under the same conditions. As in the case of ethers and esters of carboxylic acids, the presence of the chlorine atom lowers the mole fraction solubility of this gas. Interpolated mole fraction solubilities at 298.15 K and a total pressure of 1.013 bar are as follows:

diethyl carbonate	0.254
dibutyl carbonate	0.271
diisobutyl carbonate	0.284
diisopentyl carbonate	0.271
ethyl 2-chloroethyl carbonate	0.202

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Esters of Carboxylic Acids and of Carbonic Acid

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

The data for these esters of carbonic acid are self-consistent and are likely to be reliable but confirmation by comparison with independent measurements is not possible.

Cook (4) measured solubilities in several esters of unsaturated acids and of unsaturated alcohols over short temperature ranges at a total pressure equal to barometric. Under the conditions of the experiments solubilities at a partial pressure of 1.013 bar are likely to be close to the measured solubilities. Mole fraction solubilities are high relative to the reference line based upon the Raoult's law equation. Values for ethyl crotonate are close to values for crotyl acetate and to values for ethyl butanoate. Values for allyl acetate, propionate and butanoate are lower but close to each other. For the solvents in this group mole fraction solubility is lowest in propargyl butyrate. No measurements by other authors are available for comparison and the reliability of these measurements cannot be judged.

Table 3 Mole fraction solubilities of hydrogen chloride in unsaturated esters at 283.15 K and a partial pressure of 1.013 bar.

Ester		*HCl	ref.
1-Propen-2-ol acetate (allyl acetate) 2-Buten-1-ol acetate (crotyl acetate) Propionic acid, 2-propenyl ester (allyl propanoate) 2-Butenoic acid, ethyl ester (ethyl crotonate) Butanoic acid, 2-propynyl ester (propargyl butanoate) Butanoic acid, 2-propenyl ester (allyl butanoate) (Propyl acetate) (Ethyl butanoate)	C5H8O2 C6H10O2 C6H10O2 C6H10O2 C7H10O2 C7H12O2 C5H10O2 C6H12O2	0.354 0.403 0.361 0.410 0.263 0.363 0.402 0.398	(4) (4) (4) (4) (4) (1) (1)
(Propyl butanoate)	C ₇ H ₁ 4O ₂	0.410	(4)

- Gerrard, W.; Macklen, E. D. J. Appl. Chem. <u>1956</u>, 6, 241 244.
- Ionin, M. V.; Shverina, V. G. Zh. Obshch. Khim. 1965, 35, 209 211; J. Gen. Chem. USSR 1965, 35, 211 212.
- 3. Chesterman, D. R. J. Chem. Soc. 1935, 906 910.
- 4. Cook, T. M. Thesis, 1966, University of London.
- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89 - 93; 1960, 10, 115 - 121.
- Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1959, 9, 85 88.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Esters of aliphatic carboxylic acids.

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E.D.

J. Appl. Chem. 1956, 6, 241-244

VARIABLES:

T/K: See below

Total P/kPa : 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

TATERINAL VALUE.	*	Mole ratio Cl ^{/n} ester	Mole* fraction *HCl	Smoothed** mole fraction *HC1	
Formic acid, ethyl ester,	273.15			0.287	
(ethyl formate); $C_3^H 6^O_2$; [109-94-4]	281.25 283.15	0.398	0.285	0.275	
	288.35 293.15	0.316	0.240	0.210	
	297.45	0.215	0.177	0.210	
	301.75 303.15	0.170	0.145	0.132	
	306.65	0.118	0.106		
	313.15			0.070	

Smoothing equation: $\ln x_{HCl} = 381.135 - 523.963/(T/100) - 189.640 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 4.81×10^{-3}

Acetic acid, methyl ester, (methyl acetate); $C_3^H_6^{O_2}$; [79-20-9]	273.15 274.75 279.75	0.719 0.654	0.418 0.395	0.423
	283.15			0.380
	287.85	0.554	0.356	
	292.15	0.504	0.335	
	293.15			0.330
	296.45	0.454	0.312	
	299.45	0.420	0.296	
	303.15			0.276
	303.55	0.375	0.273	

Smoothing equation: $\ln x_{HC1} = 71.059 - 94.752/(T/100) - 37.051 \ln(T/100)$ Standard error in x_{HC1} about the regression line = 9.97 × 10⁻⁴

- * calculated by the compiler
 ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an all-glass apparatus.

The all-glass absorption vessel (50 cm³) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Esters: high grade specimens were distilled and attested.

ESTIMATED ERROR:

±0.1 $\delta T/K =$ $= \pm 0.02$ $\delta x_{\text{HCl}}/x_{\text{HCl}}$

0.355

0.299

0.241

0.187

Hydrogen Chloride in Non-Aqueous Solvents ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen chloride; HCl; Gerrard, W.; Macklen, E.D. [7647-01-0] J. Appl. Chem. 1956, 6, 241-244 Esters of aliphatic carboxylic (2) acids. EXPERIMENTAL VALUES: T/K Mole ratio Mole* Smoothed** fraction mole fraction ⁿHCl^{/n}ester xHCl xHC1 Acetic acid, ethyl ester, 273.15 0.418 (ethyl acetate); C4H8O2; 278.05 0.700 0.412 [141-78-6] 282.85 0.638 0.389 283.15 0.390 288.25 0.573 0.364 293.15 0.342 293.55 0.510 0.338 301.85 0.416 0.294 303.15 0.284 306.45 0.366 0.268 313.15 0.225 317.95 0.246 0.197 323.15 0.171 Smoothing equation: $\ln x_{\rm HC1} = 109.975 - 149.726/(T/100) - 55.762 \ln(T/100)$ Standard error in $x_{\rm HC1}$ about the regression line = 3.89 \times 10⁻³ Acetic acid, propyl ester; $C_5H_{10}O_2$; [109-60-4] 273.15 0.430 278.81 0.720 0.419 282.35 0.677 0.406 283.15 0.402 285.65 0.633 0.388

Smoothing equation: $\ln x_{HCl} = 100.477 - 136.692/(T/100) - 51.030 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 2.98 × 10⁻³

0.536

0.483

0.386

0.257

0.349

0.326

0.278

0.204

293.15

293.95

298.25

303.15

307.25

313.15

319.56

323.15

Acetic acid, 1-methylethyl	282.65	0.728	0.421	
ester; C ₅ H ₁₀ O ₂ ; [108-21-4]	283.15			0.416
5 10 2	289.55	0.633	0.388	
	293.15			0.372
	293.75	0.576	0.365	
	301.95	0.469	0.319	
	303.15			0.310
	307.35	0.400	0.286	
	313.15			0.243
	321.45	0.233	0.189	
	323.15		• • • • •	0.180

Smoothing equation: $\ln x_{HC1} = 141.452 - 194.592/(T/100) - 70.720 \ln(T/100)$ Standard error in x_{HC1} about the regression line = 4.38×10^{-3}

^{*} calculated by the compiler

^{**} smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS:		MEASUREMENTS	
(1) Hydrogen chloride; HCl; [7647-01-0]		W.; Macklen,	
(2) Esters of aliphatic carboxylic acids.	J. Appl.	Chem. <u>1956</u> ,	6, 241-244
EXPERIMENTAL VALUES: T/K	Mole ratio	Mole*	Smoothed**
	HCl ^{/n} ester	fraction	mole fraction
		^x HCl	xHCl
Acetic acid, 2-methylpropyl 273.15 ester; C ₆ H ₁₂ O ₂ ; [110-19-0] 279.25		0.436	0.447
283.15			0.419
287.45 293.15		0.395	0.368
293.65 303.15		0.361	0.306
303.65 308.05	0.442 0.383	0.307 0.277	
313.15			0.243
317.35 323.15	0.276	0.216	0.185
Smoothing equation: $\ln x_{} = 111.201$	- 151.463/	/(T/100) - 56	.283 ln(T/100)
Smoothing equation: $\ln x_{HCl} = 111.201$ Standard error $\ln x_{HCl}$ about the	regression	line = 4.63	× 10 ⁻³
Acetic acid, 1-methylpropyl 273.15	0.040		0.457
ester; C ₆ H ₁₂ O ₂ ; [105-46-4] 277.25 283.15	0.818	0.450	0.425
288.85 293.15	0.649	0.394	0.374
294.55		0.361	
303.05 303.15	0.459	0.315	0.312
308.65 313.15	0.392	0.282	0.249
317.85	0.280	0.219	
323.15			0.192
Smoothing equation: $\ln x_{HC1} = 102.632$ Standard error in x_{HC1} about the	- 139.384/ regression	(T/100) - 52 n line = 4.96	.133 ln(T/100) × 10 ⁻³
Acetic acid, butyl ester; 273.15 C ₆ H ₁₂ O ₂ ; [123-86-4] 277.95	0.741	0.426	0.436
283.15			0.405
283.85 292.85	0.665 0.556	0.399 0.357	
293.15			0.358
300.65	0.467	0.318	0.303
312.65 313.15	0.337	0.252	0.247
318.15	0.279	0.218	
323.15			0.195
Smoothing equation: $\ln x_{HC1} = 89.114$ Standard error in x_{HC1} about the	- 120.793/(regression	T/100) - 45. n line = 3.24	501 ln(T/100) × 10 ⁻³
Acetic acid, octyl ester; 273.15	0 747	0.400	0.434
C ₁₀ H ₂₀ O ₂ ; [112-14-1] 277.55 283.15	0.747	0.428	0.408
288.85 293.15	0.610	0.379	0.361
295.35	0.533	0.348	
303.15 303.35	0.440	0.306	0.305
310.75 313.15	0.356	0.263	0.246
320,75	0.255	0.203	
323.15	_ 137 386/	/(m/100) 51	0.192
Smoothing equation: $\ln x_{HC1} = 100.796$ Standard error in x_{HC1} about the * calculated by the compiler	regression	(17/100) = 51 1 line = 3.63	.121 ln(T/100) × 10 ⁻³
** smoothing equation and smoothed va	lues were	calculated b	y H.L. Clever

ORIGINAL MEASUREMENTS: COMPONENTS: Gerrard, W.; Macklen, E.D. Hydrogen chloride; HCl; (1) [7647-01-0] J. Appl. Chem. 1956, 6, 241-244 Esters of aliphatic carboxylic (2) Mole ratio Mole* Smoothed** **EXPERIMENTAL VALUES:** T/K ⁿHCl^{/n}ester fraction mole fraction x HCl XHCl Acetic acid, phenyl ester, 273.15 0.275 (phenyl acetate); C₈H₈O₂; 277.05 0.367 0.268 283.15 0.248 [122-79-2] 0.323 0.244 283.45 0.211 293.15 291.55 0.275 0.216 300.55 0.222 0.182 303.15 0.170 0.170 0.145 309.95 0.132 313.15 315.15 0.142 0.124 0.115 323.15 Smoothing equation: $\ln x_{HC1} = 103.449 - 139.930/(T/100) - 53.253 \ln(T/100)$ Standard error in x_{HC1} about the regression line = 2.24 × 10⁻³ 0.341 273.15 Acetic acid, phenylmethyl 277.95 0.489 0.328 ester, (benzyl acetate); 283.15 0.309 $C_9H_{10}O_2$; [140-11-4] 284.15 0.436 0.304 0.392 0.282 289.35 293.15 0.266 297.65 0.327 0.246 303.15 0.220 0.216 304.15 0.275 313.15 0.175 315.45 0.197 0.165 323.15 0.135 Smoothing equation: $\ln x_{\rm HCl}$ = 90.759 - 122.460/(T/100) - 46.776 $\ln({\rm T}/100)$ Standard error in $x_{\rm HCl}$ about the regression line = 1.10 \times 10⁻³ 273.15 0.417 Propanoic acid, ethyl ester, (ethyl propionate); C₅H₁₀O₂; 280.15 0.684 0.406 [105-37-3] 283.15 0.390 0.642 0.391 283.45 287.45 0.593 0.372 293.15 0.343 293.95 0.514 0.339 301.45 0.429 0.300 303.15 0.286 311.65 0.315 0.240 313.15 0.228 319.35 323.15 0.240 0.194 0.174 Smoothing equation: $\ln x_{\text{HCl}} = 108.525 - 147.853/(T/100) - 55.005 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 2.52 × 10⁻³ 273.15 0.428 Butanoic acid, ethyl ester, (ethyl butyrate); $C_6H_{12}O_2$; 279.25 0.707 0.414 [105-54-4] 283.15 0.398 283.35 0.652 0.395 0.351 293.15 0.472 298.56 0.321 303.15 0.296 306.15 0.391 0.281 313.15 0.240 0.237 313.75 0.311 0.211 318.55 0.267 0.188 323.15 Smoothing equation: $\ln x_{\text{HCl}} = 93.226 - 126.530/(\text{T}/100) - 47.522 \ln(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 2.03×10^{-3} * calculated by the compiler

** smoothing equation and smoothed values were calculated by H.L. Clever.

COMPONENTS:

(1) Hydrogen chloride; HCl; Chesterman, D. R.

[7647-01-0]

(2) Esters

VARIABLES:

T/K: 298.15

Total P/kPa: 101 (~1 atm)

ORIGINAL MEASUREMENTS:

Chesterman, D. R.

J. Chem. Soc. 1935, 906 - 910.

VARIABLES:

W. Gerrard

EXPERIMENTAL VALUES:

T/K Observed Solubility Mol Fraction Pressure g HCl g⁻¹ Solution p/mmHq Acetic acid, methyl ester or methyl acetate; $C_3H_6O_2$; [79-20-9] 298.15 760 0.46 0.63 Acetic acid, ethyl ester or ethyl acetate; C4H8O2; [141-78-6] 298.15 0.39 765 0.21

The mole fraction solubility values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus was that used for the conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess standard base which was back titrated with a standard acid solution.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P₂O₅.
- (2) Methyl acetate. Was stated to be the purest obtainable. Dried with phosphorus pentoxide, b.p./°C (760 mmHg) = 57.3 - 57.8.

Ethyl acetate. Was stated to be the purest obtainable. Dried with P_2O_5 , b.p./°C (765 mmHg) = 76.8 - 77.2.

COMPONENTS: ORIGINAL MEASUREMENTS: Ionin, M. V.; Shverina, V. G. Hydrogen chloride; HCl; [7647-01-0] Zh. Obshch. Khim. 1965, 35, 209-211. (2) Acetic acid, alkane esters; J. Gen. Chem. USSR (Engl. Transl.) 1965, 35, 211 - 212. $C_3H_6O_2$ and $C_4H_8O_2$ VARIABLES: PREPARED BY: T/K: 298.15 Total P/kPa: 101.3 (atmospheric) W. Gerrard EXPERIMENTAL VALUES: Refractive Index¹ *D Solution Mol Ratio Mol Fraction T/K Density n_1/n_2 $\rho/g cm^{-3}$ Acetic acid, methyl ester; C3H6O2; [79-20-9] 0.333 298.15 1.36184 0.96322 Acetic acid, ethyl ester; CAHgO2; [141-78-6] 0.2400 0.92652 0.316 1.37248 298.15 1 Pure solvent values. Mole ratio values calculated by the compiler. AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD/APPARATUS/PROCEDURE: (1) Hydrogen chloride. Prepared The ester was saturated with hydrogen from pure sodium chloride and chloride at 298.2 K and atmospheric pressure, not specified. An aliquot sulfuric acid, and dried by sulfuric acid and calcium of the solution was diluted with water and titrated with alkali. chloride. (2) Acetic acid, alkane esters. Stated to be "pure". ESTIMATED ERROR: REFERENCES:

216 Hydrogen Chloride in Non-Aqueous Solvents COMPONENTS: ORIGINAL MEASUREMENTS: Ionin, M. V.; Shverina, V. G. Hydrogen chloride; HCl; [7647-01-0] Zh. Obshch. Khim. 1965, 35, 209-211. (2) Acetic acid, alkane esters; J. Gen. Chem. USSR (Engl. Transl.) 1965, 35, 211 - 212. $C_5H_{10}O_2$ and $C_6H_{12}O_2$ **VARIABLES:** PREPARED BY: T/K: 298.15 W. Gerrard Total P/kPa: 101.3 (atmospheric) EXPERIMENTAL VALUES: Solution Mol Ratio Mol Fraction T/K Refractive Index Density n_1/n_2 p/g cm-3 Acetic acid, propyl ester; $C_5H_{10}O_2$; [109-60-4] 1.38310 0.92210 0.321 298.15 Acetic acid, 1-methyl ethyl ester; $C_5H_{10}O_2$; [108-21-4] 0.93304 0.317 298.15 1.37668 Acetic acid, butyl ester; C₆H₁₂O₂; [123-86-4] 0.90420 0.323 0.2441 298.15 1.39361 1 Pure solvent values. Mole ratio values calculated by the compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) Hydrogen chloride. Prepared The ester was saturated with hydrogen

METHOD/APPARATUS/PROCEDURE: The ester was saturated with hydrogen chloride at 298.2 K and atmospheric pressure, not specified. An aliquot of the solution was diluted with water and titrated with alkali. (1) Hydrogen chloride. Prepared from pure sodium chloride and sulfuric acid, and dried by sulfuric acid and calcium chloride. (2) Acetic acid, alkane esters. Stated to be "pure".

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Acetic acid pentyl ester or n-amyl acetate; C7H14O2; [628-63-7]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1959, 9, 85 - 88.

VARIABLES:

T/K:

279.85 - 314.75 T/k: 2/9.85 - 314.75 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC7H14O2	Mol Fraction **HCl
279.85	0.723	0.420
282.55	0.687	0.407
288.35	0.615	0.381
294.15	0.545	0.353
300.25	0.476	0.322
306.45	0.407	0.289
314.75	0.318	0.241

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = 84.774 - 114.771/(T/100) - 43.344 \ln (T/100)$

Standard error about regression line = 1.90×10^{-3}

T/K	Mol Fraction
	xHCl
283.15 293.15 303.15 313.15	0.418 0.370 0.315 0.258

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared and dried.
- (2) Acetic acid pentyl ester or n-amyl acetate. Purified, distilled, and attested by physical constants.

ESTIMATED ERROR:

 $\delta x/x = 0.01$

REFERENCES:

Gerrard, W.; Macklen, E. D.
 J. Appl. Chem. 1956, 6, 241.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Benzeneacetic acid, ethyl ester; $C_{10}^{H}_{12}^{O}_{2}$; [101-97-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1959, 9, 85 - 88.

VARIABLES:

T/K: 273.15 - 320.65 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
273.15	0.592	0.372
281.95	0.504	0.335
291.05	0.414	0.293
303.05	0.310	0.237
308.65	0.267	0.211
314.45	0.219	0.180
320.65	0.172	0.147

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HCl} = 102.728 - 138.964/(T/100) - 52.600 \ln (T/100)$

Standard error about regression line = 4.87×10^{-3}

T/K	Mol Fraction x HCl
273.15	0.367
283.15	0.334
293.15	0.287
303.15	0.235
313.15	0.184
323.15	0.138

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Self prepared and dried.
- (2) Benzeneacetic acid, ethyl ester. Purified, distilled, and attested by physical constants.

ESTIMATED ERROR:

 $\delta x/x = 0.02$

REFERENCES:

Gerrard, W.; Macklen, E. D.
 J. Appl. Chem. 1956, 6, 241.

COMPONENTS: (1) Hydrogen chloride; HCl;	;	ORIGINAL MI Cook, T. M		3:
[7647-01-0]		Thomas 10	= <i>c</i>	
(2) Esters of carboxylic ac	cids	Thesis, 190 University	of London.	
VARIABLES: T/K: See below		PREPARED BY	r: errard	
Total P/kPa : 101.325 (1 atm	n)	,,,,	zriara	
EXPERIMENTAL VALUES:				
	т/к	Mole ratio	Mole*	
	n I	HCl ^{/n} borate	fraction	
			*HCl	*HC1
1 Propon 2 ol agotato	279.35	0.652	0.395	
1-Propen-2-ol acetate, (allyl acetate); C ₅ H ₈ O ₂ ;	280.35		0.393	
[108-22-5]	281.95		0.365	
	283.15	0.549	0.354	0.361
	291.35	0.455	0.313	
	293.15			0.301
Smoothing equation: ln x _{HCl}	6 363 -	+ 15.130/(T/	100)	
Standard error in *HCl	about the	regression	line = 5.49	×10 ⁻³
2-Buten-1-ol acetate,	279.65	0.760	0.432	
(crotyl acetate); C6H10O2;		0.706	0.414	
[628-08-0]			0.400	0.403
		0.640	0.390	0.014
	293.15			0.341
Smoothing equation: $\ln x_{}$	= -5.781 +	13.796/(T/	100)	
Standard error in xHCl	Smoothing equation: $\ln x_{\text{HCl}} = -5.781 + 13.796/(\text{T}/100)$ Standard error in x_{HCl} about the regression line = 4.42 × 10 ⁻³			2×10^{-3}
* calculated by the compile ** smoothing equation and s		alues were ca	alculated h	oy H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data were cited by Gerrard (1).

Hydrogen chloride was passed into a bubbler tube containing a weighed amount of solvent at the specified temperature until the increase in weight was constant at the barometric pressure (2).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: sample of best quality was self prepared and was passed through concentrated sulfuric acid and calcium chloride.
- (2) Esters: all esters fractionally distilled.

1-propen-2-ol acetate 2-buten-1-ol acetate propanoic acid,	.Pt.(1 atm)° 102-103.5 131-132.5 121.5-123	/C Refractive Index $n_D^{21} = 1.4051$ $n_D^{20} = 1.4197$ $n_D^{23.5D} = 1.4060$	Density $d^{2} = 0.901$ $d^{2} = 0.911$ $d^{2} = 0.899$
2-propenyl ester 2-butenoic acid, ethyl ester butanoic acid,	48 155-156	$n_D^{23} = 1.4237$ $n_D^{21.5} = 1.4213$	$d^{2}_{4}^{0} = 0.919$ $d^{2}_{4}^{0} = 0.947$
2-propynyl ester butanoic acid, 2-propenyl ester	113-114	$n_D^{25} = 1.4133$	$d^{20} = 0.895$
butanoic acid, propyl ester	143.5-145	$n_D^{32} = 1.3953$	$d^{24} = 0.8695$

ESTIMATED ERROR:

 $\delta x_{\text{HCl}}/x_{\text{HCl}} = \pm 0.005$

- Gerrard, W. J. Chim. Phys. 1964, 61, 73; Solubility of Gases in Liquids, Plenum Press, New York, 1976.
 Ahmed, W.; Gerrard, W.; Maladkar, W.K. J. Appl. Chem. 1970, 20, 109.

ORIGINAL MEASUREMENTS: COMPONENTS: Cook, T. M. (1) Hydrogen chloride; HCl; [7647-01-0] Thesis, 1966, (2) Esters of carboxylic acids University of London. EXPERIMENTAL VALUES: Smoothed** T/K Mole ratio Mole* n HCl $^{/n}$ borate fraction mole fraction XHC1 x_{HCl} Propanoic acid, 2-propenyl 273.15 0.435 ester, (allyl propionate); 281.55 0.592 0.372 283.15 0.564 C₆H₁₀O₂; [2408-20-0] 0.361 0.361 0.520 286.25 0.342 293.15 0.304 Smoothing equation: $\ln x_{HCl} = -6.097 + 14.381/(T/100)$ Standard error in x_{HCl} about the regression line = 3.14×10^{-4} 0.479 2-Butenoic acid, ethyl ester, 273.15 (ethyl crotonate); C6H10O2; 0.806 0.446 277.55 0.710 0.415 [10544-63-5] 281.95 283.15 0.700 0.412 0.410 0.699 283.15 0.411 0.379 289.15 0.610 293.15 0.362 303.15 0.326 Smoothing equation: $\ln x_{\rm HCl}$ = -32.423 + 49.458/(T/100) + 13.513 $\ln(\text{T/100})$ Standard error in $x_{\rm HCl}$ about the regression line = 2.11 \times 10⁻³ Butanoic acid, 2-propynyl 273.15 0.379 0.275 281.05 ester, (propargyl butyrate); С₇H₁₀O₂; [1932-93-0] 282.55 0.362 0.266 283.15 0.356 0.263 0.263 0.256 284.75 0.344 286.85 0.327 0.246 0.225 293.15 Smoothing equation: $\ln x_{HCl} = -107.987 + 155.955/(T/100) + 49.552 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 5.79 \times 10⁻⁴ Butanoic acid, 2-propenyl ester, (allyl butyrate); 273.15 0.438 0.410 0.696 276.65 281.35 0.585 0.369 $C_7H_{12}O_2$; [2051-78-7] 283.15 0.573 0.364 0.363 0.551 0.355 284.15 285.35 0.542 0.351 0.523 287.55 0.343 0.569 291.15 0.319 293.15 0.313 Smoothing equation: $\ln x_{HCl} \approx -54.106 + 80.510/(T/100) + 23.691 \ln(T/100)$ Standard error in x_{HCl} about the regression line = 3.97×10^{-3} 0.438 0.778 281.15 Butanoic acid, propyl ester; 0.694 $C_7H_{14}O_2$; [105-66-8] 283.15 0.410 0.412 0.692 0.409 283.15 284.25 0.662 0.398 288.25 0.584 0.369 0.327 293.15 Smoothing equation: $\ln x_{HCl} = -7.653 + 19.157/(T/100)$ Standard error in x_{HCl} about the regression line = 3.98 × 10⁻³ * calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever

COMPONENTS:		ORIGINAL ME	EASUREMENTS	
(1) Hydrogen chloride; HCl; [7647-01-0]		Gerrard, W.	.; Macklen,	E.D.
(2) Halogenated esters		J. Appl. Ci	hem. <u>1956</u> ,	6, 241-244
(2) halogenated esters				
VARIABLES:		PREPARED BY	Y:	
T/K: See below Total P/kPa: 101.325 (1 atm)		W. Ge	errard	
EXPERIMENTAL VALUES:				
	т/к	Mole ratio	Mole*	Smoothed**
	n.	HCl ^{/n} ester	fraction	mole fraction
			*HCl	*HCl
Carbonochloridic acid, ethyl	273.15			0.0908
ester, (ethyl chloroformate);	277.25		0.0893	0.0300
C ₃ H ₅ O ₂ Cl; [541-41-3]	281.45	0.088	0.0809	
3 5 2	283.15			0.0794
	288.75		0.0689	
	293.15			0.0620
	293.55		0.0602	
	301.05		0.0476	
	303.15			0.0437
	306.75		0.0394	0.0000
	313.15		0 0215	0.0282
	318.25 323.15		0.0215	0.0169
Smoothing equation: ln × _{HCl} = Standard error in × _{HCl} ab	204.296 out the	- 279.047/(7 regression]	r/100) - 10 line = 1.65	$4.032 \ln(T/100) \times 10^{-3}$
				0.0959
Carbonochloridic acid, propyl ester, (1-propyl	273.15 279.55	0.099	0.0901	0.0959
chloroformate); $C_4H_7O_2C1$;	282.55		0.0842	
[109-61-5]	283.15	0.092	0.0042	0.0841
[103-01-3]	293.15			0.0672
	293.35	0.071	0.0663	0.0072
	303.15		*******	0.0494
	304.05	0.051	0.0485	• • • • •
	313.15	-	· -	0.0339
	317.45	0.029	0.0282	
	323.15			0.0219
Smoothing equation: ln x _{HCl} = Standard error in x _{HCl} ab	166.569	- 227.164/(T	r/100) - 85	.335 ln(T/100)

Smoothing equation: $\ln x_{HC1} = 166.569 - 227.164/(T/100) - 85.335 \ln(T/100)$ Standard error in x_{HC1} about the regression line = 1.01 \times 10⁻³

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was generated in an all-glass apparatus.

The all-glass absorption vessel (50 cm³) comprised an inlet bubbler tube, an outlet tube, and the part holding a weighed amount of liquid. Each tube was fitted with a tap, and either a B-19 cone, or a B-19 socket. Entrained liquid was collected and allowed for. Temperature control was within 0.1 K. The amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride: selfprepared and dried.
- (2) Halo-esters: high grade samples were distilled and attested.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$

 $\delta x_{\text{HCl}}/x_{\text{HCl}} = \pm 0.02$

COMPONENTS:	ORIGINAL M	EASUREMENTS	•
(1) Hydrogen chloride; HCl; [7647-01-0]		.; Macklen,	
(2) Halogenated esters	J. Appl. Cl	hem. <u>1956</u> ,	6, 241-244
, , , , , , , , , , , , , , , , , , , ,			
EXPERIMENTAL VALUES:			
T/K	Mole ratio MOLE ratio	Mole* fraction	Smoothed** mole fraction
	nci ester	*HCl	*HCl
Dichloroacetic acid, ethyl 273.	15		0.165
ester, (ethyl 278.	95 0.180	0.153	0.103
dichloroacetate); C ₄ H ₆ O ₂ Cl ₂ ; 282. [535-15-9] 283.		0.145	0.144
286.	35 0.158	0.136	
293. 294.		0.118	0.120
301.	95 0.108	0.0975	
303. 312.		0.0766	0.0960
313.	15		0.0743
320. 323.		0.0593	0.0559
Smoothing equation: In v = 87 31	5 - 117.286/(T	/100) _ 45	957 ln(m/100)
Smoothing equation: $\ln x_{HC1} = 87.31$ Standard error $\ln x_{HC1}$ about t	he regression	line = 8.51	× 10 ⁻⁴
Trichloroacetic acid, ethyl 283.	15		0.0992
ester, (ethyl 283.	65 0.108	0.0975	
trichloroacetate); C ₄ H ₅ O ₂ Cl ₃ ; 293. [515-84-4] 295.		0.0715	0.0749
303.	15		0.0570
303. 312.		0.0548 0.0449	
313.			0.0437 0.0338
323. 324.		0.0329	0.0336
333.	15		0.0262
Smoothing equation: $\ln x_{HCl} = 8.760$ Standard error in x_{HCl} about t	- 3.701/(T/100 he regression	0) - 9.381 line = 1.07	ln(T/100) × 10 ⁻³
Bromoacetic acid, ethyl ester, 280.	15 0.312	0.238	
(ethyl bromoacetate); 283.	15		0.228
C ₄ H ₇ O ₂ Br; [105-36-2] 287. 293.		0.212	0.193
296.	15 0.218	0.179	
301.		0.158	0.151
307. 313.		0.134	0.110
320.	35 0.092	0.0842	
323.			0.0760 0.0496
Smoothing equation: ln x _{HCl} = 158.6 Standard error in x _{HCl} about t * calculated by the compiler	84 - 217.218/(7 he regression	line = 2.92	× 10 ⁻³
** smoothing equation and smoothed	values were ca	alculated b	y H.L. Clever

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0]	Gerrard, W.; Macklen, E.D.
(2) Halogenated esters	J. Appl. Chem. <u>1956</u> , 6, 241-244
EXPERIMENTAL VALUES:	Mole ratio Mole* Smoothed**
	HCl ^{/n} ester fraction mole fraction hCl raction
2-Chloroethanol acetate, 273.1	
(2-chloroethyl acetate); 279.9	
C ₄ H ₇ O ₂ Cl; [542-58-5] 283.1 290.1	
293.1	
300.2	
303.19 306.49	
313.1	
313.4	0.161 0.139
Smoothing equation: $\ln x_{\text{HCl}} = 119.619$ Standard error in x_{HCl} about the	θ - 162.125/(T/100) - 61.153 ln(T/100) e regression line = 1.47 × 10 ⁻³
2,2,2-Trichloroethanol 283.0	0.253 0.202
acetate, C ₄ H ₅ O ₂ Cl ₃ ; [625-24-1] 283.1!	0.203
291.09 293.19	
299.8	
303.1	
305.73 312.4	
312.4	
316.69	0.126 0.112
323.1!	0.101
Smoothing equation: ln x _{HCl} = - 7.24. Standard error in x _{HCl} about the	8 + 15.993/(T/100) e regression line = 2.02 × 10 ⁻³

^{*} calculated by the compiler
** smoothing equation and smoothed values were calculated by H.L. Clever

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Carbonochloridic acid ethyl ester or Ethyl chloroformate; C₃H₅O₂Cl; [541-41-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 273.15 - 300.35 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

T/K	Mol Ratio nHC1/nC3H502C1	Mol Fraction XHC1
273.15	0.169	0.145
277.75	0.142	0.124
282.85	0.119	0.106
289.35	0.0948	0.0866
300.35	0.0666	0.0624

Smoothed Data: $\ln X_{HC1} = -11.217 + 25.368/(T/100)$

Standard Error About Regression Line = 4.30×10^{-4}

	т/к	Mol Fraction XHCl
•	273.15 283.15 293.15 303.15	0.145 0.105 0.0770 0.0579

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Carbonochloridic acid ethyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Carbonochloridic acid propyl ester or 1-propyl chloroformate; C₄H₇ClO₂; [109-61-5] VARIABLES: T/K: 274.15 - 302.35 Total P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121. W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

т/к	Mol Ratio nHCl/nC4H7ClO2	Mol Fraction
274.15 282.95 292.75 302.35	0.179 0.139 0.101 0.0761	0.152 0.122 0.0917 0.0707

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -10.1355 + 22.665/(T/100)$

Standard error about the regression line is 2.57×10^{-3}

T/K	Mol Fraction x_1
273.15	0.159
283.15	0.119
293.15	0.0904
303.15	0.0700

AUXILIARY INFORMATION

METHOD 'APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Carbonochloridic acid propyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.015$$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chloroacetic acid ethyl ester; C₄H₇ClO₂; [105-39-5]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Macklen, E. D.

J. Appl. Chem. 1959, 9, 85 - 88.

VARIABLES:

T/K: 280.45 - 316.35 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio nHCl/nC4H7ClO2	Mol Fraction ^x HCl
280.45	0.290	0.225
284.05	0.269	0.212
290.25	0.232	0.188
297.95	0.186	0.157
303.85	0.158	0.136
312.15	0.114	0.102
316.35	0.094	0.0859

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HCl} = 157.789 - 215.066/(T/100) - 80.101 \ln (T/100)$

Standard error about regression line = 1.94×10^{-3}

T/K	Mol Fraction "HC1
283.15	0.215
293.15	0.178
303.15	0.137
313.15	0.0977
323.15	0.0660

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Self prepared and dried.
- (2) Chloroacetic acid ethyl ester. Purified, distilled, and attested by physical constants.

ESTIMATED ERROR:

 $\delta x/x = 0.02$

REFERENCES:

Gerrard, W.; Macklen, E. D.
 J. Appl. Chem. 1956, 6, 241.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Carbonochloridic acid butyl ester or butyl chloroformate; C₅H₉ClO₂; [592-34-7] VARIABLES: T/K: 273.15 - 313.15 Total P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121. PREPARED BY: W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio nHC1 ^{/n} C ₅ H ₉ ClO ₂	Mol Fraction
273.15 283.15 291.75 298.75 303.15 313.15	0.192 0.140 0.110 0.0885 0.0761 0.0551	0.161 0.123 0.0991 0.0813 0.0707 0.0522

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 54.299 - 67.462/(T/100) - 31.280 \ln (T/100)$

Standard error about the regression line is 1.08×10^{-3}

т/к	Mol Fraction
273.15	0.160
283.15	0.125
293.15	0.0948
303.15	0.0709
313.15	0.0523

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Carbonochloridic acid, butyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.005$$

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) 3-Chloropropanoic acid, ethylester; C₅H₉ClO₂; [623-71-2] ORIGINAL MEASUREMENTS: Gerrard, W.; Macklen, E. D. J. Appl. Chem. 1959, 9, 85 - 88.

VARIABLES:

T/K: 273.15 - 320.15 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio nHC1/nC5H9C1O2	Mol Fraction **HC1
273.15 284.05 296.05 302.95 306.75 312.55 320.15	0.496 0.403 0.309 0.261 0.232 0.190 0.147	0.332 0.287 0.236 0.207 0.188 0.160 0.128

The mole fraction values were calculated by the compiler.

Smoothed Data: ln x_{HC1} = 103.162 - 139.249/(T/100) - 53.037 ln (T/100)

Standard error about regression line = 3.49×10^{-3}

T/K	Mol Fraction "HC1
273.15	0.329
283.15	0.296
293.15	0.251
303.15	0.203
313.15	0.158
323.15	0.118

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were those described by Gerrard and Macklen (1). The hydrogen chloride was generated in an all glass apparatus. The absorption vessel, previously weighed, was fitted with a stoppered bubbler tube, and a stoppered outlet tube. Entrained liquid was condensed at 273.15 K, and allowed for. The amount of gas absorbed by a known weight of liquid was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared and dried.
- (2) 3-Chloropropanoic acid, ethyl ester Purified, distilled, and attested by physical constants.

ESTIMATED ERROR:

 $\delta x/x = 0.01$

REFERENCES:

 Gerrard, W.; Macklen, E. D. J. Appl. Chem. <u>1956</u>, 6, 241.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Carbonochloridic acid hexyl ester or hexyl chloroformate; C₇H₁₃ClO₂; [6092-54-2]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
 Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 273.15 - 317.85 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

<u>T/K</u>	Mol Ratio	Mol Fraction
	ⁿ нс1 ^{/n} с ₇ н ₁₃ с1о ₂	x_1
273.15	0.211	0.174
279.15	0.175	0.149
284.55	0.151	0.131
292.35	0.123	0.1095
299.85	0.101	0.0917
300.75	0.0969	0.0883
308.45	0.0778	0.0722
317.85	0.0660	0.0619

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -0.622 + 8.281/(T/100) - 4.135 \ln (T/100)$

Standard error about the regression line is 1.51×10^{-3}

T/K	Mol Fraction
	x_1
$\overline{273.15}$	0.175
283.15	0.135
293.15	0.105
303.15	0.0841
313.15	0.0674
323.15	0.0545

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Carbonochloridic acid hexyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.015$$

COMPONENTS: ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; (1) Hydrogen chloride; HCl; Wyvill, P. L. [7647-01-0] J. Appl. Chem. 1960, 10, 115-121. (2) Chloroacetic acid, phenyl ester or phenyl chloroacetate; $C_8H_7O_2$; [620-73-5] **VARIABLES:** PREPARED BY: T/K: 311.15 - 323.85 W. Gerrard Total P/kPa: 101.325 (1 atm) (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio nHCl/nC8H7O2	Mol Fraction
311.15 314.65 319.15 323.85	0.0817 0.0760 0.0630 0.0446	0.0755 0.0706 0.0593 0.0427

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -17.026 + 45.1045/(T/100K)$

Standard error about the regression line is 4.81×10^{-3}

T/K	Mol Fraction
303.15	0.1168
313.15	0.0726
323.15	0.0465

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Chloroacetic acid, phenyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.025$$

COMPONENTS: 1. Hydrogen Chloride; HCl; [7647-01-0]

 Carbonic acid diethyl ester or diethyl carbonate; C₅H₁₀O₃; [105-58-8]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 198.15 - 317.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	T/K	Mol Ratio	Mol Fractio	n
		n HCl/ n C ₅ H ₁₀ O ₃	X _{HC1}	
	198.15	7.463	0.882	_
1	212.65	3.923	0.797	
	231.15	1.941	0.660	The mole fraction
	273.15	0.677	0.404	values were cal-
	279.65	0.561	0.359	culated by the
i	283.45	0.520	0.342	compiler.
	289.05	0.441	0.306	•
	300-65	0.323	0.244	

0.300

0.222

0.190

Smoothed Data: $\ln x_1 = -58.8547 + 84.5289/(T/100K) + 77.8716 \ln (T/100K) -18.7608 (T/100K)$

302.85

312.45

317.15

Standard error about the regression line = 7.69×10^{-3}

193.15	T/K	Mol Fraction x_1	T/K	Mol Fraction
203.15 0.848 273.15 0.405 213.15 0.778 283.15 0.342 223.15 0.716 293.15 0.282 233.15 0.656 303.15 0.228 243.15 0.596 313.15 0.179				
213.15 0.778 283.15 0.342 223.15 0.716 293.15 0.282 233.15 0.656 303.15 0.228 243.15 0.596 313.15 0.179	193.15	0.937	263.15	0.469
223.15 0.716 293.15 0.282 233.15 0.656 303.15 0.228 243.15 0.596 313.15 0.179	203.15	0.848	273.15	0.405
233.15	213.15	0.778	283.15	0.342
243.15 0.596 313.15 0.179	223.15	0.716	293.15	0.282
	233.15	0.656	303.15	0.228
253.15 0.533 323.15 0.138	243.15	0.596	313.15	0.179
	253.15	0.533	323.15	0.138

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed at temperatures above 273 K was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determinations below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method.

A low temperature, Teddington type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

SOURCE AND PURITY OF MATERIALS:

0.231

0.182

0.160

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Carbonic acid diethyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 \text{ below 273 K} \\ \delta X_1/X_1 = 0.015$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Carbonic acid dibutyl ester; $C_9H_{18}O_3$; [542-52-9]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 273.15 - 317.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL	VALUES:
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T/K	Mol Ratio	Mol Fraction
	ⁿ HC1/ ⁿ C ₉ H ₁₈ O ₃	X _{HC1}
273.15	0.719	0.418
279.85	0.605	0.377
289.95	0.460	0.315
297.15	0.386	0.278
306.35	0.299	0.230
317.15	0.209	0.173

Smoothed Data: $\ln X_{HC1} = 68.788 - 90.168/(T/100) - 36.478 \ln (T/100)$

Standard Error About Regression Line = 3.59×10^{-3}

т/к	Mol Fraction XHCl
273.15	0.416
283.15	0.359
293.15	0.300
303.15	0.244
313.15	0.193
323.15	0.149

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas (1) absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Carbonic acid dibutyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

Other solvent name Dibutyl carbonate

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen Chloride; HCl; Gerrard, W.; Mincer, A. M. A.; [7647-01-0] Wyvill, P. L. J. Appl. Chem. 1959, 9, 89 - 93. 2. Carbonic acid bis (2-methyl propyl) ester; CoH1803; [539-92-4] **VARIABLES:** PREPARED BY: T/K: 273.15 - 315.05 Total P/kPa: 101.325 (1 atm) W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL	VALUES:			
		T/K	Mol Ratio nHCl/nC9H18O3	Mol Fraction XHC1
		273.15 282.55 294.55 302.75 315.05	0.740 0.595 0.435 0.350 0.246	0.425 0.373 0.303 0.259 0.197

Smoothed Data: $\ln X_{HC1} = 61.946 - 80.958/(T/100) - 33.002 \ln (T/100)$ Standard Error About Regression Line = 6.90 x 10^{-4}

т/к	Mol Fraction XHCl
273.15	0.425
283.15	0.370
293.15	0.312
303.15	0.256
313.15	0.206
323.15	0.163

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The solvent was weighed in a bubbler 1. Hydrogen Chloride. Good specimen from a commercial cylinder was tube. The amount of gas absorbed was determined by reweighing to constant dried. weight. The total pressure was barometric, very nearly 1 atm 2. Carbonic acid bis (2-methy1 (101.325 kPa). propyl) ester. Carefully purified, and purity rigorously attested. ESTIMATED ERROR: $\delta x_1/x_1 = 0.01$ Other solvent name REFERENCES: Diisobutyl carbonate

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 3-Methyl-1-butanol carbonate (2:1); $C_{11}^{H}_{22}^{O}_{3}$ or (CH₃CH(CH₃)CH₂CH₂O)₂CO; [2050-95-5]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
 Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 273.15 - 315.65 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: __

т/к	Mol Ratio nHCl/nC ₁₁ H ₂₂ O ₃	Mol Fraction ^x 1
273.15	0.730	0.422
280.65	0.599	0.375
287.15	0.496	0.332
296.75	0.391	0.281
306.15	0.307	0.235
315.65	0.225	0.184

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 36.511 - 44.397/(T/100) - 20.987 \ln (T/100)$

Standard error about the regression line is 7.00×10^{-3}

	Mol Fraction
273.15	0.435
283.15	0.363
293.15	0.300
313.15	0.244
323.15	0.197

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 3-Methyl-1-butanol carbonate. Carefully purified, and purity rigorously attested.

Solvent name is isopentyl carbonate in paper, IUPAC name is diisopentyl carbonate.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.02$$

(1) Hydrogen chloride; HCl; [7647-01-0]

ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.;

Wyvill, P. L.

(2) Carbonic acid 2-chloroethyl ethyl J. Appl. Chem. 1960, 10, 115-121. ester or ethyl 2-chloroethyl carbonate; C5H9ClO3;

[50780-47-7] **VARIABLES:**

COMPONENTS:

PREPARED BY:

T/K: 273.15 - 320.15 101.325 (1 atm) Total P/kPa:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

T/K	Mol Ratio	Mol Fraction
	ⁿ нс1 ^{/n} с ₅ н ₉ с10 ₃	x_1
273.15	0.490	0.329
280.15	0.408	0.290
287.15	0.338	0.253
293.15	0.292	0.226
299.05	0.247	0.198
305.45	0.206	0.171
316.25	0.143	0.125
320.15	0.122	0.109

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 84.837 - 112.037/(T/100) - 44.727 \ln (T/100)$

Standard error about the regression line is 3.10×10^{-3}

T/K	Mol Fraction
	x_1
273.15	0.325
283.15	0.277
293.15	0.226
303.15	0.178
313.15	0.136
323.15	0.101

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Carbonic acid 2-chloroethyl ethyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.015$$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Alkanes and Halogenated Alkanes

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Halogenated Alkanes and in Halogenated Alkenes.

The solubility of hydrogen chloride in tetrachloromethane has been measured by various authors (1-4) at a total pressure equal to barometric, and over pressure ranges below 101.3 kPa by Hamai (5), by Howland et al. (6) and by Khodeeva & Rozovskii (7). The single measurement reported by Chesterman (8) is out of line with all other measurements and should be rejected. Data published by Khodeeva & Rozovskii are self-consistent except that there is an error in the reporting of constants associated with the Krichevskii-Il'inskaya equation. Data for 303.15 K and below are out of line with measurements by other authors. The evaluator considers that they are likely to be unreliable.

Mole fraction solubilities at a partial pressure of 101.3 kPa as given by other authors or as calculated from solubilities at partial pressures close to 101.3 kPa may be represented by the equation:

 $\ln x_{HC1} = -206.48 + 9800.3/(T/K) + 29.732 \ln (T/K)$

The standard deviation in values of x_{HC1} is 0.0018.

This equation is based upon data for the temperature range 266.15 K to 343.15 K. There is appreciable scatter of data as may be seen in fig 1. Values fall below a reference line based upon the Raoult's law equation, except at temperatures greater than about 320 K.

Solubility in trichloromethane was measured by Bell (1), by Howland et al.(6), by Zielinski (2) and by Vdovichenko & Kondratenko (4). Mole fraction solubilities for a partial pressure of 101.3 kPa show appreciable scatter (see fig 2) with a general tendency for values to be greater than corresponding ones for dissolution in tetrachloromethane.

The mole fraction solubility in dichloromethane at a total pressure equal to barometric pressure was measured by Vdovichenko & Kondratenko (4) at temperatures of 263.15 K, 273.15 K and 298.15 K. Values corrected to a partial pressure of 101.3 kPa for the two lower temperatures lie above the corresponding values for tetrachloromethane and below the values for trichloromethane calculated from data given by these two authors. The vapor pressure of dichloromethane at 298.15 K (> 420 mmHg) is too high for reliable estimation of the solubility corresponding to a partial pressure of 101.3 kPa at this temperature.

Solubilities in 1,2-dichloroethane have been measured by various workers. Bell (1), Zielinski (2) and also Abdullaev et al.(9) made measurements at a total pressure equal to barometric at 293.15 K, 293.15 - 313.15 K and 273.15 - 353.15 K respectively. Hamai (5) made measurements over pressure ranges at 288.15 - 298.15 K. Hannaert et al.(10) made measurements in the temperature range 273.15 - 333.15 K. Detailed results were not published but data were given for an equation for the variation in mole fraction solubility at a total pressure of 101.3 kPa over this temperature range. Treger et al.(11) made measurements over the temperature range 253 - 333 K but they also did not publish detailed results. Data were given for an equation for the variation in mole ratio solubility at a partial pressure of 101.3 kPa over this temperature range. The evaluator has calculated mole fraction solubilities at a partial pressure of 101.3 kPa from the data that have been published, making allowance for the partial pressure of the solvent where necessary. Values at 20 K intervals were estimated from the equation given by Hannaert et al. and that from Treger's measurements. Correction of the solubility at 353.15 K given by Abdullaev et al. was considered to be unreliable because the vapor pressure of the pure solvent is about 90 kPa at this temperature and this data point was disregarded. Other data points for a partial pressure of 101.3 kPa fall into a very consistent pattern (see fig 3). The variation in mole fraction solubility at a partial pressure of 101.3 kPa may be

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Alkanes

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January 1989

CRITICAL EVALUATION:

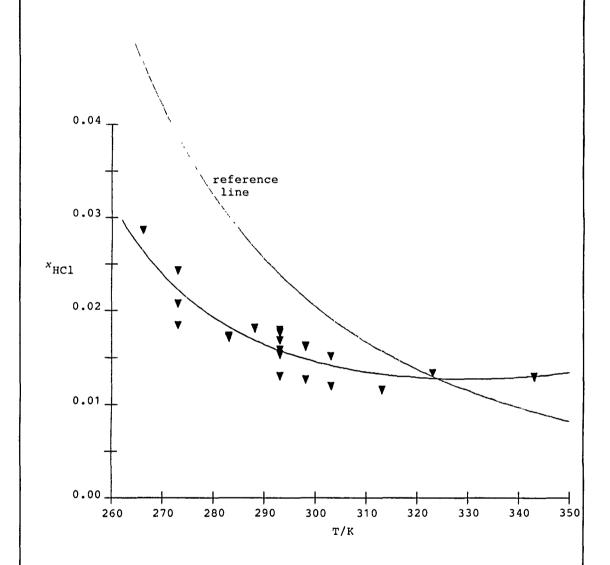


Figure 1

<u>Variation</u> with <u>temperature of experimental values of the mole fraction solubility of hydrogen chloride at a partial pressure of 101.3 kPa in tetrachloromethane.</u>

The reference line corresponds to the variation in solubility from the Raoult's law equation.

(see refs. 1-6)

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Halogenated Alkanes

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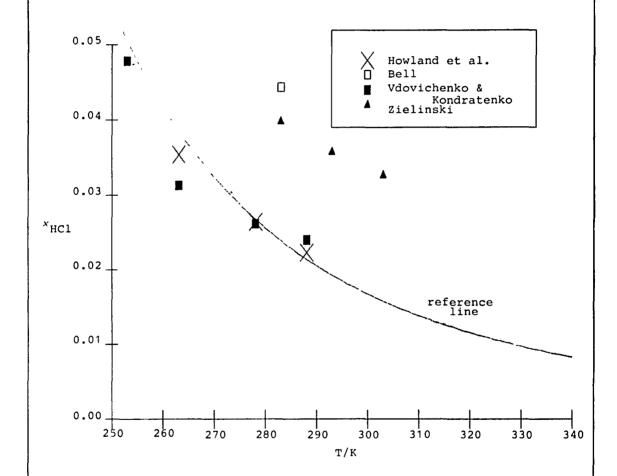


Figure 2

Variation with temperature of experimental values of the mole fraction solubility of hydrogen chloride at a partial pressure of 101.3 kPa in trichloromethane.

(see refs. 1,2,4 & 6)

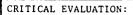
The reference line corresponds to the variation in solubility from the Raoult's law equation.

- Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Alkanes

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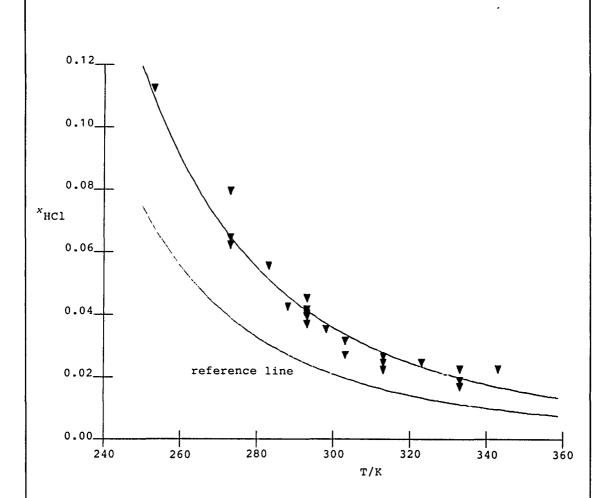


Figure 3

<u>Variation</u> with temperature of experimental values of the mole fraction solubility of hydrogen chloride at a partial pressure of 101.3 kPa in 1,2-dichloroethane.

The reference line corresponds to the variation of mole fraction solubility from the Raoult's law equation.

(see refs. 1,2,5,9-11)

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Halogenated Alkanes and Halogenated Alkenes

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

represented by the equation:

$$\ln x_{HC1} = -9.355 + 1808/(T/K)$$

The standard deviation in values of $x_{\rm HCl}$ is 0.004.

This equation is based upon measurements in the range 253.15 - 343.15 K

Danov & Golubev (12) measured the solubility in 1,1-dichloroethane over a pressure range at 204.55 K to 242.65 K. No other data for solubility in this solvent are available for comparison but the mole fraction solubilities fit an equation which is closely similar to the one given above for the 1,2 isomer. 1.e.

$$\ln x_{HC1} = -8.729 + 1646/(T/K)$$

The standard deviation in values of x_{HCl} is 0.005.

Solubility in 1,1,2-trichloroethane was measured by Hamai (5) and by Treger $et\ al.$ (11) over a pressure and temperature range. Individual solubility values have not been published by Treger $et\ al.$ but data have been given for an equation for the variation with temperature of mole fraction solubility at a partial pressure of 101.3 kPa. There is a gross discrepancy between Hamai's measurements and those of Treger $et\ al.$ The mole fraction solubility at a partial pressure of 101.3 kPa and 293.15 from Hamai's measurements is 0.0310 whereas the value from Treger's data is 0.0507. There is a similar difference between the two sets of data at 285.15 K and 288.15 K. Data published by Hamai are in better accord with the pattern of solubilities in other chlorinated ethanes (see fig 4).

Treger $et\ al.$ published data for dissolution in trichloroethene but no other measurements of the solubility in this compound are available for comparison.

Solubility in 1,1,2,2-tetrachloroethane was measured by Bell (1) and by Zielinski (2) at barometric pressure and 293.15 K and 293.15 - 313.15 K respectively. Hamai (5) measured solubilities over a pressure range at 288.15 - 298.15 K. Treger (11) reported data for an equation for the variation of mole fraction solubility with temperatures in the range 253 - 333 K. The values of the mole fraction solubility at a partial pressure of 101.3 kPa at 293.15 K from the four sets of data all lie between 0.0265 and 0.0289. Solubilities at higher temperatures from Zielinski's data are high compared with other values. Mole fraction solubilities for a partial pressure of 101.3 kPa based upon all the data may be fitted to the equation:

$$\ln x_{HC1} = -7.939 + 1281.7/(T/K)$$

The standard deviation in values of $x_{\rm HCl}$ is 0.002.

This equation is based upon data for the temperature range 253 - 333 K.

Solubility in pentachloroethane was measured by Bell (1) at 293.15 K at barometric pressure and by Hamai (5) at 285.15 - 293.15 K over a pressure range. The mole fraction solubility for a partial pressure at 293.15 K from Bell's measurement is 0.0214 which is close to the value of 0.0225 from data published by Hamai.

Solubilities in 1-chloroalkanes with 4,6,8,12 & 16 carbon atoms have been measured at different temperatures or over different temperature ranges between 197 K and 433 K (13 - 16). All measurements were made at barometric pressure except those carried out by Scher et al.(13) for 1-chlorohexadecane over a pressure range of 51 to 99 kPa. The mole fraction solubility at a partial pressure of 101.3 kPa and 313.15 K estimated from Scher's measurements is 0.0362. This is close to the value of 0.0369 for the same solvent published by Fernandes & Sharma (14).

All mole fraction solubilities for 1-chloroalkanes from the available data lie above the reference line corresponding to the Raoult's law equation. Values may

- Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Alkanes and Halogenated Alkenes

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January 1989

CRITICAL EVALUATION:

be represented approximately by the equation:

$$\ln x_{HC1} = -10.53 + 2213/(T/K)$$

The standard deviation in values of x_{HC1} is 0.011.

This equation is based upon data in the temperature range 243 K to 433 K for the five compounds mentioned above. It must be considered a general guide to the behaviour of these compounds. Solubilities in individual solvents are scattered around the values of $x_{\rm HCl}$ calculated from the equation with no general relationship between this scatter and the chain length of the solvent.

Hamai (4) measured the solubility in 1,2-dibromoethane over a pressure range at 288.15 K to 298.15 K. Bell (1) measured the solubility at 293.15 K and barometric pressure. Bell's value of the mole fraction solubility, corrected to a partial pressure of gas of 101.3 kPa, is 0.0348 and very close to the value of 0.0344 by extrapolation of Hamai's measurements. Bell also measured solubilities in bromoethane, tribromomethane and in 1,1,2,2-tetrabromoethane. No other measurements of the solubilities in these solvents are available for comparison.

The solubility in 1-bromooctane was measured by Gerrard $et\ al.$ (15) at a total pressure of 101.3 kPa at temperatures from 273.15 K to 317.15 K. Measurements in the temperature range 243.15 K to 273.15 K were made by Ahmad $et\ al.$ (16) in the same laboratory. The two values for the mole fraction solubility at 273.15 K differ by 8%. The two sets of values for the mole fraction solubility at a total pressure of 101.3 bar may be fitted to the equation:

$$\ln x_{HCl} = -96.877 + 5655.9/(T/K) + 13.156 \ln(T/K)$$

The standard deviation in values of $x_{\rm HC1}$ is 0.003.

Gerrard et al. also reported solubilities over temperature ranges in 1-bromobutane and 1-bromohexane at a total pressure of 101.3 kPa. Gerrard's data indicate that, corrected to a partial pressure of 101.3 kPa, mole fraction solubility increases with chain length from 1-bromobutane to 1-bromooctane, at temperatures at which comparison can be made (273.15 K - 298.15 K). However, the value for HCl in bromoethane at 293.15 K from Bell's measurement is 0.1019 and larger than the corresponding solubility in 1-bromooctane (0.058).

Ahmed $et\ al.$ also measured the solubility in 1-iodooctane. The data indicate that the mole fraction solubility is higher than that in 1-bromooctane under the same conditions of measurement. No other measurements are available for comparison.

The solubility in chloroethene was measured by Danov & Golubev (12) at pressures to 133.3 kPa from 204.55 K to 242.65 K. An equation for Henry's constant for dissolution in this solvent at temperatures from 213.15 K to 243.15 K has been published by Hannaert $et\ al.(10)$ Mole fraction solubilities estimated from this equation are lower than those from Danov's measurements. The mole fraction solubility for a partial pressure of hydrogen chloride of 93.3 kPa at 242.15 K is 0.1382. The value from Hannaert's equation is 0.1006. The extensive data presented by Danov are self consistent and likely to be more reliable than solubilities estimated from Hannaert's equation.

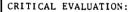
The solubility in trichloroethene was measured by Abdullaev et al.(9) at barometric pressure from 273.15 K to 353.15 K. Bell (1) measured the solubility at barometric pressure and 293.15 K. Data presented by Treger et al.(11) are ambiguous and cannot be compared with data from other authors. The mole fraction solubility at 293.15 K and a partial pressure of 101.3 kPa given by Bell is 0.0206. This is very close to the value of 0.0205 obtained by correcting Abdullaev's data for this temperature to a partial pressure of 101.3 kPa and adds support to data for other temperatures.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Alkanes

EVALUATOR:

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January 1989



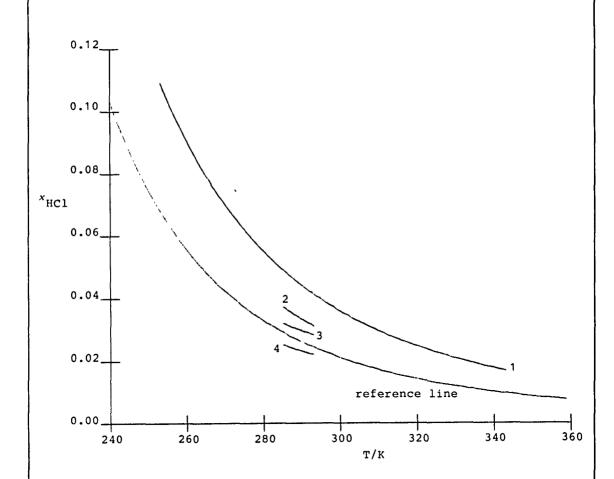


Figure 4

Variation with temperature of the mole fraction solubilities of hydrogen chloride at a partial pressure of 101.3 kPa in chloroethanes.

- 1 1,2-dichloroethane
- 3 1,1,2,2-tetrachloroethane
- 2 1,1,2-trichloroethane
- 4 pentachloroethane

The reference line corresponds to the variation in solubility from the Raoult's law equation.

(see refs. 1,2,5,9-11)

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Alkanes and Halogenated Alkenes

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

Curda & Holas (3) measured the solubility in tetrachloroethene at barometric pressure from 293.15 K to 363.15 K. The mole fraction solubility at 293.15 K corrected to a partial pressure of 101.3 kPa from these data is 0.0160. This is in good agreement with the value of 0.0163 given by Bell.

Danov & Golubev (12) measured the solubility in (E)-1,2-dichloroethene at pressures to 133.3 kPa in the range 225.15 K to 256.25 K. The measurements are self consistent but no other data for this system are available for comparison.

The solubility in 3-chloro-1-propene was measured by Cook (17) at barometric pressure from 268.95 K to 283.15 K. The interpolated value of the mole fraction solubility at 273.15 K is 0.0468. This is in sharp contrast to the value of 0.0609 from data published by Curda & Holas (3). Measurements on this system need to be repeated.

- 1. Bell, R. P. J. Chem. Soc. 1931, 1371 1382.
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- 5. Hamai, S. Bull. Chem. Soc. Japan 1935, 10, 5 16.
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- 14. Fernandes, J. B.; Sharma, M. M. Indian Chem. Eng. 1965, 7, 38 40.
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- 17. Cook, T. M. Thesis 1966, University of London.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Dichloromethane; CH₂Cl₂; [75-09-2] VARIABLES: T/K = 263.15 - 298.15 p /kPa = 101.325 (1 atm) PRIGINAL MEASUREMENTS: Vdovichenko, V. T.; Kondratenko, V. I. Khim. Prom. 1967, 43, 290 - 291. W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:		
EXFERITEMENT VALUES.	T/K	Mol Fraction
		\boldsymbol{x}_{1}
	263.15	0.031
	273.15	0.018
	298.15	0.013

The mole fraction values appear to be for a total pressure of 1 atm.

Smoothed Data: For use between 263.15 and 298.15 K.

 $\ln x_1 = -347.20 + 482.95/(T/100 \text{ K}) + 165.57 \ln (T/100 \text{ K})$

_	T/K	Mol Fraction
		x ₁
	268.15	0.023
	278.15	0.015
	288.15	0.013
	298.15	0.013

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Solubility determined at atmospheric pressure by the method described by Strepikheev and Babkin (1).	SOURCE AND PURITY OF MATERIALS: (1) Hydrogen chloride. Obtained from chemically pure sodium chloride and concentrated sulfuric acid, dried by calcium chloride and filtered through glass wool.
	(2) Dichloromethane. B.p. (1 atm)/°C = 40.0 - 40.3; density, ρ ₄ ²⁰ = 1.3260; refractive index, n _D ²⁰ = 1.4245.
	ESTIMATED ERROR:
	REFERENCES: 1. Strepikheev, Yu. A.; Babkin, B. M. Khim. Prom. 1963, (1), 38.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chloromethanes

ORIGINAL MEASUREMENTS:

- Bell, R. P.
- J. Chem. Soc. <u>1931</u>, 1371 - 1382.

VARIABLES:

T/K: 293.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K Partition Mol Fraction Coefficient x_1

c_{1,1}/c_{1,g}

Trichloromethane; CHCl₂;

293.15

[67-66-3]

13.80

0.0444

Tetrachloromethane; CCl₄; [56-23-5]

293.15

4.54

0.0181

The ideal gas concentration at $p_1 = 1$ atm is $c_{1,g}/\text{mol dm}^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO₂ free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, c/mol dm⁻³, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Chloromethanes. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

COMPONENTS:

(1) Hydrogen chloride; HCl; Chesterman, D. R.

[7647-01-0]

(2) Chloromethanes

VARIABLES:

T/K: 298.15

Total P/kPa: 101 (∿1 atm)

ORIGINAL MEASUREMENTS:

Chesterman, D. R.

J. Chem. Soc. 1935, 906 - 910.

W. Gerrard

EXPERIMENTAL VALUES:

T/K Observed Pressure g HCl g⁻¹ Solution x_1 Trichloromethane or chloroform; CHCl₃; [67-66-3]

298.15 730 0.004 0.013

Tetrachloromethane or carbon tetrachloride; CCl_4 ; [56-23-5]

298.15 765 0.001 0.004

The mole fraction solubility values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was that used for the conductivity. A sample of the saturated solution was removed, weighed, the hydrogen chloride was reacted with excess base which was back titrated with a standard acid solution.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure sodium chloride. Passed through sulfuric acid and over P_2O_5 .
- (2) Trichloromethane. Was stated to be the purest obtainable. Freed from acetone and alcohol, and dried with phosphorus pentoxide, b.p./°C (729 mmHg) = 59.5 - 59.8.

Tetrachloromethane. Was stated to be the purest obtainable. Dried with P_2O_5 ; b.p./°C (760 mmHg) = 77 - 77.5.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

Howland, J. J.; Miller, D. R. Willard, J. E.

ORIGINAL MEASUREMENTS:

(2) Trichloromethane or chloroform; CHCl₃; [67-66-3]

J. Am. Chem. Soc. 1941, 63, 2807 - 2811.

VARIABLES: T/K:

273.15 - 298.15 22.80 - 81.33 (171 - 610 mmHg) P/kPa:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure Range	Number of Determinations	Henry's, Constant ¹ 10 ⁵ K/(mmHg) ⁻¹	Mol Fraction ²
273.15	308 - 581	3	4.66 ± 0.03	0.0354
288.15	171 - 587	5	3.48 ± 0.02	0.0264
298.15	194 - 610	5	2.93 <u>+</u> 0.02	0.0223

Henry's constant, $K/(mmHg)^{-1} = x_1/(P_1/mmHg)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mercury manometer was attached to an absorption bulb. The solvent was added to the bulb, and the vapor pressure was determined. This pressure, p₂, was used to calculate the gas partial pressure, p₁, from the total pressure, p, measured by the manometer:

$$p_1 = p_t - p_2^0 (1 - x_1).$$

The amount of gas absorbed in a measured weight of solution withdrawn as a sample, was determined by a chemical titration.

The heat of solution was determined to be $-3.00 \pm 0.30 \text{ kcal mol}^{-1}$ $(-12.55 \text{ kJ mol}^{-1})$.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping sulfuric acid onto sodium chloride. The gas was passed through glass wool and calcium chloride.
- (2) Trichloromethane. Merck and Co. Technical grade, purified and distilled.

ESTIMATED ERROR:

 $\delta K/K = 0.01$

² Values of the mole fraction solubility at 101.325 kPa (1 atm, 760 mmHg) calculated by the compiler.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Trichloromethane or chloroform; CHCl₂; [67-66-3]

ORIGINAL MEASUREMENTS:

Zielinski, A. Z.

Przem. Chem. 1958, 37, 338 - 339.

VARIABLES:

$$T/K \approx 293.15 - 313.15$$

 $p_1/kPa \approx 53.14 - 83.35$
 $(398.6 - 625.2 \text{ mmHg})$

PREPARED BY:

W. Gerrard

T/K Hydrogen		Liquid Composition		Kuenen	Mol Ratio	Mol Fraction
	Chloride Pressure p ₁ /mmHg	HCl n ₁ /mmol	n_2/mmol	Coefficient S/cm ³ (STP)g ⁻¹ atm ⁻¹	n ₁ /n ₂	x ₁
293.15	625.2 625.2	2.841 3.175	84.6 93.2	7.67	0.0336 0.0341	0.0325 0.0329 0.0398 ¹
303.15	529.4 529.4	3.102 2.690	? 105.4	6.92 6.88	? 0.0255	? 0.0249 0.0357 ¹
313.15	398.6 398.6	1.719 1.793	99.1 102.6	6.21 6.26	0.0173 0.0175	0.0170 0.0172 0.03261

 $^{^{1}}$ Mean mole fraction, x_{1} , for 101.325 kPa (1 atm), assuming a linear change of x, with p,.

The mole ratio, mole fraction at p_1 of the experiment, and the mean mole fraction at 101.325 kPa (1 atm) values were calculated by the compiler.

The author took the HCl partial pressure to be the difference between the barometric pressure and the pure solvent vapor pressure.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen chloride was absorbed by the liquid in an absorption vessel described by Bichowsky and Storch (1). The amount absorbed was determined by a chemical titration.

To calculate the volume of HCl absorbed by one gram of liquid, at 760 mmHg, $22.42 \text{ dm}^3 \text{ mol}^{-1}$ was taken as the molar volume of HCl at 273.15 K and 1 atm. The volume based on the real density of HCl under these conditions is (compiler) ESTIMATED ERROR: 22.247 dm³ mol⁻¹.

SOURCE AND PURITY OF MATERIALS:

May be assumed to be of satisfactory purity.

REFERENCES:

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

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Trichloromethane or chloroform; CHCl₂; [67-66-3]

ORIGINAL MEASUREMENTS:

Vdovichenko, V. T.; Kondratenko, V. I.

Khim. Prom. 1967, 43, 290 - 291.

VARIABLES:

$$T/K = 263.15 - 298.15$$

p /kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Fraction
	x_1
263.15	0.046
273.15	0.029
288.15	0.022
298.15	0.018

The mole fraction values appear to be for a total pressure of 1 atm.

Smoothed Data: For use between 263.15 and 298.15 K.

 $\ln x_1 = -152.60 + 215.59/(T/100 \text{ K}) + 69.842 \ln (T/100 \text{ K})$

The standard error about the regression line is 2.04×10^{-3} .

T/K	Mol Fraction
	x_1
268.15	0.0365
278.15	0.026
288.15	0.021
298.15	0.0185

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubility determined at atmospheric pressure by the method described by Strepikheev and Babkin (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Obtained from chemically pure sodium chloride and concentrated sulfuric acid, dried by calcium chloride and filtered through glass wool.
- (2) Chloroform. B.p. $(1 \text{ atm})/^{\circ}C = 6\frac{1}{2} \cdot 1 61.2$; density, $\rho_{+}^{20} = 1.4892$; refractive index, $n_{D}^{20} = 1.4464$.

ESTIMATED ERROR:

REFERENCES:

Strepikheev, Yu. A.;
 Babkin, B. M.
 Khim. Prom. 1963, (1), 38.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Hamai, S.

Bull. Chem. Soc. Jpn. <u>1935</u>, 10, 5 - 16.

VARIABLES:

T/K: 288.15 - 298.15 Total P/kPa: 56.06 - 103.92 (420.5 - 779.5 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Total Pressure p/mmHg	Mol Fraction
288.15	420.5 515.5 614.0 664.0	0.00613 0.00928 0.01170 0.01270
	(760	0.01826) 1
293.15	425.0 521.0 572.0 770.5 (760	0.00563 0.00829 0.00876 0.01380
298.15`	433.5 531.5 580.0 631.5 680.5 779.5	0.00367 0.00622 0.00757 0.00817 0.00955 0.01200

These values were calculated by the compiler for a hydrogen chloride partial pressure of 760 mmHg (101.325 kPa). It was assumed that the solvent vapor pressure was the same for the solution and pure solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a U shaped gas buret, connected to a gas reservoir (335 cm³ capacity) which was connected to the absorption vessel. The volume of hydrogen chloride absorbed by 20 cm³ of the original liquid was converted into the amount of gas absorbed at a measured total pressure.

The author obtained the heat of absorption, ΔH , of -6100 cal mol⁻¹ (-25.2 kJ mol⁻¹) from the slope of a plot of log x_1 vs. 1/T.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping concentrated hydrochloric acid into pure concentrated sulfuric acid. The gas was passed through conc. sulfuric acid and twice condensed by liquid nitrogen.
- (2) Tetrachlormethane. Kahlbaum. B.p. 349.15 K.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HC1; [7647-01-0]
- (2) Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Howland, J. J.; Miller, D. R. Willard, J. E.

J. Am. Chem. Soc. 1941, 63, 2807 - 2811.

VARIABLES:

T/K: 273.15 - 298.15 P/kPa: 16.40 - 92.66 (123 - 695 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure or Pressure Range P1/mmHg	Number of Determinations	Henry's Constant ¹ 10 ⁵ K/(mmHg) ⁻¹	Mol Fraction ²
273.15	269 - 667	4	3.22 ± 0.01	0.0245
293.15	123 - 695	7	2.34 ± 0.03	0.0178
298.15	178.5 379.5 425.0 548.5 662.5		2.12 2.11 2.16 2.17 2.14	0.00379 ³ 0.00803 ³ 0.00922 ³ 0.01190 ³ 0.01415 ³
	178 - 662	5	2.14 ± 0.02	0.0163

- ¹ Henry's constant, $K/(mmHg)^{-1} = x_1/(P_1/mmHg)$.
- ² Values of the mole fraction solubility at 101.325 kPa (1 atm, 760 mmHg) calculated by the compiler.
- Mole fraction solubility values at the stated pressure. Only complete set of data given by the authors.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mercury manometer was attached to an absorption bulb. The solvent was added to the bulb, and the vapor pressure was determined. This pressure, p_0° , was used to calculate the gas partial pressure, p_1 , from the total pressure, p_t , measured by the manometer:

$$p_1 = p_t - p_2^0 (1 - x_1)$$
.

The amount of gas absorbed in a measured weight of solution with-drawn as a sample, was determined by a chemical titration.

The heat of solution was determined to be $-2.67 \pm 0.30 \text{ kcal mol}^{-1}$ (-11.17 kJ mol⁻¹).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Prepared by dropping sulfuric acid onto sodium chloride. The gas was passed through glass wool and calcium chloride.
- (2) Tetrachloromethane. Merck and Co. Technical grade, purified and distilled.

ESTIMATED ERROR:

 $\delta K/K = 0.01$

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Zielinski, A. Z. [7647-01-0] Przem. Chem. 1958, 37, 338 - 339. (2) Tetrachloromethane or carbon tetrachloride; CCl₄; [56-23-5] **VARIABLES:** PREPARED BY: T/K = 293.15 - 313.15 $p_1/kPa = 71.89 - 89.65$ W. Gerrard (539.2 - 672.4 mmHg)

EXPERIMENTAL VALUES:						
T/K	Hydrogen Chloride	Liquid C	omposition	Kuenen Coefficient	Mol Ratio	Mol Fraction
	Pressure p ₁ /mmHg	n_1/mmol	n_2/mmol	$S/\text{cm}^3 (STP) g^{-1}$ atm ⁻¹	n_{1}/n_{2}	x ₁
293.15	672.4 672.4	1.157	101.4	1.88	0.0114 0.0121	0.0113 0.0120 0.0132
303.15	613.8 613.8	0.971 1.009	97.8 101.5	1.79 1.79	0.0099 0.0099	0.0098 0.0098 0.0121 ¹
313.15	539.2 539.2	0.934 0.821	111.6 100.4	1.72 1.68	0.0084 0.0082	0.0084 0.0082 0.0117 ¹

Mean mole fraction, x_1 , for 101.325 kPa (1 atm), assuming a linear change of x_1 with p_1 .

The mole ratio, mole fraction at p_{1} of the experiment, and the mean mole fraction at 101.325 kPa (1 atm) values were calculated by the compiler.

The author took the HCl partial pressure to be the difference between the barometric pressure and the pure solvent vapor pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was absorbed by the liquid in an absorption vessel described by Bichowsky and Storch (1) The amount absorbed was determined by a chemical titration.

To calculate the volume of HCl absorbed by one gram of liquid, at 760 mmHg, $22.42~\mathrm{dm}^3~\mathrm{mol}^{-1}$ was taken as the the molar volume of HCl at 273.15 K and 1 atm. The volume based on the real density of HCl under these ESTIMATED ERROR: conditions is (compiler) 22.247 dm3 mol^{-1} .

SOURCE AND PURITY OF MATERIALS:

May be assumed to be of satisfactory purity.

REFERENCES:

Bichowsky, F. R. v.; Storch, H. J. Am. Chem. Soc. <u>1915</u>, 37, 2695.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Curda, M.; Holas, J.

Chem. Prumysl 1964, 14, 547 - 548.

VARIABLES:

T/K = 273.15 - 343.15p /kPa = 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Weight Ratio	Mol Fraction
	$g_{1}/10^{2}g_{2}$	<i>x</i> ₁
273.15	0.43	0.0178
283.15	0.39	0.0162
293.15	0.34	0.0141
303.15	0.30	0.0125
323.15	0.19	0.0080
343.15	0.06	0.0025

The mole fraction values were calculated by the compiler.

Smoothed Data: For use between 273.15 and 343.15 K.

 $\ln x_1 = -1804.630 + 2455.507 / (T/100 K) + 1691.006 \ln (T/100 K) - 291.983 (T/100K)$

The standard error about the regression line is 5.32×10^{-4} .

T/K	Mol Fraction
	x_1
283.15	0.0156
298.15	0.0136
313.15	0.0107
328.15	0.0063
343.15	0.0025

¹ The weight ratio is grams of HCl per 100 grams of tetrachloromethane.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was passed through the liquid in a jacketed bubbler tube fitted with a sampling tap at the bottom. The amount of hydrogen chloride in a sample was determined by a chemical titration.

The pressure was presumably atmospheric.

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. May be taken as of satisfactory purity.
- (2) Tetrachloromethane. Rectified
 technical grade. B.p.
 (1 atm)/°C = 77.

ESTIMATED ERROR:

EXPERIMENTAL VALUES:

T/K	Mol Fraction
	x ₁
266.15	0.028
273.15	0.020
283.15	0.016
293.15	0.015
298.15	0.014

The mole fraction values appear to be for a total pressure of one atm.

Smoothed Data: For use between 266.15 and 298.15 K.

 $\ln x_1 = -243.30 + 339.06/(T/100 \text{ K}) + 114.73 \ln (T/100 \text{ K})$

The standard error about the regression line is 7.79×10^{-4} .

T/K	Mol Praction
	$\boldsymbol{x}_{_{\boldsymbol{\mathcal{I}}}}$
268.15	0.025
278.15	0.018
288.15	0.015
298.15	0.014

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubility determined at atmospheric pressure by the method described by Strepikheev and Babkin (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Obtained from chemically pure sodium chloride and concentrated sulfuric acid, dried by calcium chloride and filtered through glass wool.
- (2) Tetrachloromethane. B.p. $(1 \text{ atm})/^{\circ}C = 76.7 76.8;$ density, $\rho_{+}^{20} = 1.5970;$ refractive index, $n_{D}^{20} = 1.4602.$

ESTIMATED ERROR:

REFERENCES:

Strepikheev, Yu. A.;
 Babkin, B. M.
 Khim. Prom. 1963, (1), 38.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrachloromethane; CCl₄;
 [56-23-5]

VARIABLES:

T/K: 293 - 323 Total p/kPa: 24.13 - 99.46 (181 - 746 mmHg)

ORIGINAL MEASUREMENTS:

Khodeeva, S.M.; Rozovskii, M.B.

Zh. Fiz. Khim. 1975, 49, 1396-1400. Russ. J. Phys. Chem. (Engl. Transl.) 1975, 49, 824-827.

PREPARED BY:

P.G.T. Fogg

EXPERIMENTAL VALUES:

The authors stated that the data were represented by the Krichevskii-Ilinskaya equation:

$$\log_{10}(p_1/\text{mmHg}) = \log_{10}((K/\text{mmHg})x_1) - \beta(1 - x_2^2)$$

where β = A/2.303 RT. Values of A, K and β were given at 5 K intervals from 293 - 323 K.

Tempera t/°C	ature T/K	A/cal mol-1	K/mmHg	β
20	293	3200	37200	2.4
25	298	1700	38300	1.4*
30	303	0	39300	0
35	308	-6700	36300	-2.4*
40	313	-8600	33700	-6.0
45	318	-15000	31600	-10.5
50	323	-25000	24600	-17.0

Mole fraction solubilities of HCl at a partial pressure of HCl of 1.013 bar, calculated by the compiler from this equation, are as follows:

$$T/K$$
 293 298 303 308 313 318 323 x_1 0.0276 0.0226 0.0193 0.0151 0.0150 0.0129 0.0121

* The value of A is not consistent with that of β . The mole fraction solubility at a partial pressure of 1.013 bar has been calculated using the value of β which has been given.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

The apparatus was similar to that described by Khodeeva (1).

Total vapor pressures over solutions of different composition were measured.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from "pure grade" hydrochloric acid, water vapor being removed at -50°C, and HCl being collected at the temperature of liquid nitrogen.
- Tetrachloromethane. Chemically pure. Distilled.

$$d_A^{20} = 1.594 \text{ g cm}^{-3}$$

ESTIMATED ERROR:

REFERENCES:

Khodeeva, S.M.
 Zh. Fiz. Khim. 1961, 35, 629.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Chloroethanes. ORIGINAL MEASUREMENTS: Bell, R. P. J. Chem. Soc. 1931, 1371 - 1382.

VARIABLES:

T/K: 293.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K Partition Mol Fraction Coefficient x_1 $c_1, t^{/c}_{1,g}$

1,2-Dichloroethane; C₂H₄Cl₂; [107-06-2]

293.15 14.74

0.0457

1,1,2,2-Tetrachloroethane; C₂H₂Cl₄; [79-34-5]

293.15

6.20

0.0265

Pentachloroethane; C₂HCl₅; [76-01-7]

293.15

3.86

0.0214

The ideal gas concentration at $p_1 = 1$ atm is $c_{1,g}/\text{mol dm}^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO₂ free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, c/mol dm⁻³, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Chloroethanes. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2-Dichloroethane; C₂H₄Cl₂; [107-06-2]

ORIGINAL MEASUREMENTS:

Hamai, S.

Bull. Chem. Soc. Jpn. <u>1935</u>, 10, 5 - 16.

VARIABLES:

T/K: 288.15 - 298.15 Total P/kPa: 45.66 - 97.53

45.66 - 97.53 (342.5 - 731.5 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Total Pressure p/mmHg	Mol Fraction
288.15	342.5 422.0 533.5 550.0 (760.0	0.0188 0.0229 0.0298 0.0300 0.04377) 1
293.15	520.5 526.5 540.0 600.0 731.5 (760.0	0.0253 0.0258 0.0261 0.0303 0.0350 0.03993) 1
298.15	467.5 500.0 584.0 680.0 (760.0	0.0198 0.0213 0.0252 0.0291 0.03576) 1

These values were calculated by the compiler for a hydrogen chloride partial pressure of 760 mmHg (101.325 kPa). It was assumed that the solvent vapor pressure was the same for the solution and pure solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a U shaped gas buret, connected to a gas reservoir (335 cm³ capacity) which was connected to the absorption vessel. The volume of hydrogen chloride absorbed by 20 cm³ of the original liquid was converted into the amount of gas absorbed at a measured total pressure.

The author obtained the heat of absorption, ΔH , of -3500 cal mol⁻¹ (-14.64 kJ mole⁻¹) from the slope of a plot of log x_1 vs. 1/T.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping concentrated hydrochloric acid into pure concentrated sulfuric acid. The gas was passed through concentrated sulfuric acid and twice condensed by liquid nitrogen.
- (2) 1,2-Dichloroethane. Takeda. B.p. 356.15 K.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2-Dichloroethane; C2H4Cl2; [107-06-2] 1,1,2-Trichloroethane; C2H3Cl3; [79-00-5] 1,1,2,2-Tetrachloroethane; C₂H₂Cl₄ [79-34-5]

Trichloroethene; C2HCl3;[79-01-6]

VARIABLES: T/K = 253 - 333 $p_1/kPa = 26.7 - 101.325$

ORIGINAL MEASUREMENTS:

Treger, Yu. A.; Flid, R. M.; Pimenov, I. F.; Avet'yan, M. G.;

Zh. Fiz. Khim. 1967, 41, 2967 - 8.

Russ. J. Phys. Chem. (Engl. Transl.) <u>1967</u>, *41*, 1596 - 8.

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

Liquid	Enthalpy of Dissolution ΔH/cal mol ⁻¹	Entropy of Dissolution ΔS/cal K ⁻¹ mol ⁻¹
1,2-Dichloroethane	-4150 ± 50	-20.5
1,1,2-Trichloroethane	-4070 ± 100	-19.7
1,1,2,2-Tetrachloroethane	-2820 ± 100	-16.7
Trichloroethene	-3230 ± 100	-18.9

The authors state that they have determined the solubility of hydrogen chloride in the compounds named above at temperatures from 253 to 333 K and at partial pressures of hydrogen chloride of 200 to 760 mmHg (26.7 to 101.325 kPa). Numerical data of solubilities were not recorded, but small, unsatisfactory diagrams were given.

Two measures of solubility are mentioned in the paper. The mole ratio, $K/\text{mol mol}^{-1}$, and Henry's constant, $K_{\chi} = p_1/c_1$. Neither values or units of Henry's constant are given. Apparently the thermodynamic properties of dissolution were calculated from the mole ratio, $K/mol\ mol^{-1}$

 $\log (K/\text{mol mol}^{-1}) = -(\Delta H/\text{cal mol}^{-1})/(2.3R(T/K)) + (\Delta S/\text{cal }K^{-1}\text{mol}^{-1})/2.3R$

AUXILIARY INFORMATION

(Continued from above) One diagram showed plots of $10^2 K/\text{mol mol}^{-1} vs$. p_1/mmHg . Each line was shown as being straight, but the temperature was not stated. Their Fig. 2 showed plots of $\log (K/\text{mol mol}^{-1}) vs. 1/(T/K)$. Each line was drawn as straight, but a value of 1/T was missing. The pressure for the K value was not given.

The equation above should be used with caution. It gives values of K of the magnitude in figure 1, but it does not reproduce the order of solubility ESTIMATED ERROR: shown in the figure.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Purified and dried.
- (2) Chlorocarbons. No information.

 $\delta T/K = \pm 0.1$ $\delta K/K = \pm 0.01$

METHOD/APPARATUS/PROCEDURE:

Gas was passed into a cell containing a definite quantity of liquid. The pressure of HCl was measured with a mercury manometer. Helium was used for measurements at lower partial pressures of HCl (details are lacking). The contents of the cell were weighed, a sample was withdrawn, treated with water, and the HCl content determined by "titrating."

Results were stated to be reproducible to ± 1 per cent.

Hydrogen Chloride in Non-Aqueous Solvents 259 ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] Danov, S. M.; Golubev, Yu. D. Khim. Prom_st. (Moscow) 1968, (2) 1,1-Dichloroethane; C₂H₄Cl₂; [75-34-3] 44 (2), $11\overline{6}$ - 120. VARIABLES: PREPARED BY: T/K = 204.55 - 242.65W. Gerrard $p_1/kPa = (100 - 1000 mmHg)$ **EXPERIMENTAL VALUES:** SEE NEXT PAGE AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were stated to be measured by a static method. The pressures were stated to have been measured to an accuracy of 1 mmHg on a mercury column.

Note that in the authors' table the pressures were given in steps of 100 mmHg. This appears to indicate a smoothing of primary data.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Probably of satisfactory purity.
- (2) 1,1-Dichloroethane. Purity checked by chromatography.

ESTIMATED	ERROR:
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Hydrogen chloride; [7647-01-0]

1,1-Dichloroethane; $C_2H_4Cl_2$; [75-34-3]

Khim. Prom st. (Moscow) 1968, 44 (2), 116 - 120.

ORIGINAL MEASUREMENTS:

Golubev,

T/K	20	04.55	20	09.65	2	15.15	2:	20.65	2:	26.15	2	31.15	23	36.65	242	2.65
p/mmHg	S 1	x ₁	S1	x 2 2	S1	x ₁ ²	S 1	x_1^2	S 1	x_1^2	S 1	x_1^2	S 1	x_1^2	S ¹	x_1^2
100	16.2	0.0674	12.9	0.0547	10.4	0.0444	8.4	0.0364	6.6	0.0288	5.9	0.0257	4.8	0.0213	4.1	0.0187
200	34.9	0.1348	27.5	0.1094	21.8	0.0888	17.6	0.0728	13.7	0.0576	12.1	0.0514	9.9	0.0426	8.4	0.0362
300	56.7	0.2022	44.0	0.1641	34.4	0.1332	27.4	0.1092	21.2	0.0864	18.7	0.0771	15.3	0.0639	12.8	0.0543
400	82.6	0.2696	62.8	0.2188	48.4	0.1776	38.1	0.1456	29.1	0.1152	25.6	0.1028	20.9	0.0852	17.5	0.0724
500	113.8	0.3370	84.4	0.2735	64.0	0.2200	49.7	0.1820	37.7	0.1440	33.1	0.1285	26.7	0.1065	22.3	0.0905
600			109.6	0.3282	81.4	0.2664	62.5	0.2184	46.8	0.1728	40.8	0.1542	32.9	0.1278	27.3	0.1086
700					114.2	0.3377	85.5	0.2764	62.8	0.2190	54.3	0.1953	43.4	0.1623	35.8	0.1379
800							91.9	0.2910	67.1	0.2305	57.9	0.2056	46.1	0.1708	38.0	0.1452
900							109.0	0.3274	78.4	0.2593	67.4	0.2313	53.3	0.1921	43.7	0.1632
1000									90.6	0.2881	77.4	0.2570	60.8	0.2134	49.6	0.1813
Henry's Constant K/mmHq		184		326		250	2	749	2	1 70	2.	891	468		-	510

¹ Kuenen coefficient, S/cm3 (STP) g-1 atm-3.

 $^{^{2}}$ Mole fraction hydrogen chloride, \boldsymbol{x}_{1} .

³ Henry's constant, $K/mmHg = (p_1/mmHg)/x_1$.

- Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2-Dichloroethane; C2H4Cl2; [107-06-2]

ORIGINAL MEASUREMENTS:

Zielinski, A. Z.

Przem. Chem. 1958, 37, 338 - 339.

VARIABLES: T/K = 293.15 - 313.15 $p_1/kPa = 79.74 - 92.62$

(598.1 - 694.7 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Hydrogen Chloride	Liquid Composition		Kuenen Coefficient	Mol Ratio	Mol Fraction
	Pressure	HCl n ₁ /mmol	C ₂ H ₄ Cl ₂ n ₂ /mmol	S/cm ³ (STP) g ⁻¹ atm ⁻¹	n_{1}/n_{2}	x ₁
293.15	694.7 694.6	4.336 4.409	122.2 125.7	8.79 8.69	0.0355 0.0351	0.0343 0.0339 0.0374 ¹
303.15	661.1 661.2	2.989 2.690	121.6 108.4	6.40 6.45	0.0246 0.0248	0.0240 0.0242 0.02751
313.15	598.1 598.1	2.466 2.504	134.9 134.6	5.26 5.29	0.0183 0.0186	0.0180 0.0183 0.02271

Mean mole fraction, x_1 , for 101.325 kPa (1 atm), assuming a linear change of x_1 with p_1 .

The mole ratio, mole fraction at p_1 of the experiment, and the mean mole fraction at 101.325 kPa (1 atm) values were calculated by the compiler.

The author took the HCl partial pressure to be the difference between the barometric pressure and the pure solvent vapor pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was absorbed by the May be assumed to be of satisliquid in an absorption vessel described by Bichowsky and Storch (1). The amount absorbed was determined by a chemical titration.

To calculate the volume of HCl absorbed by one gram of liquid, at $760~\mathrm{mmHg}$, $22.42~\mathrm{dm}^3~\mathrm{mol}^{-1}$ was taken as the molar volume of HCl at 273.15 K and 1 atm. The volume based on the real density of HCl under these conditions is (compiler) 22.247 dm³ mol⁻¹.

SOURCE AND PURITY OF MATERIALS:

factory purity.

ESTIMATED ERROR:

REFERENCES:

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

262 Hydrogen Chloride in Non-Aqueous Solvents COMPONENTS: ORIGINAL MEASUREMENTS: Hannaert, H.; Haccuria, M.; Mathieu, M. P. Hydrogen chloride; HCl; [7647-01-0] (2) 1,2-Dichloroethane; C₂H₄Cl₂; Ind. Chim. Belge 1967, 32, [107-06-2] 156 - 164. VARIABLES: PREPARED BY: T/K = 273.15 - 333.15p/kPa = 101.325 (1 atm) W. Gerrard EXPERIMENTAL VALUES: Kπv/atm¹ Hydrogen Temperature Enthalpy of Constant Interval of Chloride at Dissolution 293.15 K Measurements Mol % Range $10^2 x_1/\text{mol }$ % $\Delta H/\text{kcal mol}^{-1}$ T/K

24.6

¹ log $(K\pi\nu/atm) = A - (\Delta H/cal mol^{-1})/(2.3R(T/K))$

1 - 3

The author's definitions are:

273.15-333.15

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$
,

3.54

4.04

 $\pi/atm = total pressure,$

v = coefficient of fugacity.

The function, $K\pi\nu/atm$, is equivalent to a Henry's constant in the form $H_{1,2}/\text{atm} = (f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe three methods:

- 1.A. [Saturat. nº 1]. A measure of the static pressure of saturation in an apparatus which gave a precision (2) 1,2-Dichloroethane. Attested by of 10 - 15 %.
- 1.B. [Saturat. n° 2]. A measure of the static pressure of saturation in an apparatus which gave a precision of 2 - 5%.
- 2. [Chromato]. A Gas liquid chromato- ESTIMATED ERROR: graphic method estimated to have a precision of 2 - 5%.
- 3. [Anal. directe]. Direct analysis of the gaseous and liquid phases.

Method 1.B. was used for this system.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. BASF. Purity stated to be greater than 99.9 %.
- spectroscopy and gas chromatography as having purity greater than 99.9 per cent.

REFERENCES .

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2-Dichloroethane; C2H4Cl2: [107-06-2]

ORIGINAL MEASUREMENTS:

Abdullaev, A. I.; Aliev, A. M.; Mamedov, M. B.

Uch. Zap. Azerb. Gos. Univ., Ser. Khim. Nauk 1968, No. 3, 80 - 83.

Ref. Zh. Khim. 1969, Abstr. No. 11B1279.

VARIABLES:

T/K = 273.15 - 353.15Total pressure = barometric

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Hydrogen Chloride $w_{_{1}}/w$ t %			Hydrogen C	hloride1	Mol Ratio	Mol Fraction	
	a	<i>w</i> ₁ /wс b	Mean	g HCl per 100 g (2)	cm HCl per l cm (2)	n_1/n_2	x_1	
273.15	2.94	3.14	3.04	3.13	23.32	0.0850	0.0783	
283.15	2.02	2.11	2.06	2.10	16.00	0.0570	0.0539	
293.15	1.47	1.46	1.46	1.47	11.46	0.0399	0.0384	
303.15	1.01	1.08	1.05	1.06	7.99	0.0288	0.0280	
313.15	0.82	0.77	0.80	0.80	6.10	0.0217	0.0215	
323.15	0.66	0.64	0.65	0.65	4.95	0.0178	0.0175	
333.15	0.50	0.46	0.48	0.48	3.68	0.0132	0.0130	
343.15	0.33	0.30	0.32	0.32	2.45	0.0087	0.0086	
353.15	0.16	0.16	0.16	0.16	1.23	0.0043	0.0043	

¹ Based on the mean weight per cent.

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a flask in which HCl is generated, a bubbler tube containing concentrated sulfuric acid, a bubbler absorption tube containing about 50 cm3 of dichloroethane.

The gas was passed for 3 hours, the bubbler tube cooled to $258\ \mathrm{K}$ and a sample withdrawn for titration with 0.5 N KOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure sodium chloride and concentrated sulfuric acid.
- (2) 1,2-Dichloroethane. information.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1,2-Trichloroethane; C₂H₃Cl₃; [79-00-5]

ORIGINAL MEASUREMENTS:

Hamai, S.

Bull. Chem. Soc. Jpn. 1935, 10, 207 - 211.

VARIABLES:

T/K: 285.15 - 293.15 Total P/kPa: 67.79 - 88.93

(508.5 - 667.0 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total Pressure p/mmHg	Mol fraction
285.15	508.5 556.5 601.5 649.0 (760.0	0.02514 0.02705 0.02935 0.03195 0.03715) 1
288.15	516.0 655.0 562.0 (760.0	0.02378 0.03056 0.02588 0.03463) ¹
293.15	523.5 523.5 620.0 620.0 640.5 667.0 (760.0	0.02166 0.02171 0.02488 0.02489 0.02633 0.02781 0.03101) 1

These values were calculated by the compiler for a hydrogen chloride partial pressure of 760 mmHg (101.325 kPa). It was assumed that the solvent vapor pressure was the same for the solution and pure solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a U shaped gas buret, connected to a gas reservoir (335 cm³ capacity) which was connected to the absorption vessel. The volume of hydrogen chloride absorbed by 20 cm³ of the original liquid was converted into the amount of gas absorbed at a measured total pressure.

The author obtained the heat of absorption, ΔH , of -3600 cal mol⁻¹ (-15.06 kJ mole⁻¹) from the slope of a plot of log x_1 vs. 1/T.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping concentrated hydrochloric acid into pure concentrated sulfuric acid. The gas was passed through concentrated sulfuric acid and twice condensed by liquid nitrogen.
- (2) 1,1,2-Trichloroethane. Eastman, twice distilled. B.p. 385.65 -386.15 K.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1,2,2-Tetrachloroethane; C₂H₂Cl₄; [79-34-5]

ORIGINAL MEASUREMENTS:

Hamai, S.

Bull. Chem. Soc. Jpn. 1935, 10, 5 - 16.

VARIABLES:

T/K: 288.15 - 298.15

Total P/kPa: 51.26 - 98.53

(384.5 - 739.0 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total Pressure p/mmHg	Mol Fraction
288.15	384.5 573.5 663.5 722.5 (760.0	0.0155 0.0231 0.0261 0.0281 0.03006) 1
293.15	390.0 582.0 621.5 631.5 680.0 731.5 (760.0	0.0140 0.0211 0.0225 0.0229 0.0243 0.0258 0.02744) 1
298.15	396.0 442.0 493.5 541.0 614.5 739.0 (760.0	0.0128 0.0146 0.0161 0.0178 0.0201 0.0239 0.02481) ¹

These values were calculated by the compiler for a hydrogen chloride partial pressure of 760 mmHg (101.325 kPa). It was assumed that the solvent vapor pressure was the same for the solution and pure solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a U shaped gas buret, connected to a gas reservoir (335 cm³ capacity) which was connected to the absorption vessel. The volume of hydrogen chloride absorbed by 20 cm³ of the original liquid was converted into the amount of gas absorbed at a measured total pressure.

The author obtained the heat of absorption, ΔH , of -3300 cal mol⁻¹ (-13.81 kJ mole⁻¹) from the slope of a plot of log x_1 vs. 1/T.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping concentrated hydrochloric acid into pure concentrated sulfuric acid. The gas was passed through concentrated sulfuric acid and twice condensed by liquid nitrogen.
- (2) 1,1,2,2-Tetrachloroethane. Kahlbaum, twice distilled. B.p. 416.65 - 417.15 K.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,1,2,2-Tetrachloroethane; C₂H₂Cl₄; [79-34-5]

ORIGINAL MEASUREMENTS:

Zielinski, A. Z.

Przem. Chem. 1958, 37, 338 - 339.

VARIABLES: T/K = 293.15 - 313.15 $p_1/kPa = 98.25 - 100.10$ (736.9 - 750.8 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL	VALUES:
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T/K	Hydrogen Chloride	Liquid Composition		Kuenen Coefficient	Mol Ratio	Mol Fraction
	Pressure p ₁ /mmHg	HCl n ₁ /mmol	C ₂ H ₂ Cl ₄ n ₂ /mmol	S/cm ³ (STP) g ⁻¹ atm ⁻¹	n ₁ /n ₂	x ₁
293.15	750.8 750.8 750.8	2.879 2.802 2.841	95.5 95.8 98.2	4.07 3.95 3.91	0.0301 0.0292 0.0289	0.0293 0.0284 0.0281 0.0289 ¹
303.15	761.7 761.7	2.652 2.244	97.3 81.7	3.63 3.66	0.0273 0.0275	0.0265 0.0267 0.02651
313.15	736.9 736.9	2.318 2.541	90.8 98.2	3.51 3.57	0.0255 0.0259	0.0249 0.0252 0.0258 ¹

 $^{^{1}}$ Mean mole fraction, x_{1} , for 101.325 kPa (1 atm), assuming a linear change of x_{1} with $p_{\,1}.$

The mole ratio, mole fraction at $p_{\,1}$ of the experiment, and the mean mole fraction at 101.325 kPa (1 atm) values were calculated by the compiler.

The author took the HCl partial pressure to be the difference between the barometric pressure and the pure solvent vapor pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was absorbed by the liquid in an absorption vessel described by Bichowsky and Storch (1). The amount absorbed was determined by a chemical titration.

To calculate the volume of HCl absorbed by one gram of liquid, at 760 mmHg, 22.42 dm³ mol-¹ was taken as the molar volume of HCl at 273.15 K and l atm. The volume based on the real density of HCl under these conditions is (compiler) 22.247 dm³ mol-¹.

SOURCE AND PURITY OF MATERIALS:

May be assumed to be of satisfactory purity.

ESTIMATED ERROR:

REFERENCES:

 Bichowsky, F. R. v.; Storch, H. J. Am. Chem. Soc. <u>1915</u>, 37, 2695.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Pentachloroethane; C₂HCl₅; [76-01-7]

ORIGINAL MEASUREMENTS:

Hamai, S.

Bull. Chem. Soc. Jpn. 1935, 10, 207 - 211.

VARIABLES:

T/K: 285.15 - 293.15 Total P/kPa: 45.26 - 95.73

Total P/kPa: 45.26 - 95.73 (339.5 - 718.0 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total Pressure p/mmHg	Mol Fraction
285.15	560.5 611.5 657.5 712.5 (760.0	0.01865 0.02018 0.02199 0.02381 0.02502) 1
288.15	562.0 611.5 661.5 (760.0	0.01790 0.01934 0.02096 0.02396) ¹
293.15	339.5 565.5 614.0 666.0 718.0 (760.0	0.009946 0.01666 0.01838 0.01937 0.02125 0.02250) 1

These values were calculated by the compiler for a hydrogen chloride partial pressure of 760 mmHg (101.325 kPa). It was assumed that the solvent vapor pressure was the same for the solution and pure solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a U shaped gas buret, connected to a gas reservoir (335 cm³ capacity) which was connected to the absorption vessel. The volume of hydrogen chloride absorbed by 20 cm³ of the original liquid was converted into the amount of gas absorbed at a measured total pressure.

The author obtained the heat of absorption, ΔH , of -2200 cal mol⁻¹ (-9.20 kJ mole⁻¹) from the slope of a plot of log x_1 vs. 1/T.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping concentrated hydrochloric acid into pure concentrated sulfuric acid. The gas was passed through concentrated sulfuric acid and twice condensed by liquid nitrogen.
- (2) Pentachloroethane. Eastman, twice distilled. B.p. 431.65 -432.65 K.

ESTIMATED ERROR:

COMPONENTS: ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; (1) Hydrogen chloride; HCl; [7647-01-0] Wyvill, P. L. (2) 1-Chlorobutane; C_AH_qCl; J. Appl. Chem. 1959, 9, 89 - 93. [109-69-3] VARIABLES: PREPARED BY: T/K: 273.15 - 293.55 W. Gerrard Total P/kPa: 101.325 (1 atm) (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio ⁿ HCl/ ⁿ C ₄ H ₉ Cl	Mol Fraction ^x HCl
273.15	0.0843	0.0777
277.05	0.0759	0.0705
282.15	0.0701	0.0655
293.55	0.0520	0.0494

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = -8.995 + 17.607/(T/100)$

Standard error about regression line = 1.54×10^{-3}

T/K	Mol Fraction
	xHCl
273.15	0.0782
283.15	0.0622
293.15	0.0503

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1-Chlorobutane. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.015$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Chlorohexane; C₆H₁₃Cl; [544-10-5]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 197.15 - 315.95 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC6H13Cl	Mol Fraction ^x HCl
197.15 208.15 229.65 243.45 251.15 261.65 273.45 279.15 287.65	2.639 1.194 0.468 0.261 0.179 0.124 0.0885 0.0771 0.0699 0.0555	0.725 0.544 0.319 0.207 0.152 0.110 0.0813 0.0716 0.0653 0.0526
303.45 309.25 315.95	0.0452 0.0417 0.0325	0.0432 0.0400 0.0315

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = 7.457 - 4.071/(T/100) - 8.348 \ln (T/100)$ Standard error about regression line = 1.68 x 10⁻²

T/K	Mol Fraction	T/K	Mol Fraction
	x HCl		xHCl
203.15	0.629	263.15	0.115
213.15	0.463	273.15	0.0888
223.15	0.344	283.15	0.0693
233.15	0.258	293.15	0.0545
243.15	0.195	303.15	0.0431
253.15	0.149	313.15	0.0343

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

For determination at temperatures below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method. A low temperature, Teddington-type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1-Chlorohexane. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 < 273K$ $\delta x/x = 0.035$

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 1-Chlorooctane; C₈H₁₇Cl; [111-85-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 273.15

Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC8H17Cl	Mol Fraction XHC1
273.15	0.12	0.107

The mole fraction solubility was calculated from the mole ratio by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- 2. 1-Chlorooctane. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.05$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972,
 22, 623 650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Chlorododecane or lauryl chloride; C₁₂H₂₅Cl; [112-52-7]

ORIGINAL MEASUREMENTS:

Fernandes, J. B.; Sharma, M. M.

Indian Chem. Eng. 1965, 7, 38 - 40.

VARIABLES:

T/K: 313.15 - 433.15

HC1 P/kPa: 101.325 (760 mmHg)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction #1
313.15	0.0276	0.0269
333.15	0.0174	0.0171
353.15	0.0132	0.0130
393.15	0.0072	0.00715
433.15	0.0037	0.00369

The compiler calculated the mole fraction solubility values.

Smoothed Data: $\ln x_1 = -10.572 + 21.825/(T/100K)$

Standard error about the regression line = 7.27×10^{-4} .

T/K	Mol Fraction		
313.15	0.0273		
333.15	0.0179		
353.15	0.0124		
373.15	0.0089		
393.15	0.0066		
413.15	0.0050		
433.15	0.0040		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was bubbled into the solvent for more than an hour. Approximately 1 cm3 of the solution was transferred to a weighed sample tube and the whole re-weighed. The contents were transferred to water, and the chloride content determined by the Volhard method.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared by the method of Sloan (1).
- (2) 1-Chlorododecane. Prepared from dodecanol by the interaction of hydrogen chloride in the presence of zinc chloride at 393 - 453 K.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta x_1/x_1 = 0.05$

REFERENCES:

1. Sloan, A. D. B. Chem. Ind. 1964, 574.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Chlorohexadecane or cetyl chloride; C₁₆H₃₃Cl; [4860-03-1]

ORIGINAL MEASUREMENTS:

Fernandes, J. B.; Sharma, M. M.

Indian Chem. Eng. 1965, 7, 38 - 40.

VARIABLES:

T/K: 313.15 HCl P/kPa: 101.325 (760 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction	
313.15	0.0383	0.0369	

The compiler calculated the mole fraction solubility values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was bubbled into the solvent for more than an hour. Approximately 1 cm³ of the solution was transferred to a weighed sample tube and the whole re-weighed. The contents were transferred to water, and the chloride content determined by the Volhard method.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared by the method of Sloan (1).
- (2) 1-Chlorohexadecane. Prepared from 1-hexadecanol and hydrogen chloride in the presence of zinc chloride at 393-453 K.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta x_1/x_1 = 0.05$

REFERENCES:

1. Sloan, A. D. B. Chem. Ind. 1964, 574.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Chlorohexadecane; C₁₆H₃₃Cl; [4860-03-1]

ORIGINAL MEASUREMENTS:

Scher, M.; Gill, W. N.; Jelinek, R. V.

Ind. Eng. Chem., Fundam. 1963, 2, 107 - 112.

VARIABLES:

T/K: 313.15

P/kPa: 50.66 - 98.66 (380-740 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's Constants		Number of Points	Percent Mean	Mol Fraction
	K'/mmHg dm ³ mol ⁻¹	K/mmHg	or roines	Deviation	<i>x</i> ₁
313.15	6460	20,980	4	±0.6	0.0362

Henry's constants:

 $K'/mmHg dm^3 mol^{-1} = (p_1/mmHg)/(c_1/mol dm^{-3})$

 $K/mmHg = (p_1/mmHg)/x_1$

The compiler calculated the mole fraction solubility value at 101.325 kPa (760 mmHg).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was measured in an apparatus designed to determine the kinetic rate of catalyzed hydrochlorination of hexadecene in the presence of ferric chloride. The volume of gas absorbed by the pure liquid at increasing pressures, 380 - 740 mmHg, was measured. The individual solubility values are presented in a graph. The Henry's constants were tabulated.

The paper references a value of Henry's constant in 2-chlorohexa-decane (1) which was not available for compilation.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Matheson Co. Sublimed at high vacuum and liquid air temperature, and distilled into storage and supply system.
- (2) 1-Chlorohexadecane. Not stated.

ESTIMATED ERROR:

REFERENCES:

1. Domash, L. K. Ph. D. thesis, <u>1952</u> Purdue University

274 Hydrogen Chloride in Non-Aqueous Solvents COMPONENTS: ORIGINAL MEASUREMENTS: Bell, R. P. (1) Hydrogen chloride; HCl; [7647-01-0] J. Chem. Soc. 1931, 1371 - 1382. (2) Bromine substituted alkanes **VARIABLES:** PREPARED BY: T/K: 293.15 W. Gerrard P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES: Partition Mol Fraction T/K Coefficient c_{1,l}/c_{1,g} Bromoethane; C₂H₅Br; [74-96-4] 293.15 35.15 0.1019

293.15 10.3 0.0348

Tribromomethane; CHBr₃; [75-25-2]

4.78

1,2-Dibromoethane; C2H4Br2;

[106-93-4]

293.15

1,1,2,2-Tetrabromoethane; $C_2^{H_2Br_4}$; [79-27-6]

0.0306

293.15 3.93 0.0236

The ideal gas concentration is $c_{1,\sigma} = n/V = p/RT = 0.0417 \text{ mol dm}^{-3}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO₂ free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, c/mol dm⁻³, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Bromine substituted alkanes. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

(1) Hydrogen chloride; HCl; [7647-01-0]

(2) 1,2-Dibromoethane; C₂H₄Br₂; [106-93-4]

ORIGINAL MEASUREMENTS:

Hamai, S.

Bull. Chem. Soc. Jpn. 1935, 10, 5 - 16.

VARIABLES:

T/K: 288.15 - 298.15 Total P/kPa: 37.20 - 95.86

37.20 - 95.86 (279.0 - 719.0 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Total Pressure p/mmHg	Mol Fraction
288.15	354.0 531.0 672.0 719.0 (760.0	0.0180 0.0266 0.0325 0.0348 0.03754) ¹
293.15	362.0 453.5 496.0 679.5 (760.0	0.0165 0.0207 0.0225 0.0309 0.03441) ¹
298.15	279.0 368.5 507.0 601.0 672.0 (760.0	0.0117 0.0153 0.0206 0.0242 0.0269 0.03116) 1

These values were calculated by the compiler for a hydrogen chloride partial pressure of 760 mmHg (101.325 kPa). It was assumed that the solvent vapor pressure was the same for the solution and pure solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a U shaped gas buret, connected to a gas reservoir (335 cm³ capacity) which was connected to the absorption vessel. The volume of hydrogen chloride absorbed by 20 cm³ of the original liquid was converted into the amount of gas absorbed at a measured total pressure.

The author obtained the heat of absorption, ΔH , of -3200 cal mol⁻¹ (-13.39 kJ mole⁻¹) from the slope of a plot of $\log x_1 \ vs. \ 1/T.$

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping concentrated hydrochloric acid into pure concentrated sulfuric acid. The gas was passed through concentrated sulfuric acid and twice condensed by liquid nitrogen.
- (2) 1,2-Dibromoethane. Takeda, twice distilled. B.p. 402 K.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Bromobutane; C₄H₉Br; [109-65-9]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 274.65 - 296.65 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio ⁿ HCl/ ⁿ C ₄ H ₉ Br	Mol Fraction ^x HCl
274.65	0.0800	0.0741
280.15	0.0699	0.0653
286.15	0.0608	0.0573
296.65	0.0440	0.0421

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{\rm HC1} = 110.656 - 147.474/(T/100) - 58.957 \ln (T/100)$ Standard error about regression line = 7.07 x 10^{-4}

Mol Fraction
xHCl
0.0760
0.0614
0.0469
0.0341

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1-Bromobutane. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.01$

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHC1/nC6H13Br	Mol Fraction "HCl
273.15	0.0896	0.0822
282.35	0.0709	0.0662
293.15	0.0567	0.0537
298.15	0.0508	0.0483
304.15	0.0464	0.0443
315.65	0.0340	0.0329

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = -9.064 + 17.961/(T/100)$

Standard error about regression line = 1.34×10^{-3}

T/K	Mol Fraction ^x HCl
273.15	0.0830
283.15	0.0658
293.15	0.0530
303.15	0.0433
313.15	0.0359
323.15	0.0300

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1-Bromohexane. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.015$

COMPONENTS: (1) Hydrogen chloride; HCl; Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. (2) 1-Bromooctane; C₈H₁₇Br; J. Appl. Chem. 1959, 9, 89 - 93. VARIABLES: T/K: 273.15 - 317.15 Total P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89 - 93. W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC ₈ H ₁₇ Br	Mol Fraction ^x HCl
273.15	0.0958	0.0874
280.15	0.0820	0.0758
289.15	0.0687	0.0643
296.75	0.0601	0.0567
302.55	0.0540	0.0512
310.45	0.0439	0.0421
317.15	0.0371	0.0358

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = 47.221 - 61.914/(T/100) - 26.875 \ln (T/100)$ Standard error about regression line = 1.19 x 10⁻³

T/K	Mol Fraction **HC1
273.15	0.0862
283.15	0.0730
293.15	0.0606
303.15	0.0494
313.15	0.0396
323.15	0.0314

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) 1-Bromooctane. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.01$

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. 1-Bromooctane; C₈H₁₇Br;
 [111-83-1]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 273.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K M	Mol Ratio	Mol Fraction
пно	C1/ ⁿ C ₈ H ₁₇ Br	X _{HC1}
243.15	0.363	0.266
263.15	0.146	0.127
273.15	0.105	0.095

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $1n X_{HC1} = -10.764 + 22.939/(T/100)$

Standard error about regression line = 2.82×10^{-3}

T/K	Mol Fraction
	XHCl
243.15 263.15	0.265 0.129
273.15	0.094

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For the first temperature a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- 1-Bromooctane. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. 1-Iodooctane; C₈H₁₇I; [629-27-6]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W. Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 213.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	_ Mol_Ratio	Mol Fraction
	"HC1/"C8H17I	X _{HC1}
213.15	0.70	0.412
223.15	0.47	0.320
233.15	0.35	0.259
243.15	0.27	0.213
253.15	0.215	0.177
263.15	0.17	0.145
273.15	0.13	0.115
283.15	0.10	0.0909
293.15	0.08	0.0740

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln x_{HC1} = 14.263 - 14.459/(T/100) - 11.088 \ln (T/100)$ Standard error about regression line = 6.37 x 10^{-3}

T/K.	Mol Fraction
	x_{HC1}
213.15	0.401
223.15	0.327
233.15	0.266
243.15	0.215
253.15	0.174
263.15	0.141
273.15	0.113
283.15	0.0821
293.15	0.0746

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K a chemical titration was performed.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- 1-Iodooctane. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.025$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972,
 623 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Chloroethene or vinyl chloride; C₂H₃Cl; [75-01-4] (ARIABLES: p/kPa = 101.325 (1 atm) ORIGINAL MEASUREMENTS: Hannaert, H.; Haccuria, M.; Mathieu, M. P. Ind. Chim. Belge. 1967, 32, 156 - 164. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

Temperature Interval of Measurement T/K	Hydrogen Chloride Mol % Range $10^2x_1/\text{mol}$ %	Kπν/atm¹ at 293.15 K	Enthalpy of Solution ΔH/kcal mol ⁻¹	Constant A
213.15-243.15	1 - 5	(42)	4.26	4.80

 $\log (K\pi v/atm) = A - (\Delta H/cal mol^{-1})/(2.3R(T/K))$

The function, $K\pi\nu/atm$, is equivalent to a Henry's constant in the form $K/atm = (f_1/atm)/x_1$ where f_1 is the fugacity.

The author's definitions are $K = y_1/x_1 = \frac{\text{mole fraction HCl in the gas}}{\text{mole fraction HCl in the liquid,}}$

 $\pi/atm = total pressure,$

ν = coefficient of fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe three methods.

- 1.A. A measure of the static pressure
 of saturation in an apparatus
 which gave a precision of 10 15 %.
- 1.B. A measure of the static pressure
 of saturation in an apparatus
 which gave a precision of 2 5
 per cent.
- A Gas Liquid Chromatographic method estimated to have a precision of 2 - 5 per cent.
- Direct analysis of the gaseous and liquid phases.

Method 1.B. was used for this system.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. BASF. Purity stated to be greater than 99.9 %.
- (2) Chloroethene. BASF. Degassed by repeated fusions in a vacuum. Purity greater than 99.9 %. Several values of both vapor pressure and density are given in the paper.

ESTIMATED ERROR:

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]	ORIGINAL MEASUREMENTS: Danov, S. M.; Golubev, Yu. D.
(2) Chloroethene or vinyl chloride; C ₂ H ₃ Cl; [75-01-4]	Khim. Prom_st. (Moscow) 1968, 44 (2), 116 - 120.
VARIABLES: T/K = 204.55 - 242.65 $p_1/kPa = (100 - 1000 \text{ mmHg})$	PREPARED BY: W. Gerrard
EXPERIMENTAL VALUES:	
See next	nage
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AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE: Solubilities were stated to be	SOURCE AND PURITY OF MATERIALS: (1) Hydrogen chloride. Probably of
measured by a static method. The pressures were stated to have been	satisfactory purity.
measured to an accuracy of 1 mmHg on a mercury column.	(2) Chloroethene. Purity of vinyl chloride was checked by chromato-
Note that in the authors' table the	graphy; stated to be not less than 99.99%.
pressures were given in steps of 100 mmHg. This appears to indicate a	chan 55.555%.
smoothing of primary data.	
	ESTIMATED ERROR:
	REFERENCES:

Danov,

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M.; Golubev,

ORIGINAL MEASUREMENTS:

(1) Hydrogen chloride; HCl; [7647-01-0]

Hydrogen
Chloride in I
Non-Aqueous
ous Solvents

T/K	20	14.55	20	09.65	2	15.15	2	20.65	23	26.15	23	31.15	2	36.65	24	12.65
p/mmHg	S1	x ₁ ¹	S^1	x ₁ ²	S1	x_1^2	<i>S</i> ¹	x_1^2	S1	x ₁ ²	S ¹	x_1^2	S ¹	x_1^2	S 1	x_1^2
100	25.9	0.0675	20.9	0.0554	16.9	0.0448	13.6	0.0366	10.6	0.0289	9.3	0.0254	7.8	0.0214	6.6	0.0182
200	55.8	0.1350	44.6	0.1108	35.3	0.0896	28.3	0.0732	22.0	0.0578	19.1	0.0508	16.0	0.0428	13.5	0.0364
300	90.9	0.2025	71.3	0.1662	55.7	0.1344	44.1	0.1098	34.0	0.0867	29.5	0.0762	24.5	0.0642	20.6	0.0546
400	132.4	0.2700	101.9	0.2216	78.3	0.1692	61.4	0.1464	46.9	0.1156	40.4	0.1016	33.5	0.0856	28.1	0.0728
500	182.4	0.3375	137.1	0.2770	103.5	0.2240	80.2	0.1830	60.6	0.1445	52.0	0.1270	42.9	0.1070	42.9	0.0910
600			178.2	0.3324	131.9	0.2688	100.8	0.2196	75.3	0.1734	64.3	0.1524	52.7	0.1284	43.8	0.0109
700					185.3	0.3411	138.1	0.2783	101.1	0.2202	85.5	0.1928	69.5	0.1627	57.4	0.1382
800							148.3	0.2930	108.0	0.2930	91.2	0.2030	73.9	0.1712	60.9	0.1455
900							176.0	0.3296	126.3	0.2607	³ 105.9	0.2284	85.4	0.1926	70.1	0.1637
1000									146.1	0.2896	121.7	0.2538	97.5	0.2140	79.6	0.1819
Henry's Constan K/mmHq	t	181	13	305	2:	228	2.	730	3,	150	31	340	4	671	54:	0.6

¹ Kuenen coefficient, S/cm³ (STP) g⁻¹ atm⁻³.

 $^{^{2}}$ Mole fraction hydrogen chloride, $\boldsymbol{x}_{1}.$

³ Value appears to be in error.

[&]quot;Henry's constant, $K/mmHg = (p_1/mmHg)/x_1$.

COMPONENTS:	ORIGINAL MEASUREMENTS:
<pre>(1) Hydrogen chloride; HC1; [7647-01-0]</pre>	Danov, S. M.; Golubev, Yu. D.
(2) (E)-1,2-Dichloroethene or trans-dichloroethene; C ₂ H ₂ Cl ₂ ; [156-60-5]	Khim. Prom_st. (Moscow) 1968, 44 (2), 116 - 120.
VARIABLES:	PREPARED BY:
T/K = 225.15 - 256.15 $p_1/kPa = (100 - 1000 \text{ mmHg})$	W. Gerrard
EXPERIMENTAL VALUES:	
See next p	page
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were stated to be measured by a static method. The pressures were stated to have been measured to an accuracy of 1 mmHg on a mercury column. Note that in the authors' table the pressures were given in stages of 100 mmHg. This appears to indicate a smooting of primary data.	 (1) Hydrogen chloride. Probably of satisfactory purity. (2) (E)-1,2-dichloroethene or trans-dichloroethene. Purity checked by chromatography.
	ESTIMATED ERROR:
	REFERENCES:

Hydrogen chloride; [7647-01-0]

HCl;

(E)-1,2,-Dichloroethene or dichloroethene; C₂H₂Cl₂; [156-60-5]

Khim. 116 -

Prom_st. 120.

(Moscow) 1968,

Ö

EXPERIMENTAL MEASUREMENTS:

EVALUATOR:

Danov, S. M.;

T/K	225.1	.5	229.6	5	235.	15	241.6	5	251.	15	256.1	5
p/mmHg	SI	x_1	S1	x_1^2	SI	x_1^2		x_{1}^{2}	- <u></u>	x_1^2	- gr	x_1^2
100	4.5	0.0193	3.9	0.0168	3.4	0.0146	2.8	0.0121	2.2	0.0096	1.9	0.0084
200	9.2	0.0386	8.0	0.0336	6.7	0.0292	5.7	0.0242	4.1	0.0192	4.0	0.0168
300	14.2	0.0579	12.2	0.0504	10.6	0.0438	8.7	0.0363	6.9	0.0288	5.9	0.0252
400	19.3	0.0772	16.6	0.0672	14.3	0.0584	11.7	0.0484	9.2	0.0384	8.0	0.0336
500	24.7	0.0965	21.1	0.0840	18.2	0.0730	18.2	0.0630	11.6	0.0480	10.1	0.0420
600	30.3	0.1158	25.8	0.1008	22.2	0.0876	16.7 ³	0.0726	14.2	0.0576	12.3	0.0504
760	39.8	0.1470	33.7	0.1275	28.8	0.1111	23.4	0.0920	18.3	0.0734	15.7	0.0640
800			35.8	0.1342	30.6	0.1169	24.7	0.0968	19.7	0.0772	16.6	0.0674
900					35.0	0.1315	23.2	0.1089	22.0	0.0868	18.1	0.0758
1000					39.5	0.1461	31.2	0.1210	24.5	0.0964	21.2	0.0842
enry's onstant'												
K/mmHg	5169		5957		683	9	8260		1035	0	1187	0

¹ Kuenen coefficient, S/cm³ (STP) g⁻¹ atm⁻¹.

 $^{^{2}}$ Mole fraction hydrogen chloride, x_{1} .

³ Value appears to be in error.

⁴ Henry's constant, K/mmHg = $(p_1/mmHg)/x_1$.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chloroethenes

ORIGINAL MEASUREMENTS:

Bell, R. P.

J. Chem. Soc. 1931, 1371 - 1382.

VARIABLES:

T/K: 293.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K Partition Mol Fraction Coefficient x_1 $c_{1,t}/c_{1,q}$

Trichloroethene; C₂HCl₃; [79-01-6]

293.15

5.79

0.0206

Tetrachloroethene; C₂Cl₄; [127-18-4]

293.15

3.88

0.0163

The ideal gas concentration at one atm is $c_{1,g}/\text{mol dm}^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO₂ free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, $c/\text{mol dm}^{-3}$, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Chloroethenes. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Trichloroethene; C2HCl3; [79-01-6]

ORIGINAL MEASUREMENTS:

Abdullaev, A. I.; Aliev, A. M.; Mamedov, M. B.

Uch. Zap. Azerb. Gos. Univ., Ser. Khim. Nauk. 1968, No. 3, 80 - 83.

From Ref. Zh. Khim. 1969, Abstr. No. 11B 1279.

VARIABLES:

T/K = 273.15 - 353.15Total pressure = barometric PREPARED BY:

W. Gerrard

0.00541

0.00538

EXPERIMENT	AL VALU	ES:					
T/K	Hydro	gen Ch.	loride	Hydrogen C	hloride1	Mol Ratio	Mol Fraction
l		w_{γ}/wt	≒ %			n /n	
	a	b	Mean	g HCl per 100 g (2)	cm HCl per l cm (2)	n_{1}/n_{2}	x ₁
							
273.15	0.88	0.90	0.89	0.90	8.00	0.0324	0.0314
283.15	0.62	0.73	0.68	0.68	6.07	0.0245	0.0239
293.15	0.50	0.58	0.54	0.54	4.90	0.0195	0.0191
303.15	0.44	0.46	0.45	0.45	4.10	0.0162	0.0160
313.15	0.38	0.36	0.37	0.37	3.31	0.0133	0.0132
323.15	0.31	0.29	0.30	0.30	2.71	0.0108	0.0107
333.15	0.24	0.22	0.23	0.23	2.03	0.00829	0.00822
343.15	0.17	0.19	0.18	0.18	1.59	0.00649	0.00645

¹ Based on the mean weight per cent.

0.15

0.15

The mole ratio and mole fraction values were calculated by the compiler.

1.35

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

353.15 0.16 0.14

The apparatus consists of a flask in which HCl is generated, a bubbler tube containing concentrated sulfuric acid, a bubbler absorption tube containing about 50 cm³ of the trichloroethylene.

The gas was passed for 3 hours, the bubbler tube was cooled to 258 K, and a sample of the solution was withdrawn for titration with 0.5 N KOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure sodium chloride and concentrated sulfuric acid.
- (2) Trichloroethene. No information.

ESTIMATED ERROR:

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) Tetrachloroethene; C₂Cl₄; [127-18-4] VARIABLES: T/K = 293.15 - 363.15 p /kPa = 101.325 (1 atm) PREPARED BY: (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:		Weight ratio	Mol Fraction
		$g_1/10^2g_2$	x 1
	293.15	0.35	0.0157
	303.15	0.31	0.0139
	323.15	0.22	0.0099
	343.15	0.15	0.0068
	363.15	0.08	0.0036

The mole fraction values were calculated by the compiler.

Smoothed Data: For use between 293.15 and 363.15 K.

 $\ln x_1 = 95.045 - 137.022/(T/100 \text{ K}) - 48.788 \ln (T/100 \text{ K})$

 T/K	Mol Fraction
	x_{1}
298.15	0.0148
313.15	0.0122
328.15	0.0092
343.15	0.0065
358.15	0.0043

¹ The weight ratio is grams of HCl per 100 grams of tetrachloroethene.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The gas was passed through the liquid (1) Hydrogen chloride. May be in a jacketed bubbler tube fitted taken as of satisfactory with a sampling tap at the bottom. purity. The amount of hydrogen chloride in a sample was determined by a chemical (2) Tetrachloroethene. Rectified technical grade. B.p. (1 atm)/°C = 120. titration. The pressure was presumably atmospheric. **ESTIMATED ERROR:** REFERENCES:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen chloride; HCl; Curda, M.; Holas, J. [7647-01-0] Chem. Prumys1 1964, 14, 547 - 548. (2) 3-Chloro-1-propene or allyl chloride; C₃H₅Cl; [107-05-1] VARIABLES: PREPARED BY: T/K = 273.15W. Gerrard p / kPa = 101.325 (1 atm)EXPERIMENTAL VALUES: Weight Ratio 1 Mol Fraction T/K $g_1/10^2g_2$ 273.15 3.05 0.0609 $^{\mathrm{1}}$ The weight ratio is grams of HCl per 100 grams of 1-chloropropene. The mole fraction value was calculated by the compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The gas was passed through the liquid (1) Hydrogen chloride. May be taken as of satisfactory in a jacketed bubbler tube fitted with a sampling tap at the bottom. purity. The amount of hydrogen chloride in a sample was determined by a chemical (2) 1-Chloropropene. Redistilled. titration. B.p. $(1 \text{ atm})/^{\circ}C = 44.$ The pressure was presumably atmospheric. ESTIMATED ERROR: REFERENCES:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. 3-Chloro-1-propene or allyl
 chloride; C₃H₅Cl; [107-05-1]

ORIGINAL MEASUREMENTS:

Cook, T. M.

Thesis, <u>1966</u> University of London

VARIABLES:

T/K: 268.95 - 283.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

т/к	Mol Ratio nHCl/nC3H5Cl	Mol Fraction X _{HCl}
268.95	0.0536	0.0509
273.65	0.0484	0.0462
274.65	0.0475	0.0453
278.15	0.0407	0.0391
283.15	0.0320	0.0310

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln X_{HCl} = 485.138 - 655.137/(T/100) - 247.155 \ln (T/100)$

Standard Error About Regression Line = 4.12×10^{-4}

T/K	Mol Fraction XHC1
263.15	0.0520
273.15	0.0468
283.15	0.0309

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data were cited by Gerrard (1).

Hydrogen chloride was passed into a bubbler tube containing a weighed amount of solvent at the specified temperature until the increase in weight was constant at the barometric pressure (2).

For temperatures below 273 K a weighed amount (excess) of pyridine was quantitatively injected into the absorption vessel at the temperature of the thermostat. The tube was then weighed at room temperature.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Sample of best quality was self prepared, and was passed through concentrated sulfuric acid and calcium chloride.
- 2. 3-Chloropropene. Fractionally
 distilled, boiling point (1 atm) =
 45-45.5°C, and refractive index,
 n_D²⁰ = 1.4151.

ESTIMATED ERROR:

$$\delta X_1/X_1 = 0.02$$

- 1. Gerrard, W.
 J. Chim. Phys. 1964, 61, 73;
 Solubility of Gases in Liquids,
 Plenum Press, New York, 1976.
- 2. Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Aromatic Compounds

EVALUATOR:

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Department of Applied Chemistry
and Life Sciences,
Polytechnic of North London,
Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

Solubility of Hydrogen Chloride in Halogenated Aromatic Compounds.

Solubility in chlorobenzene has been measured at barometric pressure by Bell (1), Gerrard et al.(2), and by Zetkin et al.(3). Measurements were made over a pressure range below 101.3 kPa by O'Brien (4,5) and by Wyrzykwoska-Stankiewicz et al.(6) and over a pressure range to 5050 kPa by Strepikheev & Babkin (7). Measurements by these various authors extend over the temperature range 273 to 391 K. Mole fraction solubilities for a partial pressure of 101.3 kPa calculated from the available data are shown in fig 1. The value for 391 K, estimated from measurements by Strepikheev & Babkin, can be disregarded because of the high vapor pressure of the solvent at this temperature. Other values may be fitted to the equation:

$$\ln x_{HC1} = -82.804 + 5275.3/(T/K) + 10.802 \ln(T/K)$$

The standard deviation in values of $x_{\rm HCl}$ is 0.0021.

Solubility in bromobenzene at barometric pressure was measured by Bell (1) at 293.15 K and by Gerrard (2) over the temperature range 273.45 K to 316.75 K. O'Brien & Byrne (4) made measurements at 298.15 K over a pressure range to 38.7 kpa. The mole fraction solubilities for a partial pressure of 101.3 kPa estimated from the published data may be fitted to the equation:

$$\ln x_{HC1} = 231.01 - 8259.3/(T/K) - 36.315 \ln(T/K)$$

The standard deviation in values of $x_{\rm HCl}$ is 0.0012.

O'Brien & Byrne (4) also measured solubilities in fluorobenzene and iodobenzene at 298.15 K over a pressure range to 35 kPa. No other measurements on this system are available for comparison. The compiler has estimated mole fraction solubilities for a partial pressure of 101.3 kPa from the average value of the Henry's constants reported by O'Brien. An alternative method is to fit the data to a form of the Krichevskii-Il'inskaya equation applicable to moderate pressures. i.e.

$$\log_{10} = \frac{P_{HC1}/mmHg}{x_{HC1}} = \log_{10} (H/mmHg) - B (1 - x_{solvent})$$

where B is a constant and H is the limiting value of Henry's constant defined as: $H = \lim_{x \to 0} (P_{HC1}/x_{HC1})$

The corresponding values of mole fraction solubilities for a partial pressure of 101.3 kPa from O'Brien's data estimated in this way then fall in the order fluorobenzene (0.048) > chlorobenzene (0.027) > bromobenzene (0.026) > iodobenzene (0.022).

Zetkin et al.(3) measured solubility in 1,2-dichlorobenzene at barometric pressure over the temperature range 288.15 K to 333.15 K. Lavrova & Tudorovskaya (8) made measurements over the range 293.15 K to 438.15 K, also at barometric pressure, but corrected the values to a partial pressure of 101.15 kPa before publication. The data given by Zetkin, corrected to a partial pressure of 101.325 kPa is in good agreement with that given by Lavrova except at 293.15 K. Mole fraction solubilities at this temperature are 0.0209 (Zetkin) and 0.0220 (Lavrova). Mole fraction solubilities from the two sets of data may be represented by the equation:

$$\ln x_{HC1} = 18.049 - 106.766/(T/K) - 3.8027 \ln(T/K)$$

The standard deviation in values of $x_{\rm HC1}$ is 0.00090. This equation is based upon data for the range 288 K to 438 K.

The solubility in 1,2,4-trichlorobenzene was measured by Zetkin $et\ al.(3)$ at barometric pressure in the temperature range 288.15 K to 333.15 K. These values are self-consistent and probably as reliable as other

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Halogenated Aromatic Compounds

EVALUATOR:

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January 1989



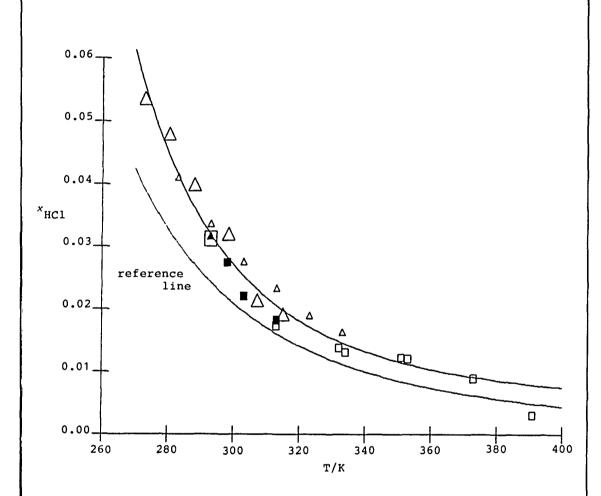


Figure 1

Variation with temperature of experimental values of the mole fraction solubility of hydrogen chloride at a partial pressure of 101.3 kPa in chlorobenzene.

The reference line corresponds to the variation in solubility from the Raoult's law equation.

- \triangle Gerrard et a1. (2)
- A Zetkin et al. (3)
- Wyrzykwoska-Stankiewicz et 81. (6)
- Strepikheev & Babkin (7)
- ▲ Bell (1)
- O'Brien (4,5)

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Halogenated Aromatic Compounds

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

measurements by these authors of the solubilities in the chlorobenzenes. There are, however, no other measurements on this system with which comparison may be made.

Bell (1) measured the solubility in (chloromethyl)benzene at barometric pressure and 293.15 K. No other measurements on this system are available for comparison.

The solubility in (trichloromethyl)benzene at barometric pressure was also measured by Bell (1) at 293.15 K and by Gerrard et al.(2) over the temperature range 273.65 K to 315.95 K. The mole fraction solubility of 0.0275 from Bell's measurement is in sharp contrast to the value of 0.0449 at this temperature by interpolation of Gerrard's measurements. Gerrard's measurements are consistent over the temperature range and are likely to be the more reliable.

The solubility in (trifluoromethyl)benzene has been measured by Ushakov et al.(9) at a total pressure equal to barometric pressure over the temperature range 279 K to 353 K. The measurements are self consistent but there are no other measurements on this system with which comparisons may be made. These authors also published data for solubility in mixtures of this solvent with chloro- and dichloro(triluoromethyl)benzenes. The compiler has noted errors in the presentation of data for these mixtures.

Ahmed (10) reported the solubility in benzoyl chloride at a total pressure equal to barometric pressure over the temperature range 253.15 K to 293.15 K. Mole fraction solubilities from these measurements are self-consistent and lower than values for chlorobenzene and other solvents containing the carbonyl group. No other measurements on this system are available for comparison.

- 1. Bell, R. P. *J. Chem. Soc.* <u>1931</u>, 1371 1382.
- 2. Gerrard, W.; Mincer, A. M.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89 93.
- Zetkin, V. I.; Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V. Khim. Prom. 1971, 47, 102 103.; Soviet Chem. Ind. 1971, 3, 89 90.
- 4. O'Brien, S. J.; Byrne, J. B. J. Am. Chem. Soc. 1940, 62, 2063 2065.
- 5. O'Brien, S. J. J. Am. Chem. Soc. 1941, 63, 2709 2712.
- Wyrzykwoska-Stankiewicz, D.; Szfranski, A.; Kaminski, M. Bull. Acad. Polon. Sci., Ser. Sci. Chim. 1971, 19, 199 - 205.
- 7. Strepikheev, Yu. A.; Babkin, B. M. Khim. Prom_st (Moscow) 1963, No. 1, 38 39.
- 8. Lavrova, E. M.; Tudorovskaya, G. L. Zh. Prikl. Khim. (Leningrad) <u>1977</u>, 50, 2105 2106.; J. Appl. Chem. USSR <u>1977</u>, 50, 2005 2006.
- 9. Ushakov, A. A.; Kosorotov, V. I.; Stul, B. Ya.; Motsarev, G. V.; Dzhagatspanyan, R. V. Zh. Prikl. Khim. (Leningrad) 1977, 50, 425 - 427.; J. Appl. Chem. USSR 1977, 50, 403 - 405.
- 10. Ahmed, W. Thesis, 1970, University of London.

COMPONENTS: (1) Hydrogen chloride; HCl;

[1) Hydrogen chloride; HCl; [7647-01-0]

(2) Fluorobenzene; C₆H₅F; [462-06-6]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Byrne, J. B.

J. Am. Chem. Soc. <u>1940</u>, 62, 2063 - 2065.

VARIABLES: T/K:

T/K: 298.15

P/kPa: 6.52 - 34.55 (48.9 - 259 mmHq) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	48.9	0.0208	3.09	0.00200	0.00199
	69.9	0.0277	3.32	0.00266	0.00265
	95.3	0.0402	3.12	0.00386	0.00384
	202	0.085	3.10	0.00816	0.00809
	259	0.121	2.82	0.0116	0.0115
	(760	0.331	3.02 av.	0.0318	0.0308) ²

 $^{^{1}}$ k/atm mol⁻¹ kg = $(p_{1}/atm)/(m_{1}/mol kg^{-1})$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Fluorobenzene. Eastman Kodak Co. Attested by refractive index, $n_{\rm D}^{20}$, 1.4650.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. 1937, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0281 to 0.0329 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) (Trifluoromethyl)-benzene or benzotrifluoride; C7H5F3; [98-08-8]

ORIGINAL MEASUREMENTS:

Ushakov, A. A.; Kosorotov, V. I.; Stul, B. Ya.; Motsarev, G. V.; Dzhagatspanyan, R. V.

Zh. Prikl. Khim. (Leningrad) 1977, 50, 425 - 427. J. Appl. Chem. USSR (Engl. Transl.) 1977, 50, 403 - 405.

VARIABLES:

T/K = 279 - 353p/kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Hydrogen	Chloride	Mol Fraction
	w_{τ}/wt %	Mol Ratio	$oldsymbol{x_1}$
		$\frac{n_1/n_2}{}$	
279	1.280	0.0512	0.0487
298	0.540	0.0216	0.0211
313	0.342	0.0137	0.0135
323	0.245	0.0098	0.0097
333	0.176	0.0071	0.00705
353	0.086	0.0036	0.0036

Smoothed Data: For use between 278 and 353 K.

 $\ln x_1 = -15.1689 + 33.8866/(T/100 K)$

The standard error about the regression line is 7.55 x 10-4.

T/K	Mol Fraction
	$x_{_{1}}$
278	0.0508
₩,0	0.0300
288	0.0333
200	0 0004
298	0.0224
212	0 0120
313	0.0130
323	0.0093
	0.0093
333	0.0068
242	0.0000
343	0.0050
353	0.0038
253	0.0036

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Determined under atmospheric pressure (1) Hydrogen chloride. Prepared in a thermostated cylindrical vessel of 200 cm3 capacity fitted with a reflux condenser and a bubbler.

Every 20 minutes a sample was removed (2) (Trifluoromethyl)-benzene. and the HCl content determined by alkalimetry, until a constant concentration was attained.

SOURCE AND PURITY OF MATERIALS:

- from cp grade NaCl and concentrated H₂SO₄. Dried by CaCl₂.
- Rectified, purity 99.8 per cent.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) (Trifluoromethyl)-benzene or benzotrifluoride; C₇H₅F₃; [98-08-8]
- (3) Chloro(trifluoromethyl)-benzene; C₇H_dC1F₃; [52181-51-8]

ORIGINAL MEASUREMENTS:

Ushakov, A. A.; Kosorotov, V. I.; Stul, B. Ya.; Motsarev, G. V.; Dzhagatspanya, R. V.

2h. Prikl. Khim. (Leningrad) 1977, 50, 425 - 427.

J. Appl. Chem. USSR (Engl. Transl.) 1977, 50, 403 - 405.

VARIABLES:

$$T/K = 298 - 353$$

p/kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Composition of Initial Mixture	Hydro	gen Chloride
	C7 ^H 5 ^F 3 C7 ^H 4 ^{ClF} 3 wt % wt %	w ₁ /wt %	$n_1/(n_2 + n_3)$
298 313 323 333 353	84.84 15.16	0.544 0.348 0.258 0.188 0.102	0.0116 (0.0225) 1 0.0074 (0.0144) 1 0.0055 (0.0107) 1 0.0040 (0.0078) 1 0.0024 (0.0042) 1

Values in () are mole ratios calculated by the compiler from the weight per cent data. The compiler could reproduce the papers values of the chlorine mole ratio, but not the hydrogen chloride mole ratio. The probable source of the discrepancy is that the authors used the Cl molecular weight in place of the HCl molecular weight.

The authors tabulated values of the Gibbs energy, enthalpy, and entropy of dissolution based on the mole ratio values. The values need to be recalculated from the corrected mole ratio values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Determined under atmospheric pressure in a thermostated cylindrical vessel of 200 cm capacity fitted with a reflux condenser and a bubbler. Every 20 minutes a sample was removed, and the HCl content determined by alkalimetry, until a constant concentration was attained.

Component (3) is probably mostly 1-chloro-3-(trifluoromethyl)-benzene [98-15-7].

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from cp grade NaCl and concentrated H₂SO₄. Dried by CaCl₂.
- (2, 3) Mixture. Prepared by chlorination of (trifluoromethyl) benzene at 60°C in the presence of FeCl₃.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) (Trifluoromethyl)-benzene or benzotrifluoride; C₇H₅F₃;[98-08-8]
 (3) Chloro(trifluoromethyl)-benzene;
- C₇H₄ClF₃; [52181-51-8] (4) Dichloro(trifluoromethyl)-benzene;
- $C_7H_3Cl_2F_3$; [30498-35-2]

VARIABLES:

T/K = 298 - 353p/kPa = 101.325 (1 atm)

ORIGINAL MEASUREMENTS:

Ushakov, A. A.; Kosorotov, V. I.; Stul, B. Ya.; Motsarev, G. V.; Dzhagatspanya, R. V.

2h. Prikl. Khim. (Leningrad) 1977, 50, 425 - 427.

J. Appl. Chem. USSR (Engl. Transl.) 1977, 50, 403 - 405.

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K C	/K Composition of Initial Mixture		tial Mixture	Hydro	ogen Chlo	
	C7H5F3	C7H4ClF3	C7H3Cl2F3	w ₁ /wt %	$n_1/(n_2$	atio + n ₃ + n ₄ ,
298 313 323 333 353	58.29	39.47	2.24	0.540 0.362 0.280 0.212 0.140	0.0123 0.0082 0.0064 0.0048 0.0031	(0.0237) (0.0159) (0.0123) (0.0093) (0.0061)
298 313 323 333 353	22.82	60.86	16.32	0.550 0.374 0.302 0.230 0.152	0.0138 0.0094 0.0076 0.0058 0.0035	(0.0266) ¹ (0.0181) ¹ (0.0146) ¹ (0.0111) ¹ (0.0073) ¹

1 Values in () are mole ratios calculated by the compiler from the weight per cent data. The compiler could reproduce the papers values of the chlorine mole ratio, but not the hydrogen chloride mole ratio. The probable source of the discrepancy is that the authors used the ${\rm Cl}_2$ molecular weight in place of the HCl molecular weight.

The authors tabulated values of the Gibbs energy, enthalpy, and entropy of dissolution based on the mole ratio values. The values need to be recalculated from the corrected mole ratio values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Determined under atmospheric pressure in a thermostated cylindrical vessel of 200 cm³ capacity fitted with a reflux condenser and a bubbler. Every 20 minutes a sample was removed, and the HCl content determined by alkalimetry, until a constant concentration was attained.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from cp grade NaCl and concentrated H₂SO₄. Dried by CaCl₂.
- (2, 3, 4) Mixture. Prepared by chlorination of (trifluoromethyl)-benzene at 60 °C in the presence of FeCl3.

ESTIMATED ERROR:

Component (3) is probably mostly 1-chloro-3-(trifluoromethyl)-benzene [98-15-7]. Component (4) is a mixture of mostly 1,2-dichloro-4-(trifluoromethyl)-benzene [328-84-7], 1,4-dichloro-2-(trifluoromethyl)-benzene [320-50-3], and 2,4-dichloro-1-(trifluoromethyl)-benzene [320-60-5].

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chlorobenzene and (chloromethy1) 1371 1382. benzenes

ORIGINAL MEASUREMENTS:

Bell, R. P.

J. Chem. Soc. 1931,

VARIABLES:

T/K: 293.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K Partition Mol Fraction Coefficient x_1 $c_{1,l}/c_{1,g}$

Chlorobenzene; C₆H₅Cl; [108-90-7]

293.15

7.63

0.0315

(Chloromethyl)benzene; C₇H₇Cl; [100-44-7]

293.15

9.75

0.0448

(Trichloromethyl)benzene; $C_7^{H_5}Cl_3$; [98-07-7]

293.15

4.77

0.0275

The ideal gas concentration at $p_I = 1$ atm is $c_{1,g}/\text{mol dm}^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 cm³ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO₂ free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, c/mol dm⁻³, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Chlorobenzene and (chloromethy1)benzenes. Good specimens were dried over calcium chloride, and distilled. Boiling points are given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chlorobenzene; C₆H₅Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Byrne, J. B.

J. Am. Chem. Soc. 1940, 62, 2063 - 2065.

VARIABLES: T/K:

298.15

P/kPa: 4.01 - 45.29

(30.1 - 340 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant	Mol Ratio	Mol Fraction
30.1	0.0081	4.85	0.00091	0.00091
48.0	0.0152	4.16	0.00171	0.00171
108	0.0310	4.58	0.00349	0.00346
193	0.0578	4.39	0.00650	0.00646
198	0.0597	4.31	0.00672	0.00667
340	0.1027	4.35	0.0116	0.0114
(760	0.228	4.38 av.	0.0257	0.0251)2
	30.1 48.0 108 193 198 340	p ₁ /mmHg m ₁ /mol kg ⁻¹ 30.1 0.0081 48.0 0.0152 108 0.0310 193 0.0578 198 0.0597 340 0.1027	p1/mmHg m1/mol kg-1 Constant k1 30.1 0.0081 4.85 48.0 0.0152 4.16 108 0.0310 4.58 193 0.0578 4.39 198 0.0597 4.31 340 0.1027 4.35	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$

 $k/atm mol^{-1} kg = (p_1/atm)/(m_1/mol kg^{-1})$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

- SOURCE AND PURITY OF MATERIALS:
 (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Chlorobenzene. Eastman Kodak Co. Attested by refractive index, $n_{\rm D}^{\rm 20}$, 1.5240.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0227 to 0.0263 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chlorobenzene; C₆H₅Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.

J. Am. Chem. Soc. 1941, 63, 2709 - 2712.

VARIABLES: T/K:

303.15, 313.15 3.03 - 33.73 (22.7 - 253 mmHg) P/kPa:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure p ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
303.15	22.7	0.0058	5.16	0.000652	0.000652
	23.9	0.0069	4.59	0.000776	0.000775
	113	0.0311	4.78	0.00350	0.00349
	103	0.0312	4.30	0.00351	0.00350
	156	0.0449	4.58	0.00505	0.00803
	253	0.0726	4.76	0.00817	0.00810
313.15	38.8	0.0093	5.48	0.00105	0.00105
	75.2	0.0170	5.82	0.00191	0.00191
	118	0.0291	5.34	0.00327	0.00326
	139	0.0314	5.82	0.00353	0.00352
	203	0.0470	5.68	0.00529	0.00526

At 303.15 K the author's overall mean value of k = 4.65; this gives $m_1(1 \text{ atm})$ equal to 0.215, and equivalent to $x_1 = 0.0236$ for 101.325 kPa.

At 313.15 K the author's overall mean value of k = 5.71; this gives m_1 (1 atm) equal to 0.175, and equivalent to $x_1 = 0.0193$ for 101.325 kPa. (760 mmHg).

¹ The units of Henry's constant, k, are atm mol⁻¹ kg.

 $k/atm mol^{-1} kg = (p_1/atm)/(m_1/mol kg^{-1})$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of (1) Hydrogen chloride. Prepared Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Chlorobenzene. Stored over calcium chloride and distilled, $n_{\rm D}^{20}$, 1.5420.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0]

(2) Chlorobenzene; C₆H₅Cl; [108-90-7] ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 273.15 - 315.15 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio "HCl/"C6H5Cl	Mol Fraction **HCl
273.15	0.0561	0.0531
280.55	0.0498	0.0474
288.15	0.0408	0.0392
298.55	0.0322	0.0312
307.35	0.0210	0.0206
315.15	0.0185	0.0182

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = 97.858 - 130.990/(T/100) - 52.571 \ln (T/100)$

Standard error about regression line = 1.63×10^{-3}

T/K	Mol Fraction ^x HCl
273.15	0.0538
283.15	0.0442
293.15	0.0345
303.15	0.0258
313.15	0.0186
323.15	0.0130

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Chlorobenzene. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.01$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chlorobenzene; C₆H₅Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Strepikheev, Yu. A.; Babkin, B. M.

Khim. Prom_st (Moscow) 1963, No. 1, 38 - 39.

VARIABLES:

T/K = 293-391, 443-523 Total p/kPa = 101.3 - 5050(1 - 50 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

	T/K	Mol Fraction
		x_{1}
	293	0.0265 - 0.0320 (4 points)
	313	0.0172, 0.0175
	332	0.0127
	334	0.0119
	351	0.0101
	353	0.0098
	373	0.0050, 0.0060
	391	0.0010
_		

Numerical data were not recorded. The data are displayed in two diagrams. The data above were obtained from Fig. 1 by the compiler. The figure shows a plot of (HCl, mol %) (total pressure atmospheric) $vs.\ t/^{\circ}C$. The increasing effect of the vapor pressure due to the chlorobenzene is clearly seen as a drifting downward of the concave upward plot over the 333 to 393 K (60 - 120°C) range.

Temper	ature	Total Pressure	Mol Fraction
t/°C	T/K	p/atm	$oldsymbol{x}_{1}$
170	443	50	0.29
190	463		0.24
210	483		0.22
230	503		0.17
250	523		0.155

The data above were read by the compiler from Fig. 2 which shows a plot of mol % HCl vs. total pressure in atm for five isotherms from 443 to 523 K (170 - 250°C).

(Figure numbers refer to the original paper.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into 750 cm³ of freshly distilled chlorobenzene in a flask of 1 dm³ capacity. After saturation a sample was removed, weighed, and the HCl content determined by acid-alkali titration.

An autoclave was used for measurements at the higher pressures, HCl being obtained from a cylinder. The pressure was measured to within 0.5 atm, the temperature to within ± 1°C. The withdrawn sample of solution was weighed to within 0.05 g (10 to 20 g of sample), and the HCl content determined by an acid-alkalititration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by action of concentrated sulfuric acid on chemically pure sodium chloride, dried with calcium chlorides, and filtered through glass wool.
- (2) Chlorobenzene. Dried over calcium chloride and distilled. B.p. (1 atm)/°C = 132 ± 0.2.

ESTIMATED ERROR:

For the high pressure measurements

$$\delta T/K = \pm 1$$

$$\delta p/atm = \pm 0.5$$

- Hydrogen chloride; HCl; [7647-01-0]
- (2) Chlorobenzene; C₆H₅Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Wyrzykwoska-Stankiewicz, D.; Szafranski, A.; Kaminski, M.

Bull. Acad. Polon. Sci., Ser. Sci. Chim. 1971, 19, 199 - 205.

VARIABLES:

K = 293.15kPa = 20.265 - 101.325(152 - 760 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Hydrogen Chloride	Mol Fraction
	p ₁ /mmHg	<i>x</i> ₁
293.15	152	0.0059
	204	0.0081
	380	0.0151
	500	0.0203
	608	0.0248
	760	0.0312

By a calorimetric determination the "heat of solution" was found to have a mean value of 3.70 \pm 0.06 kcal mol⁻¹.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The design of the equilibrium cell was stated to be based on the static method, or on the dynamic method; and although each procedure was described, and diagram of each was drawn, it is not clear which data were obtained by (2) Chlorobenzene. Technical grade. a particular method. The dynamic B. p. (755 mmHg)/ C = 131.5; method required a bubble tube. The hydrogen chloride in a sample of the saturated solution was determined by titration with standard alkali in the presence of bromothymol blue and phenol red.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride was obtained by treating analytical reagent grade sodium chloride with concentrated sulfuric acid.
- B. p. (755 mmHg)/ C = 131.5; refractive index, $n_D^{2^0} = 1.5245$; density $\rho_+^{2^0}/g$ cm⁻³ = 1.106.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Chlorobenzene; C₆H₅Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Zetkin, V. I.; Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V.

Khim. Prom. 1971, 47, 102 - 103.

Soviet Chem. Ind. 1971, 3, 89 - 90.

VARIABLES:

T/K = 283.15 - 333.15p/kPa = 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Temperature		Mol Fraction
t/°C	T/K	x_1
10	283.15	0.0407
20	293.15	0.0331
30	303.15	0.0269
40	313.15	0.0224
50	323.15	0.0178
60	333.15	0.0148

The measurements were stated to be for atmospheric pressure.

Smoothed Data: For use between 283.15 and 333.15 K.

 $\ln x_1 = 15.0758 - 17.0226/(T/100 \text{ K}) - 11.7856 \ln (T/100 \text{ K})$ The standard error about the regression line is 2.51×10^{-4} .

T/K	Mol Fraction x ₁
283.15	0.0407
293.15	0.0332
298.15	0.0299
303.15	0.0270
313.15	0.0221
323.15	0.0180
333.15	0.0147

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas absorbed at atmospheric pressure as described by Zetkin and Kosorotov (1). The amount of gas absorbed was determined by a chemical titration.

The author's fitted the data to the linear equation

$$\log x_1 = -4.54 + 900/(T/K).$$

However, the three constant equation above fits the data much better. The ESTIMATED ERROR: author's equation gives an enthalpy of solution of -4.1 kcal mol-1.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared from sodium chloride and concentrated sulfuric acid. Dried with sulfuric acid.
- (2) Chlorobenzene. Purity stated to be greater than 99%. Dried with calcium chloride.

REFERENCES:

1. Zetkin, V. I.; Kosorotov, V. I. Zh. Fiz. Khim. 1970, 44, 830.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2-Dichlorobenzene; C₆H₄Cl₂; [95-50-1]

ORIGINAL MEASUREMENTS:

Zetkin, V. I.; Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V.

Khim. Prom. 1971, 47, 102 - 103.

Soviet Chem. Ind. 1971, 3, 89 - 90.

VARIABLES:

$$T/K = 288.15 - 333.15$$

 $p/kPa = 101.325 (1 atm)$

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Temp	erature	Mol Fraction
t/°C	T/K	x_1
15	288.15	0.0209
20	293.15	0.0186
30	303.15	0.0166
40	313.15	0.0158
50	323.15	0.0144
60	333.15	0.0135

The measurements were stated to be for atmospheric pressure.

Smoothed Data: For use between 288.15 and 333.15 K.

 $\ln x_1 = -42.6859 + 60.6173/(T/100 K) + 16.7806 \ln (T/100 K)$ The standard error about the regression line is 4.82×10^{-4} .

T/K	Mol Fraction
	x_1
288.15	0.0204
293.15	0.0191
298.15	0.0179
303.15	0.0169
313.15	0.0154
323.15	0.0143
333.15	0.0136

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas absorbed at atmospheric pressure as described by Zetkin and Kosorotov (1). The amount of gas absorbed was determined by a chemical titration.

The author's fitted the data to the linear equation

$$\log x_1 = -2.86 + 330/(T/K)$$

However, the three constant equation above fits the data much better. The author's equation gives an enthalpy of solution of -1.5 kcal mol⁻¹.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared from sodium chloride and concentrated sulfuric acid. Dried with sulfuric acid.
- (2) 1,2-Dichlorobenzene. Purity stated to be greater than 99%. Dried with calcium chloride.

ESTIMATED ERROR:

REFERENCES:

Zetkin, V. I.; Kosorotov, V. I.
 Zh. Fiz. Khim. <u>1970</u>, 44, 830.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2-Dichlorobenzene; C₆H₄Cl₂; [95-50-1]

ORIGINAL MEASUREMENTS:

Lavrova, E. M.; Tudorovskaya, G. L. Zh. Prikl. Khim. (Leningrad) 1977, *50*, 2105 - 2106.

J. Appl. Chem. USSR (Engl. Transl.) <u>1977</u>, 50, 2005 - 2006.

VARIABLES:

T/K = 293 - 438Total p/kPa = 101.3 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Ratio Mol Fraction 2
n_2 x_1
0.0220
00 [sic] 0.0157
0.0128
0.00916
0.00892
0.00781
3 0.00624
0.00447
֡

¹corrected by authors to $p_1 = 101.3$ kPa; ²calculated by the compiler Smoothed Data: For use between 293 and 438 K.

 $\ln x_1 = \pm 8.2612 + 12.9657/(T/100 K)$

The standard error about the regression line is 6.90 x 10⁻⁴.

T/K	Mol Fraction
	\boldsymbol{x}_{1}
293	0.0216
313	0.0163
333	0.0127
353	0.0102
373	0.0084
393	0.0070
413	0.0060
438	0.0050

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas was passed into the liquid in (1) Hydrogen chloride. Prepared a bubbler tube, to which a reflux condenser was fitted. The HCl content in a sample of the saturated solution (p_{total}, 1 atm) was determined by an acid-alkali titration.

The compiler's smoothed data equation confirms the authors thermodynamic values for the enthalpy and entropy of dilution

> $\Delta H/kcal mol^{-1} = -2.603$ $\Delta S/cal K^{-1} mol^{-1} = -16.464$

However the signs in the authors smoothed data equation appear to be reversed and the calculated values of mol mol⁻¹ and wt % of Table 1 appear to be in error.

SOURCE AND PURITY OF MATERIALS:

- from sulfuric acid and chemically pure concentrated hydrochloric acid, and dried.
- (2) 1,2-Dichlorobenzene. Distilled. B.p. $(1 \text{ atm})/^{\circ}C = 183$.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1,2,4-Trichlorobenzene; C₆H₃Cl₃; [120-82-1]

ORIGINAL MEASUREMENTS:

Zetkin, V. I.; Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V.

Khim. Prom_st. (Moscow) 1971, 47, 102 - 103.

Sov. Chem. Ind. (Engl. Transl.) $\underline{1971}$, 3, 89 - 90.

VARIABLES:

$$T/K = 288.15 - 333.15$$

 $p/kPa = 101.325 (1 atm)$

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Temperature		erature	Mol Fraction
	t/°C	T/K	x_1
	15	288.15	0.0301
	20	293.15	0.0251
	30	303.15	0.0186
	40	313.15	0.0151
	50	323.15	0.0141
	60	333.15	0.0117

The measurements were stated to be for atmospheric pressure.

Smoothed Data: For use between 288.15 and 333.15 K

 $\ln x_1 = -113.4479 + 169.1467/(T/100 K) + 48.4095 \ln (T/100 K)$ The standard error about the regression line is 6.35 x 10^{-4} .

T/K	Mol Fraction
	x_1
288.15	0.0298
293.15	0.0251
298.15	0.0217
303.15	0.0190
313.15	0.0154
323.15	0.0133
333.15	0.0120

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas absorbed at atmospheric pressure as described by Zetkin and Kosorotov (1). The amount of gas absorbed was determined by a chemical titration.

The author's fitted the data to the linear equation

$$\log x_{7} = -4.83 + 940/(T/K).$$

However, the three constant equation above fits the data much better. The author's equation gives an enthalpy of solution of -4.4 kcal mol⁻¹.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Self prepared from sodium chloride and concentrated sulfuric acid. Dried with sulfuric acid.
- (2) 1,2,4-Trichlorobenzene. Purity stated to be greater than 99%. Dried with calcium chloride.

ESTIMATED ERROR:

REFERENCES:

Zetkin, V. I.; Kosorotov, V. I.
 Zh. Fiz. Khim. 1970, 44, 830.

COMPONENTS: (1) Hydrogen chloride; HCl; [7647-01-0] (2) (Trichloromethyl) benzene; C7^H5^{Cl}3; [98-07-7] VARIABLES: T/K: 273.65 - 315.95 Total P/kPa: 101.325 (1 atm) EXPERIMENTAL VALUES: T/K Mol Ratio Mol Fraction

T/K	Mol Ratio nHCl/nC7H5Cl3	Mol Fraction #HCl
273.65 279.15 285.15 293.75 294.85 303.65 315.95	0.0751 0.0664 0.0600 0.0465 0.0457 0.0340 0.0275	0.0699 0.0623 0.0566 0.0444 0.0437 0.0329 0.0268

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln x_{HC1} = 20.018 - 22.099/(T/100) - 14.488 \ln (T/100)$ Standard error about regression line = 1.75 x 10^{-3}

Mol Fraction ^x HCl
HCI
0.0720
0.0569
0.0449
0.0354
0.0280
0.0221

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) (Trichloromethyl) benzene. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.03$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Bromobenzene; C₆H₅Br; [108-86-1]

ORIGINAL MEASUREMENTS:

Bell, R. P.

J. Chem. Soc. 1931, 1371 - 1382.

VARIABLES:

T/K: 293.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Partition Coefficient c1,1/c1,g	Mol Fraction
293.15	7.13	0.0305

The ideal gas concentration at $p_1 = 1$ atm is $c_{1,g}/mo1 dm^{-3} = n/V = p/RT = 0.0417$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a 50 ${\rm cm}^3$ bulb extended at the top as a graduated tube, and sealed at the bottom to a capillary U-tube. The liquid was saturated with gas at atmospheric pressure. The gas was displaced from the saturated solution by a current of dry CO, free air, absorbed in water, and titrated with a solution of NaOH.

The solubility, $c/\text{mol dm}^{-3}$, was converted to a partition coefficient by dividing by the ideal gas concentration of HCl in the gas phase.

The mole fraction solubility was calculated on the assumption that the density of the solution obeys the ideal mixture law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared by dropping pure concentrated hydrochloric acid into pure sulfuric acid.
- (2) Bromobenzene. Good specimen was dried over calcium chloride, and distilled. Boiling point is given in paper.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta c/c = 0.01$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Bromobenzene; C₆H₅Br; [108-86-1]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Byrne, J. B.

J. Am. Chem. Soc. <u>1940</u>, 62, 2063 - 2065.

VARIABLES:

T/K: 298.15

P/kPa: 7.09 - 38.71 (53.2 - 290 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	53.2	0.0131	5.35	0.00206	0.00205
	110	0.0272	5.30	0.00427	0.00425
	116	0.0278	5.51	0.00436	0.00435
	128	0.0328	5.12	0.00515	0.00512
	134	0.0346	5.11	0.00543	0.00540
	189	0.0447	5.57	0.00702	0.00700
	290	0.0686	5.56	0.0108	0.0107
	(760	0.185	5.40	0.0291	0.0283)2

 $^{^{1}}$ k/atm mol⁻¹ kg = $(p_{1}/atm)/(m_{1}/mol kg_{1}^{-1})$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
 - (2) Bromobenzene. Eastman Kodak Co. Attested by refractive index, n_D^{20} , 1.3741.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- O'Brien, S. J.; Kenny, C. L.
 Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

 $^{^2}$ Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0274 to 0.0298 for the mole fraction solubility at one atm (101.325 kPa).

(1) Hydrogen chloride; HCl; [7647-01-0]

(2) Bromobenzene; C₆H₅Br; [108-86-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

COMPONENTS:

T/K: 273.45 - 316.75 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio ⁿ HC1 ^{/n} C6 ^H 5 ^{Br}	Mol Fraction ^x HCl
273.45	0.0545	0.0517
279.55	0.0469	0.0448
287.15	0.0384	0.0370
296.95	0.0313	0.0303
306.15	0.0228	0.0223
316.75	0.0151	0.0149

Smoothed Data: $\ln x_{\text{HCl}} = 110.939 - 149.228/(T/100) - 58.997 \ln (T/100)$

Standard error about regression line = 1.15×10^{-3}

T/K	Mol Fraction
	xHCl
273.15	0.0510
283.15	0.0421
293.15	0.0328
303.15	0.0243
313.15	0.0172
323.15	0.0118

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Bromobenzene. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x/x = 0.02$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Iodobenzene; C₆H₅I; [591-50-4]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Byrne, J. B.

J. Am. Chem. Soc. 1940, 62, 2063 - 2065.

VARIABLES: T/K: 298.15

5.57 - 34.96 P/kPa: (41.8 - 262 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction ^x l
298.15	41.8	0.0064	8.56		0.00131
	71.8	0.0118	8.47		0.00241
	85.8	0.0133	8.48		0.00271
	113	0.0168	8.82		0.00343
	164	0.0247	8.75	0.00504	0.00504
	262	0.0403	8.56	0.0082	0.0082
	(760	0.117	8.58 av.	0.0238	0.0232)2

- 1 k/atm mol⁻¹ kg = $(p_{1}/atm)/(m_{1}/mol kg^{-1})$
- ² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0226 to 0.0235 for the mole fraction solubility at one atm (101.325 kPa).

Note: Iodobenzene was incorrectly named bromobenzene in the original paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Iodobenzene. Eastman Kodak Co. Attested by refractive index, $n_{\rm D}^{20}$, 1.6192.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Benzoyl Chloride; C₇H₅ClO;
 [98-88-4]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC7H5C10	Mol Fraction XHCl
253.15	0.200	0.167
258.15	0.172	0.147
263.15	0.143	0.125
268.15	0.117	0.105
273.15	0.098	0.089
278.15	0.090	0.083
283.15	0.080	0.074
288.15	0.072	0.067
293.15	0.067	0.063

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -65.829 + 95.702/(T/100) + 28.273 \ln (T/100)$

Standard Error About Regression Line = 3.05×10^{-3}

T/K	Mol Fraction XHCl
253.15	0.171
263.15	0.122
273.15	0.0923
283.15	0.0740
293.15	0.0624

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the weighed amount of benzoyl chloride in a bubbler tube, as described in the main paper (1). For temperatures below 268 K the final mixture was quantitatively treated with water and the total chloride was estimated by titration.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Benzoyl chloride. The best specimen was purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.02$

REFERENCES:

 Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109.

COMPONENTS:		
 Hydrogen 	Chloride;	HCl;
[7647-01	-0]	

2. Solvents Containing Nitrogen

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
Polytechnic of North London,
Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

Solubility of Hydrogen Chloride in Solvents Containing Nitrogen.

Solubility in nitrobenzene has been measured at barometric pressure over a temperature range by Zetkin et al.(1) and by Ahmed et al.(2). O'Brien (3) measured solubilities at various temperatures over a partial pressure range to 69.8 kPa. The evaluator has estimated solubilities at a partial pressure of 101.3 kPa from O'Brien's measurements by assuming that the change in mole fraction solubility with partial pressure can be approximated by an equation of the the Krichevskii-Il'inskaya type. The evaluator has also estimated mole fraction solubilities at a partial pressure of 101.3 kPa from mole fraction solubilities of total pressures of approximately 101.3 kPa published by Zetkin et al. and by Ahmed et al. Mole fraction solubilities at a partial pressure of 101.3 kPa in the range 253.15 K to 433.15 K from the three sources fit the equation:

$$\ln x_{HC1} = -39.613 + 3208.7/(T/K) + 4.5790 ln (T/K)$$

Standard deviation in values of $x_{\rm HCl} = 5.02 \times 10^{-3}$

The solubility of hydrogen chloride in nitrobenzene in the presence of water for partial pressures of gas up to 133.5 kPa at 298.15 K may be calculated from data published by Wynne-Jones (4). The mole fraction solubility for a partial pressure of 101.3 kPa has been estimated from these data by the evaluator to be 0.070. The value for solubility in dry nitrobenzene from the equation given above is 0.063 \pm 0.005. The presence of water may therefore have little effect on the solubility of hydrogen chloride in nitrobenzene.

Solubility in chloronitrobenzenes and dichloronitrobenzenes were measured by Zetkin et al.(1) over temperature ranges. Measurements indicate that substitution of chlorine into the benzene nucleus reduces mole fraction solubility of hydrogen chloride as can be seen in the following table:

Mole fraction solubilities at $P_{HC1} = 101.3 \text{ kPa}$

	333.15 K	373.15 K
Nitrobenzene (1)	0.0332	0.0196
1-Chloro-2-nitrobenzene	0.0250	0.0150
1-Chloro-3-nitrobenzene	0.0228	0.0140
1-Chloro-4-nitrobenzene		0.0175
1,2-Dichloro-4-nitrobenzene	0.0206	0.0127
1,3-Dichloro-2-nitrobenzene	0.0222	0.0112

Data presented by Zetkin are self-consistent and may be accepted on a tentative basis. No measurements by other workers on these chlorinated compounds are available for comparison.

O'Brien et al.(5) measured the solubility of hydrogen chloride over pressure ranges below barometric pressure in 1-methyl-2-nitrobenzene at 298.15 K and in 1-methyl-3-nitrobenzene at 298.15 K and 308.15 K. Mole fraction solubilities for partial pressures of 1.013 bar may be found by extrapolation of measurements at lower pressures. These are slightly higher than corresponding values for nitrobenzene itself as estimated from the smoothing equation given above.

	NENTS: Hydrogen Chloride; HCl; [7647-01-0]	EVALUATOR: Peter G. T. Fogg Department of Applied Chemistry and Life Sciences,
2.	Solvents Containing Nitrogen	Polytechnic of North London, Holloway, London, N7 8DB, U.K.
 		January 1989

CRITICAL EVALUATION:

Mole fraction solubilities at $P_{HCl} = 101.3 \text{ kPa}$

2	98.	1	5	v	308.	15	v
	.90.	, ,	2	v	200.	13	L

Nitrobenzene	0.0632	0.0518
1-Methyl-2-nitrobenzene	0.0719	
1-Methyl-3-nitrobenzene	0.0767	0.0618

No other measurements on these methylnitrobenzenes are available for comparison but the data may be accepted on a tentative basis until further work is published on the systems.

Kosorotov $et\ al.$ (6) measured solubilities in chlorinated methylpyridines under barometric pressure in the temperature range 333 K to 473 K. The following compounds were studied:

```
2-(trichloromethyl)pyridine (A)
2-chloro-6-(trichloromethyl)pyridine (B)
3,5-dichloro-2-(trichloromethyl)pyridine (C)
3,4,5-trichloro-2-(dichloromethyl)pyridine (D)
```

Solubilities were reported as molar concentrations except in the case of A at 378 K. In this case they reported the mole ratio composition of the "thick pasty substance" which was formed. Solvents B, C & D, show a linear variation of log (Solubility/mol dm⁻³) with 1/(T/K). Solvent A behaves in a similar manner above about 423 K. Between 378 K and 423 K there is a marked decrease in the molar concentration and mole fraction of hydrogen chloride. The mole fraction of hydrogen chloride in the "pasty substance" at 378 K is 0.28. The mole fractions in the liquid phase at 393 K, 408 K and 423 K are about 0.24, 0.063, and 0.026, respectively. This decline is consistent with decreasing stability of an ionic compound from the components.

Molar concentrations of hydrogen chloride in the four solvents at the same temperature are in the order: A > C = D > B. This is not in order of increasing chlorine content. Densities of B, C, and D are not available and mole fraction solubilities cannot be compared.

There is no reason to doubt the reliability of the measurements which may be accepted on a tentative basis. Further measurements are required for confirmation of the data.

- Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.;
 Dzhagatspanyan, B. V. Khim. Prom_st. (Moscow) 1966, 42, (8), 624-626.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109-115.
- O'Brien, S. J.; Kenny, C. L.; Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504-2507; O'Brien, S. J. J. Am. Chem. Soc. 1941, 63, 2709-2712.
- 4. Wynne-Jones, V. F. K. J. Chem. Soc. 1930, 1064 1071.
- O'Brien, S. J.; Kenny, C. L. J. Am. Chem. Soc. 1940, 62, 1189-1192.
 O'Brien, S. J.; King, C. V. J. Am. Chem. Soc. 1949, 71, 3632-3634.
- Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanyan, R. V. Zh. Prikl. Khim. (Leningrad) 1978, 51, 887-889;
 J. Appl. Chem. USSR 1978, 51, 8858-860.

- Hydrogen chloride; HCl; [7647-01-0]
- (2) Nitrobenzene; C6H5NO2; [98-95-3]
- (3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Wynne-Jones, W. F. K.

J. Chem. Soc. 1930, 1064 - 1071.

VARIABLES:

T/K: 298.15 p_1/kPa : 0.404 - 133.3 (3.03 - 1000 mmHg)

PREPARED BY:

W. Gerrard

EMBEDIACHTAI MAINEC.

T/K		Water Phase	Nitrobenzene Phase	HCl Activity	Mole Fraction
	p ₁ /mmHg	$m_1/\text{mol kg}^{-1}$	$m_1/\text{mol kg}^{-1}$	10 ⁻⁵ a ₁	x_1
298.15	3.03	9.635	0.0027	0.0828	0.000332
	3.34	9.766	0.0029	0.0912	0.000357
	8.87	11.147	0.0080	0.242	0.000983
	12.13 ³	11.61	0.0109	0.331	0.00134
	26.4	12.84	0.0229	0.721	0.00281
	48.7	13.84	0.0396	1.33	0.00485
	86.8	14.84	0.0707	2.37	0.00862
	101.5	14.93	0.0773	2.77	0.00942
	107.4	15.21	0.0833	2.93	0.0101
	208.9	16.46	0.164	5.70	0.0198
	303.4	17.19	0.223	8.28	0.0267
	388.	17.76	0.292	10.6	0.0347
	436.	18.05	0.335	11.9	0.0396
	491.	18.38	0.394	13.4	0.0462
	689.(760)	6 19.334	0.556 ⁵	18.8	0.0640
	751.	19.52	0.603	20.5	0.0690
	1000.	20.42	0.833	27.3	0.0929

1 Calculated by the compiler from the HCl activity and the equation $\log \gamma = \log (a_{\pm}/m_1) = \log (a_1^{2}/m_1) = \log (p_1^{2}/m_1) + 1.718$ which rearranges to $\log a_1 = \log p_1 + (2)(1.718)$. [p₁/mmHg and m₁/mol kg⁻¹] ² The mole fraction of HCl in nitrobenzene was calculated by the compiler. 3 This experiment done by the stoppered bottle method.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

liquid being in one limb, and the other in the other limb. Equilibrium was stated to be attained through the vapor phase. The vessel was shaken occasionally over a period of 2-5 days. An acid base titration was used to determine the amount of HCl in weighed samples of each liquid phase. In one experiment the two liquids were shaken in a stoppered bottle.

- * The average of two runs of a separate experiment in which HCl was passed into water. Author corrected value to 760 mmHg HCl.
- ⁵ The average of three runs of a separate experiment in which HCl was passed into water saturated nitrobenzene. Author corrected value to 760 mmHg HCl.
- ⁶ The author states the molalities are for an HCl pressure of 760 mmHg. The vapor pressure curve (1,2) and the equation indicate a lower HCl partial pressure.

SOURCE AND PURITY OF MATERIALS:

- obtained by dropping hydrochloric
- (2) Nitrobenzene. "Pure" quality nitrobenzene was shaken with caustic soda, and distilled from P_2O_5 at 20 mmHg.
- (3) Water. Not stated.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$

- Randall, M.; Young, L. E.
 J. Am. Chem. Soc. 1928, 50, 989.
- 2. International Critical Tables Volume III, page 301 McGraw Hill Co., New York, 1928.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Nitrobenzene; C₆H₅NO₂; [98-95-3]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Kenny, C. L.; Zeurcher, R. A.

J. Am. Chem. Soc. 1939, 61, 2504 - 2507.

VARIABLES:

T/K: 298.15

P/kPa: 5.98 - 69.81

(0.059 - 0.689 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

VALUES:				
T/K	Pressure p ₁ /atm	Molality m ₁ /mol kg ⁻¹	Mol Ratio	Mol Fraction
298.15	0.059 0.213 0.278 0.312 0.428 0.654 0.636 0.689	0.030 0.110 0.146 0.161 0.225 0.319 0.323 0.338	0.00369 0.0135 0.0180 0.0198 0.0277 0.0392 0.0397 0.0416	0.00368 0.0133 0.0176 0.0194 0.0269 0.0378 0.0382 0.0399
	(1.0			0.06)1

¹ Value from the compiler's graphical extrapolation of the plot of the above x_1 vs. p_1 data.

The data are credited to unpublished M.S. theses of Schmelzle and Westfall, Creighton University, Omaha, NB.

The mole ratio and mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are almost identical to those of Saylor (1). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) Nitrobenzene. Eastman Kodak Co. Used as received.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

REFERENCES:

1. Saylor, J. H.
J. Am. Chem. Soc. 1937, 59, 1712.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Nitrobenzene; C₆H₅NO₂; [98-95-3]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.

J. Am. Chem. Soc. 1941, 63, 2709 - 2712.

EXPERIMENTAL VALUES:

T/K	Pressure	Molality	Mol Ratio	Mol Fraction
	p ₁ /mmHg	m ₁ /mol kg ⁻¹	ⁿ 1 ^{/n} 2	<i>x</i> ₁
293.15	56	0.0507	0.00624	0.00620
	64	0.0549	0.00675	0.00670
	111	0.0896	0.0110	0.0109
	160	0.1310	0.0161	0.0159
	288	0.239	0.0294	0.0286
	305	0.249	0.0306	0.0297
	(760			0.072)1
298.15	42.4	0.0319	0.00392	0.00391
	45.1	0.0332	0.00408	0.00407
	102	0.075	0.00923	0.00914
	127	0.092	0.0113	0.0112
	173	0.126	0.0155	0.0153
	171	0.134	0.0165	0.0162
	(760			0.067)1
303.15	20.7	0.0140	0.00172	0.00172
	24.1	0.0156	0.00192	0.00192
	74.8	0.047	0.00578	0.00575
	99	0.063	0.00775	0.00769
	144	0.093	0.0114	0.0113
	214	0.132	0.0162	0.0160
	248	0.157	0.0193	0.0189
	318	0.203	0.0250	0.0244
	402	0.253	0.0311	0.0302
	(760			0.057)1
313.15	4.1	0.0023	0.00028	0.00028
	7.5	0.0038	0.00047	0.00047
	90.6	0.0490	0.00603	0.00600
	95.8	0.0500	0.00615	0.00611
	351	0.169	0.0208	0.0204
	391	0.201	0.0247	0.0241
	(760			0.047)1

 $^{^{1}}$ Obtained from a speculative extrapolation of the nonlinear plot of $x_{1}\ vs.\ p_{1}$ up to 101.325 kPa (760 mmHg).

The mole ratio and mole fraction values were calculated by the compiler.

A summary of the author's Henry's constant values is on the next page.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Nitrobenzene; C₆H₅NO₂; [98-95-3]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.

J. Am. Chem. Soc. <u>1941</u>, 63, 2709 - 2712.

VARIABLES:

293.15 - 313.15 0.547 - 53.60 (4.1 - 402 mmHg) T/K: P/kPa:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

See preceeding page.

-						
	T/K	Henry's constant	, k/atm mol ⁻¹ kg	Mol Fraction at 1	.01.325 kPa	
		Range	Mean	Range	Mean	
						
	293.15	1.46 - 1.611	1.59 ± 0.04	0.0710 - 0.0777	0.0718	
	298.15	1.68 - 1.82	1.77 ± 0.05	0.0633 - 0.0682	0.0650	
	303.15	1.95 - 2.09	2.08 ± 0.04	0.0555 - 0.0593	0.0558	
	313.15	2.351- 2.731	2.51 ± 0.12	0.0431 - 0.0497	0.0467	

¹ Values recalculated by the compiler.

Henry's constant, $k/atm mol^{-1} kg = (\pi_1/atm)/(m_1/mol kg^{-1})$

The mole fraction solubility at 101.325 kPa HCl values from the mean Henry's constant and from the extremes of the range of Henry's constant values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saylor (1) as modified by O'Brien et The main difference is the al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- The method and apparatus are those of |(1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
 - (2) Nitrobenzene. Purified and distilled, m.p. 278.63 K.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

COMPONENTS: ORIGINAL MEASUREMENTS: (1)Hydrogen chloride; HCl; Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.; [7647-01-0] Dzhagatspanyan, B. V. Khim. Prom_st. (Moscow) 1966, (2) Nitrobenzene, chloro- $42 (8), 62\overline{4} - 626.$ and dichloronitrobenzenes PREPARED BY: VARIABLES: T/K: 313 - 433 W. Gerrard P/kPa : 101.325 (1 atm) EXPERIMENTAL VALUES: Smoothed** T/K Wt8 Mole ratio Mole* of fraction mole fraction n_{HC1}/n_2 HC1 x HCl x HCl Nitrobenzene; C₆H₅NO₂; 313 1.479 0.0499 0.0475 0.0475 0.0343 [98-95-3] 333 1.017 0.0332 0.0339 0.0263 353 0.780 0.0256 0.0252 0.593 0.459 373 0.0200 0.0196 0.0193 0.0200 393 0.0153 0.0152 0.365 0.0123 413 0.0122 0.0122 0.296 0.0100 0.0099 433 0.0100 $\Delta H^{\circ}/kcal\ mol^{-1} = -3.61$; $\Delta S^{\circ}/cal\ K^{-1}\ mol^{-1} = -17.50\ S$ Smoothing equation: $\ln x_{HCl} = -8.6539 + 17.5522/(T/100)$ (for use between 313 K and 433 K) Standard error in $x_{\rm HC1}$ about the regression line = 4.16 \times 10⁻⁴ 0.820 0.0354 0.0342 0.593 0.0256 0.0250 0.459 0.0198 0.0194 0.352 0.0152 0.0150 0.0342 1-Chloro-2-nitro-313 0.0252 333 benzene; C₆H₄ClNO₂; [88-73-3] 0.0192 353 373 0.0150 0.285 0.0123 0.0122 393 0.0121 0.0100 0.0083 0.0099 413 0.232 0.0099 433 0.192 0.0082 0.0083 $\Delta H^{\circ}/kcal \ mol^{-1} = -3.21$; $\Delta S^{\circ}/cal \ K^{-1} \ mol^{-1} = -16.9 \$ § Smoothing equation: $\ln x_{HC1} = -8.5017 + 16.0531/(T/100)$ (for use between 313 K and 433 K) Standard error in x_{HC1} about the regression line = 1.56 \times 10⁻⁴ * calculated by the compiler ** smoothing equation and smoothed values were calculated by H.L. Clever § the authors used a van't Hoff type equation to calculate enthalpy and entropy of solution from the mole ratio values.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

Gas was passed into 0.5 mole of component (2) in a flask of 10 cm³ capacity; a sample was removed every ten minutes for acid-alkali titration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from sodium chloride, and dried by calcium chloride.
- (2) Nitrobenzene. Distilled through a column of 20 theoretical plates.
- 1-Chloro-2-nitrobenzene. Purified by crystallization.
 1-Chloro-3-nitrobenzene. Self prepared by the chlorination of nitrobenzene. Purified by distillation and crystallization.
 - 1-Chloro-4-nitrobenzene. Purified by crystallization.

 - 1,2-Dichloro-4-nitrobenzene. Self prepared by chlorination of 1,4-chloronitrobenzene. Purified by distillation and crystallization. 1,3-Dichloro-2-nitrobenzne. Purified by crystallization.

COMPONENTS: ORIGINAL MEASUREMENTS: Zetkin, V. I.; Kolesnikov, I. M.; Zakharov, E. V.; (1) Hydrogen chloride; HCl; [7647-01-0] Dzhagatspanyan, B. V. Khim. Prom_st. (Moscow) 1966, 42 (8), 624 - 626. (2) Nitrobenzene, chloroand dichloronitrobenzenes EXPERIMENTAL VALUES: Smoothed** T/K Wt% Mole ratio Mole* of fraction mole fraction n_{HC1}/n_2 HCl x HCl xHC1 333 0.540 0.0233 0.0228 1-Chloro-3-nitro-0.0181 0.0178 benzene; C₆H₄ClNO₂; 353 0.419 0.0182 0.0142 0.0104 0.0082 [121-73-3] 373 0.329 0.0140 0.0135 0.237 393 0.0103 0.0103 413 0.192 0.0081 0.0081 0.150 0.0065 433 0.0065 0.0065 $\Delta H^{\circ}/\text{kcal mol}^{-1} = -3.66$; $\Delta S^{\circ}/\text{cal } K^{-1} \text{ mol}^{-1} = -18.40 \text{ }$ Smoothing equation: $\ln x_{HC1} = -9.5528 + 19.5784/(T/100)$ (for use between 353 K and 433 K) Standard error in x_{HC1} about the regression line = 3.63 \times 10⁻⁴ 0.412 0.0178 0.0175 0.0175 373 1-Chloro-4-nitrobenzene; C₆H₄ClNO₂; [100-00-5] 393 0.306 0.0132 0.0130 0.0130 0.232 0.0100 0.183 0.0079 0.0099 413 0.0099 433 0.183 0.0079 0.0078 0.0078 $\Delta H^{\circ}/kcal\ mol^{-1} = -4.34$; $\Delta S^{\circ}/cal\ K^{-1}\ mol^{-1} = -19.65$ § Smoothing equation: $\ln x_{HC1} = -9.8883 + 21.7914/(T/100)$ (for use between 373 K and 433 K) Standard error in $x_{\rm HC1}$ about the regression line = 2.71 \times 10⁻⁵ 333 0.399 0.0210 353 0.312 0.0164 373 0.245 0.0129 0.0206 0.0207 1,2-Dichloro-4-nitrobenzene; C₆H₃Cl₂NO₂; 0.0160 0.0161 [99-54-7] 0.0127 0.0128 0.0107 0.0087 0.0074 393 0.203 0.0106 0.0104 413 0.165 0.0086 0.0087 433 0.141 0.0073 0.0073 $\Delta H^{\circ}/kcal \ mol^{-1} = -3.00$; $\Delta S^{\circ}/cal \ K^{-1} \ mol^{-1} = -16.65 \$ Smoothing equation: $\ln x_{HCl} = -8.3733 + 14.9693/(T/100)$ (for use between 333 K and 433 K) Standard error in x_{HC1} about the regression line = 1.18 \times 10⁻⁴ 0.0227 0.0160 1,3-Dichloro-2-nitro-333 0.432 0.0222 0.0224 0.304 0.0155 353 benzene; C₆H₃Cl₂NO₂; [601-88-7] 0.0157 0.0144[sic]¹0.0112 0.0083 0.0082 0.0064 0.0064 373 0.217 0.01115 0.158 0.0083 393 0.122 413 0.0064 0.095 433 0.0050 0.0050 0.0050 The value appears to be in error. The authors also gawhich corresponds to the value of 0.0112. $\Delta H^{\circ}/kcal \text{ mol}^{-1} = -4.36 ; \Delta S^{\circ}/cal K^{-1} \text{ mol}^{-1} = -20.6 \text{ }$ The authors also gave a ΔG° value Smoothing equation: $\ln x_{HCl} = -10.2882 + 21.6070/(T/100)$ (for use between 333 K and 433 K) Standard error in $x_{\rm HCl}$ about the regression line = 1.49 \times 10⁻⁴

^{*} calculated by the compiler

^{**} smoothing equation and smoothed values were calculated by H.L. Clever \$ the authors used a van't Hoff type equation to calculate enthalpy and entropy of solution from the mole ratio values.

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. Nitrobenzene; C₆H₅NO₂; [98-95-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

 $\label{eq:W.Gerrard} \mbox{W. Gerrard} \\ \mbox{(smoothed data calculated by H.L. Clever)}$

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	n HC1/ n C $_{6}$ H $_{5}$ NO $_{2}$	X _{HC1}
253.15	0.245	0.197
263.15	0.185	0.156
273.15	0.140	0.123
283.15	0.105	0.0950
293.15	0.085	0.0783

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = 5.322 - 1.372/(T/100) - 6.890 \ln (T/100)$

Standard error about regression line = 1.97×10^{-3}

T/K	Mol Fraction
	X _{HC1}
253.15	0.198
263.15	0.155
273.15	0.122
283.15	0.0969
293.15	0.0776

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For temperatures below 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- Nitrobenzene. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.015$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. <u>1972</u>, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Methyl-2-nitrobenzene or onitrotoluene; C7H7NO2; [88-72-2]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Kenny, C. L.

J. Am. Chem. Soc. 1940, 62, 1189 - 1192.

VARIABLES:

T/K: 298.15

4.25 - 45.33P/kPa: (31.9 - 340 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure p ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction ^x l	-
298.15	31.9 53.1 112 113 224 269 340	0.0233 0.0382 0.0821 0.0839 0.164 0.202 0.259	1.80 1.82,1.83 ³ 1.79 1.78,1.77 ³ 1.79,1.80 ³ 1.75 1.72,1.73 ³	0.00320 0.00524 0.0113 0.0115 0.0225 0.0277 0.0355	0.00319 0.00521 0.0111 0.0114 0.0220 0.0270 0.0343	

¹ k/atm mol 1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of (1) Hydrogen chloride.

Saylor (1) as modified by O'Brien et from chemically pur al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) 1-Methyl-2-nitrobenzene. Eastman Kodak Co. Attested by refractive index, $n_{\rm D}^{20}$, 1.5476.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0701 to 0.0738 for the mole fraction solubility at one atm (101.325 kPa).

³ Values as calculated by compiler.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Methyl-3-nitrobenzene or mnitrotoluene; C₇H₇NO₂;
 [99-08-1]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Kenny, C. L.

J. Am. Chem. Soc. 1940, 62, 1189 - 1192.

VARIABLES:

T/K: 298.15

P/kPa: 1.85 - 22.27

(13.9 - 167 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	13.9 44.3 56.7 116 122 132 167	0.0116 0.0343 0.0438 0.0918 0.0939 0.1037 0.1385	1.58 1.69,1.70 ³ 1.70 1.67 1.71 1.68 1.54,1.59 ³	0.0016 0.0047 0.0060 0.0126 0.0129 0.0142 0.0190	0.0016 0.0047 0.0060 0.0124 0.0127 0.0140 0.0186
	(760	0.606	1.65 av.	0.0831	0.0767)2

¹ k/atm mol 1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Prepared from chemically pure potassium chloride and sulfuric acid. Dried by phosphorus pentoxide.
- (2) 1-Methyl-3-nitrobenzene. Eastman Kodak Co. Attested by refractive index, n_D^{20} , 1.5479.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0742 to 0.0818 for the mole fraction solubility at one atm (101.325 kPa).

³ Values recalculated by compiler.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 1-Methyl-3-nitrobenzene or m-nitro toluene; C₇H₇NO₂; [99-08-1]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; King, C. V.

J. Am. Chem. Soc. 1949, 71, 3632 - 3634.

VARIABLES:

T/K: 298.15, 308.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Henry's Constant'	Mol Ratio	Mol Fraction
298.15	1.65 ± 0.05^3	0.0830 0.0830 ²	0.0768 0.0767²
308.15	2.08 <u>+</u> 0.04	0.0654 0.0659 ²	0.0614 0.0618 ²

- 1 k/atm mol $^{-1}$ kg = $(p_{1}/atm)/(m_{1}/mol kg^{-1})$
- ² Values as recalculated by the compiler.
- Previously reported by O'Brien, S. J.; Kenny, C. L. J. Am. Chem. Soc. 1940, 62, 1189.

All of the mole ratio values were calculated by the compiler.

The experimental measurements were probably carried out at pressures below one-half atm partial pressure of HCl. The Henry's constant values are the mean of from 2 to 6 values followed by the average deviation of the mean.

From the slope of $\log x_1$ vs. 1/T. The enthalpy of solution is -3.90 k cal mol⁻¹(-16.32 kJ mol⁻¹).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution is added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HCl in the upper bulb is quantitatively removed and titrated with NaOH. The HCl partial pressure is calculated from the bulb volume and the number of moles of HCl assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated. Probably prepared from potassium chloride and sulfuric acid as in previous work (2).
- (2) 1-Methyl-3-nitrobenzene. Eastman Kodak Co. Dried and distilled.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A.
 J. Am. Chem. Soc. 1939, 61, 2504.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2-(Trichloromethyl)pyridine; C₆H₄Cl₃N; [4377-37-1]

ORIGINAL MEASUREMENTS:

Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanya, R. V.

2h. Prikl. Khim. (Leningrad) 1978, 51, 887 - 889.

J. Appl. Chem. USSR (Engl. Transl.) 1978, 51, 858 - 860.

VARIABLES:

T/K = 378.15 - 473.15 $p_1/kPa = 101.325$ (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

<i>T</i> /K	$\begin{array}{c} {\rm Hydrogen~Chloride} \\ {\rm Solubility} \\ c_1/{\rm mol~dm^{-3}} \end{array}$
378.15 393.15 408.15 423.15 443.15 473.15	0.39 ¹ 2.3 0.50 0.20 0.15 0.103

¹ This value is mole ratio, n_1/n_2 .

The authors stated that at 378.15 and 393.15 K the solubilities are "very high". At 378.15 K (105°C) the system consisted of a "thick pasty substance," therefore the solubility at that temperature was given as a mole ratio.

In the author's diagram the plot of $\log(c_1/p_1)$ v_8 . 1/T was shown as straight from 473 to 423 K, at which point the line rose steeply to 393 K. No parameters for the straight line portion were given.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid was saturated with gas at atmospheric pressure. The amount of gas absorbed was determined by "a back titration. The results were subsequently reduced to 760 mmHg pressure."

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder, and dried by sulfuric acid.
- (2) 2-(Trichloromethyl)pyridine. Self prepared, and purified. Purity assessed as 95-99% by chromatography.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 2-Chloro-6-(trichloromethy1)pyridine; $C_6H_3Cl_4N$; [1929-82-4]

ORIGINAL MEASUREMENTS:

Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanya, R. V.

2h. Prikl. Khim. (Leningrad) 1978, 51, 887 - 889.

J. Appl. Chem. USSR (Engl. Transl.) 1978, 51, 858 - 860.

VARIABLES:

$$T/K = 363.15 - 423.15$$

 $p_1/kPa = 101.325$ (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

<i>T</i> /K	Hydrogen Chloride Solubility c ₁ /mol dm ⁻³
363.15	0.062
393.15	0.046
408.15	0.037
423.15	0.032

It was stated that the plot of log [solubility] $vs.\ 1/T$ was a straight line. The equation

$$log(c_1/p_1) = (\Delta H/2.303 RT) - A$$

was given with p_1 = the HCl partial pressure in atm.

$$\Delta H/kcal\ mol^{-1} = 3.4$$

A = 3.23

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid was saturated with gas at atmospheric pressure. The amount of gas absorbed was determined by "a back titration. The results were subsequently reduced to 760 mmHg pressure."

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder, and dried by sulfuric acid.
- (2) 2-Chloro-6-(trichloromethyl)pyridine. Self prepared and purified. Purity assessed as 95-99% by chromatography.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 3,5-Dichloro-2-(trichloromethyl)pyridine; C₆H₂Cl₅N; [1128-16-1]

ORIGINAL MEASUREMENTS:

Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanya, R. V.

Zh. Prikl. Khim. (Leningrad) <u>1978</u>, 51, 887 - 889.

J. Appl. Chem. USSR (Engl. Transl.) 1978, 51, 858 - 860.

VARIABLES:

T/K = 333.15 - 423.15 $p_1/kPa = 101.325$ (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

<i>T</i> /K	Hydrogen Chloride Solubility $c_1/\text{mol dm}^{-3}$
333.15	0.30
363.15	0.10
393.15	0.07
423.15	0.051

It was stated that the plot of log [solubility] $v_{\mathcal{E}}$. 1/T was a straight line. The equation

 $log(c_1/p_1) = (\Delta H/2.303 RT) - A$

was given with p_1 = the HCl partial pressure in atm.

 $\Delta H/kcal mol^{-1} = 3.6$

A = 3.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid was saturated with gas at atmospheric pressure. The amount of gas absorbed was determined by "a back titration. The results were subsequently reduced to 760 mmHg pressure."

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder, and dried by sulfuric acid.
- (2) 3,5-Dichloro-2-(trichloromethyl)pyridine. Self prepared, and purified. Purity assessed as 95-99% by chromatography.

ESTIMATED ERROR:

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) 3,4,5-Trichloro-2-(dichloromethyl)-pyridine; C₆H₂Cl₅N; [7041-22-7]

ORIGINAL MEASUREMENTS:

Kosorotov, V. I.; Stul, B. Ya.; Dzhagatspanya, R. V.

2h. Prikl. Khim. (Leningrad) 1978, 51, 887 - 889.

J. Appl. Chem. USSR (Engl. Transl.) 1978, 51, 858 - 860.

VARIABLES:

T/K = 363.15 - 408.15 $p_1/kPa = 101.325$ (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

<i>T</i> /K	Hydrogen Chloride Solubility c ₁ /mol dm ⁻³
363.15	0.1
378.15	0.08
393.15	0.07
408.15	0.052

It was stated that the plot of log [solubility] $vs.\ 1/T$ was a straight line. The equation

$$log(c_1/p_1) = (\Delta H/2.303 \text{ RT}) - A$$

was given with p_1 = the HCl partial pressure in atm.

 $\Delta H/kcal mol^{-1} = 3.6$

A = 3.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid was saturated with gas at atmospheric pressure. The amount of gas absorbed was determined by "a back titration. The results were subsequently reduced to 760 mmHg pressure."

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder, and dried by sulfuric acid.
- (2) 3,4,5-Trichloro-2-(dichloro-methyl)-pyridine. Self pre-pared, and purified. Purity assessed as 95-99% by chromatography.

ESTIMATED ERROR:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Sulfur

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
and Life Sciences,
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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Solvents Containing Sulfur.

The solubilities of hydrogen chloride in a wide range of sulfur compounds have been measured by Gerrard and co-workers (1-3) at a total pressure equal to barometric pressure and at one or more temperatures.

The mole fraction solubility in sulfuric acid at 273.15 K and 1.013 bar is low (< 0.0196) but is appreciably higher in the butyl esters of sulfonic acids in which one of the hydroxyl groups in sulfuric acid has been replaced by an alkyl or aryl group and the other hydroxyl group esterified. Solubility is greater in alkyl sulfonic acids than in benzenesulfonic acid. Substitution of a methyl group into the benzene nucleus of benzenesulfonic acid increases the solubility. Substitution of a chlorine atom lowers the solubility.

Mole fraction solubilities are high in sulfones in which both hydroxyl groups of sulfuric acid have been replaced by alkyl groups. Solubility is appreciably lower but still above the reference line value in benzene sulfuryl chloride in which one group has been replaced by the phenyl group and the other by chlorine. Solubility falls below the reference line in the case of sulfuryl chloride in which both hydroxyl groups have been replaced by chlorine.

The available mole fraction solubility data are in the order :

sulfuric acid < sulfuryl chloride < benzene sulfonyl chloride <
methanesulfonyl chloride < ethanesulfonyl chloride < chlorosulfonic acid
butyl ester < 2-propanesulfonyl chloride < 4-chlorobenzenesulfonic acid,
butyl ester < benzenesulfonic acid, butyl ester < 4-methylbenzenesulfonic
acid, butyl ester < methanesulfonic acid, butyl ester < ethanesulfonic
acid, butyl ester < tetrahydrothiophene-1,1-dioxide (tetramethylene
sulfone) < 1,1'-sulfonylbispropane (dipropyl sulfone) <
1,1'-sulfonylbisbutane (dibutyl sulfone) < 2,2'-sulfonylbispropane
(disopropyl sulfone)</pre>

There is a discrepancy between the mole fraction solubility in sulfuryl chloride at 273.15 K and a total pressure of 1.013 bar from Ahmed's (3) data (0.043), and that from Charalambous $et\ al.(2)$ (0.031). There is also a discrepancy between data from these two sources for mole fraction solubility at 298.15 K and this total pressure in benzenesulfonyl chloride. The value from Charalambous $et\ al.$ is 0.0403 but the value from an extrapolation of Ahmed's data is 0.046.

In general the data for sulfuric acid and its derivatives fall into a consistent overall pattern and there is no reason to doubt the reliability of this pattern. Further work is needed to confirm the precise magnitude of solubilities in this class of solvents.

The solubility in thionyl chloride, at a total pressure equal to barometric, was measured by Ahmed in the temperature range 248.15 K to 273.15 K and by Domeniconi et al.(4) at 298.15 K. Extrapolation of Ahmed's data indicates a mole fraction solubility of 0.0095 at 298.15 K. This is in sharp contrast to the value of 0.0195 from the data published by Domeniconi et al. Further work on this system is required.

The measurement of the solubility in liquid hydrogen sulfide by Quam & Wilkinson (5) must be considered to be semi-quantitative. The solubility in several solvents, in which one or both hydrogen atoms have been replaced by an alkyl or the phenyl group, have been measured by Frazer and Gerrard (1). Data for 273.15 K and a total pressure of 101.3 kPa indicate that the mole fraction solubilities in the compounds studied lie above the reference line value corresponding to Raoult's law and are in the order:

benzenethiol < 1-butanethiol < 1,1'-thiobisbenzene < 2-propanethiol < 1,1'-thiobisbutane < 1,1'-thiobispropane.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Sulfur

EVALUATOR:

Peter G. T. Fogg
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January 1989

CRITICAL EVALUATION:

Frazer & Gerrard (1) also reported solubilities in thiophene and tetrahydrothiophene at 273.15 K and a total pressure equal to barometric. In line with the behaviour of other sulfur compounds, the solubility was markedly greater in tetrahydrothiophene than in the unsaturated thiophene.

The data for thiols, thioethers, thiophene and tetrahydrothiophene published by Frazer & Gerrard are self consistent and likely to be reliable. However further measurements on these systems are needed for confirmation of data.

Solubilities at a total pressure equal to barometric pressure have been reported by Ahmed (3) for dissolution in sulfur dioxide over the temperature range 218.15 K to 253.15 K and by Chesterman (6) for dissolution in carbon disulfide at 298.15 K. Data for these two solvents require confirmation by other workers.

- 1. Frazer, M. J.; Gerrard, W. Nature, 1964, 204, 1299-1300.
- Charalambous, J.; Frazer, M. J.; Gerrard, W. J. Chem. Soc. 1964, 1520-1521.
- 3. Ahmed, W. Thesis, 1970, University of London.
- Domeniconi, M.; Klinedinst, K.; Marincic, N.; Schlaikjer, C.; Staniewicz, R.; Swette, L. ONR Contract & NO0014-76-C-0524 Interim Report Jan. 1976 - Oct. 1977.
- Quam, G. N. J. Am. Chem. Soc. 1925, 47, 103-108.;
 Quam, G. N.; Wilkinson, J. A. J. Am. Chem. Soc. 1925, 47, 989-994.
- Chesterman, D. R. J. Chem. Soc. <u>1935</u>, 906-910.

COMPONENTS: ORIGINAL MEASUREMENTS:			
(1) Hydrogen chloride; HCl; [7647-01-0]	Charalambous, J.; Frazer, M. J.; Gerrard, W.		
(2) Organic compounds of sulfur	J. Chem. S	Soc. <u>1964</u> , 1520) - 1521.
VARIABLES:	PREPARED B	BY:	
T/K: 273.15, 298.15 Total P/kPa : 101.3 (barometric, nearly 1 atm)	W. Gerrard		
EXPERIMENTAL VALUES:	т/к	Mole ratio "HC1 ^{/n} 2	Mole fraction* ^X HCl
Sulfuric acid; H ₂ O ₄ S; [7664-93-9]	273.15	<0.020	<0.0196
Dichlorosulfuric acid, (sulfuryl chloride); Cl ₂ O ₂ S; [7791-25-5] The solvent was too volatile at 298.1	273.15	0.032	0.0310
Methanesulfonyl chloride; CH ₃ ClO ₂ S; [124-63-0]	298.15	0.044	0.0421
The observation was restricted to that was solid at 273.15 K. The solvent	t for 298.15 structure is	K because the CH ₃ SO ₂ C1.	e system
Ethanesulfonyl chloride; C ₂ H ₅ ClO ₂ S; [594-44-5] The solvent structure is C ₂ H ₅ SO ₂ Cl.	273.15 298.15		0.089 0.053
2-Propanesulfonyl chloride; C ₃ H ₇ ClO ₂ S [10147-37-2]	; 273.15	0.126	0.112
The solvent was too volatile at 298.1 The solvent structure is ${}^{i}C_{3}H_{7}SO_{2}Cl$.	5 K for a me	easurement to b	oe taken.
* calculated by the compiler			
AUXILIARY	INFORMATION		

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

The amount of hydrogen chloride absorbed at a total pressure, very nearly 1 atm, was measured by weighing the absorption vessel as described by Gerrard and Macklen (1), except that a U-tube was used instead of a bubbler tube.

In the case of the sulfones the gas was passed into the melt for 0.5 hour, and the system was cooled to the recorded temperature. Even after this treatment the 1,1'-sulfonylbisbutane/HCl system was solid at 273.15 K.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen, dried by sulfuric acid.
- 2. Ethanesulfonic acid, butyl ester: self prepared.

Benzenesulfonic acid, butyl ester: self prepared.

- 4-Methylbenzene sulfonic acid,
- butyl ester: self prepared. 4-Chlorobenzenesulfonic acid,
- butyl ester: self prepared.
 2-Propanesulfonyl chloride:
 prepared by the chlorination of
 the disulfide.
- Other solvents were commercial specimens. All solvents were carefully purified and rigorously attested.

ESTIMATED ERROR:

REFERENCES:

 Gerrard, W.: Macklen, E. D. J. Appl. Chem. <u>1956</u>, 6, 241.

Hydrogen Chloride in P	von-Aqueous Solvents 3
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen chloride; HCl; [7647-01-0]	Charalambous, J.; Frazer, M. J.; Gerrard, W.
(2) Organic compounds of sulfur	J. Chem. Soc. <u>1964</u> , 1520 - 1521.
EXPERIMENTAL VALUES:	T/K Mole ratio Mole "HCl ^{/n} 2 fraction* "HCl
Benzenesulfonyl chloride; C ₆ H ₅ ClO ₂ S;	298.15 0.042 0.0403
[98-09-9] Even after the gas had been passed int the system was solid at 273.15 K. The	to the melt at higher temperatures, e solvent structure is ${^C}_6{^H}_5{^{SO}}_2{^{Cl}}$.
Chlorosulfuric acid, butyl ester, (butyl chlorosulfate); C ₄ H ₉ ClO ₃ S; [763-23-5] The solvent structure is Cl-SO ₂ -OC ₄ H ₉ .	273.15 0.117 0.105 298.15 0.057 0.0539
Methanesulfonic acid, butyl ester, (butyl methanesulfonate); C ₅ H ₁₂ O ₃ S; [1912-32-9] The structure is CH ₃ -SO ₂ -OC ₄ H ₉ .	273.15 0.510 0.338 298.15 0.255 0.203
Ethanesulfonic acid, butyl ester, (butyl ethanesulfonate); $^{\rm C}_6{^{\rm H}_1}{^4^{\rm O}_3}{^{\rm S}};$ [14245-63-7] The structure is $^{\rm C}_2{^{\rm H}_5}{^{\rm -SO}_2}{^{\rm -OC}_4}{^{\rm H}_9}.$	273.15 0.630 0.387 298.15 0.316 0.240
Benzenesulfonic acid, butyl ester, (butyl benzenesulfonate); $^{\rm C}_{10}^{\rm H}_{14}^{\rm O}_{3}^{\rm S}$; [80-44-4] The structure is $^{\rm C}_{6}^{\rm H}_{5}^{\rm -SO}_{2}^{\rm -OC}_{4}^{\rm H}_{9}$.	273.15 0.419 0.295 298.15 0.213 0.176
4-Methylbenzenesulfonic acid, butyl ester, (butyl p-toluenesulfonate); $C_{11}^{H}_{16}^{O}_{3}^{S}$; [778-28-9] The structure is $p-CH_3-C_6H_4-SO_2-OC_4H_9$.	273.15 0.445 0.308 298.15 0.249 0.199
4-Chlorobenzenesulfonic acid, butyl ester, (butyl p-chlorobenzenesulfonate); $C_{10}^{H}_{13}^{Clo}_{3}^{S}$; [6421-41-6] The structure is $p-Cl-C_{6}^{H}_{4}-SO_{2}-OC_{4}^{H}_{9}$.	273.15 0.210 0.174 298.15 0.083 0.0766
1,1'-Sulfonylbispropane, (dipropyl-sulfone); $C_{6}^{H}_{14}^{O}_{2}^{S}$; [598-03-8] The structure is $(C_{3}^{H}_{7})_{2}^{SO}_{2}$	273.15 1.010 0.502 298.15 0.622 0.383
2,2'-Sulfonylbispropane, (diisopropylsulfone); $C_{6}^{H}_{14}^{O}_{2}^{S}$; [595-50-6] The structure is $(iC_{3}^{H}_{7})_{2}^{SO}_{2}$	- 273.15 1.174 0.540 298.15 0.712 0.416
1,1'-Sulfonylbisbutane, $(dibuty1 sulfone)$; $C_8H_{18}O_2S$; [598-04-9] The structure is $(C_4H_9)_2SO_2$.	298.15 0.627 0.385
Tetrahydrothiophene-1,1-dioxide, (tetramethylene sulfone); C ₄ H ₈ O ₂ S; [126-33-0] The structure is CH ₂ -CH ₂ SO ₂ CH ₂ -CH ₂	273.15 0.763 0.463 298.15 0.402 0.287
* calculated by the compiler	

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Thiols, thioethers, thiophene and tetrahydrothiophene

VARIABLES:

T/K: 273.15

Total P/kPa : 101.3 (barometric,

nearly 1 atm)

ORIGINAL MEASUREMENTS:

Frazer, M. J.; Gerrard, W.

Nature 1964, 204, 1299 - 1300

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

EXPERIMENTAL VALUES:			
	т/к	Mole ratio	Mole fraction* ^X HCl
2-Propanethiol, (2-propylmercaptan); C ₃ H ₈ S; [75-33-2]	273.15	0.225	0.184
1-Butanethiol, (<i>l-butylmercaptan</i>); C ₄ H ₁₀ S; [109-79-5]	273.15	0.125	0.111
Benzenethiol, (thiophenol, mercapto- benzene); C ₆ H ₆ S; [108-98-5]	273.15	0.093	0.085
2,2'-Thiobispropane, (diisopropyl sulfide); C ₆ H ₁₄ S; [625-80-9]	273.15	0.659	0.397
1,1'-Thiobisbutane, (<i>dibutyl sulfide</i>); C ₈ H ₁₈ S; [544-40-1]	273.15	0.640	0.390
1,1'-Thiobisbenzene, (diphenyl sulfide); C ₁₂ H ₁₀ S; [139-66-2]	273.15	0.144	0.126
Thiophene; C ₄ H ₄ S; [110-02-1]	273.15	0.034	0.0329
Tetrahydrothiophene; C ₄ H ₈ S; [110-01-0]	273.15	0.673	0.402

^{*} calculated by the compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

The gas was passed into a weighed amount of solvent (about 2 g) in a U-tube kept at 273.15 K. The pressure was atmospheric, approximately 1 atm. The maximum amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Self made and carefully purified.
- Sulfur compounds. The purities were checked by boiling points and gas-liquid chromatography. After each measurement of solubility the gas was removed by treatment with water, the liquid was recovered and identified with the original compound.

ESTIMATED ERROR:

- 1. Hydrogen Chloride; HCl; [7647-01-0
- 2. Sulfuryl Chloride; Cl₂O₂S;
 [7791-25-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 248.15 - 288.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nCl2O2S	Mol Fraction XHCl
248.15	0.127	0.113
253.15 263.15	0.109 0.075	0.0983
273.15	0.045	0.0698 0.0431
283.15 288.15	0.024 0.016	0.0234 0.0157

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HCl} = 234.626 - 302.781/(T/100) - 126.317 \ln (T/100)$

Standard Error About Regression Line = 1.38×10^{-3}

T/K	Mol Fraction XHCl	
243.15	0.119	
253.15	0.0998	
263.15	0.0705	
273.15	0.0428	
283.15	0.0229	
293.15	0.0109	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a weighed amount of sulfuryl chloride in a bubbler tube as described in the main paper (1). The final liquid was treated quantitatively with water. Total acid and total chloride were determined by titrations.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Sulfuryl chloride. Best specimen was purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.02$

REFERENCES:

 Ahmed, W.; Gerrard, W.; Maladkar, V. K.
 J. Appl. Chem. 1970, 20, 109.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Benzenesulfonyl Chloride; C₆H₅ClO₂S; [98-09-9]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC6H5ClO2S	Mol Fraction XHCl
253.15 258.15 263.15 268.15 273.15 278.15 283.15 288.15	0.262 0.192 0.159 0.131 0.099 0.089 0.075	0.208 0.161 0.137 0.116 0.090 0.082 0.070 0.060

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -42.713 + 67.585/(T/100) + 15.537 \ln (T/100)$

Standard Error About Regression Line = 3.38×10^{-3}

T/K	Mol Fraction X _{HCl}
253.15	0.205
263.15	0.136
273.15	0.0946
283.15	0.0690
293.15	0.0524

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a weighed specimen of the sulfur compound in a bubbler tube as described in the main paper (1). For temperatures below 268 K the final mixture was quantitatively treated with water and the total chloride estimated by titration.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Benzenesulfonyl chloride. The best specimen was purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.02$

REFERENCES:

 Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Thionyl chloride; Cl₂OS;
 [7719-09-7]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 248.15 - 273.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nCl ₂ OS	Mol Fraction XHCl
248.15	0.115	0.103
253.15	0.096	0.0876
263.15	0.061	0.0575
273.15	0.038	0.0366

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = 108.293 - 133.863/(T/100) - 62.293 \ln (T/100)$

Standard Error About Regression Line = 1.11×10^{-3}

T/K	Mol Fraction X _{HCl}
243.15	0.121
253.15	0.0868
263.15	0.0579
273.15	0.0365

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed through a weighed amount of liquid in a bubbler tube as described in the main paper (1). The final liquid was quantitatively treated with water. The sulfurous acid and total chloride were determined by titrations. Repeated observations ensured that saturation has been reached.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Thionyl chloride. The best specimen was purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.01$

REFERENCES:

 Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109.

COMPONENTS: ORIGINAL MEASUREMENTS: Domeniconi, M.; Klinedinst, K.; Hydrogen chloride; HCl; [7647-01-0] Marincic, N.; Schlaikjer, C.; Staniewicz, R.; Swette, L. (2) Thionyl chloride; SOCl₂; ONR Contract # N00014-76-C-0524 [7719-09-7] Interim Report Jan. 1976 - Oct. 1977. VARIABLES: PREPARED BY: H. L. Clever T/K: 298 Atmospheric P:

EXPERIMENTAL VALUES:

Weight changes observed on passing argon and hydrogen chloride at the same flow rate for one hour through 40 ml of thionyl chloride at(298 ± 2) K.

Gas	Experiment	Weight Change g	Average weight change/ g
Argon	1	-0.0590	
-	2	-0.0500	
	3	-0.0546	
	4	-0.0608	
			-0.0561
Hydrogen	<i>.</i> 1	0.3433	
chloride	2	0.3463	
	3	0.3652	
			0.3516

Mol HCl dm⁻³ SOCl₂ = (0.3516 + 0.0561)g HCl/(36.45 g mol⁻¹) $(0.040 \ l)$ $= 0.28_0$

The HCl was also bubbled through a solution which was 2 mol AlCl $_3$ dm $^{-3}$ SOCl $_2$ solution. The weight change indicated only the change expected for the HCl solubility in SOCl $_2$.

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The solubility of HCl was determined gravimetrically. Argon was first bubbled through the thionyl chloride to determine the solvent weight loss from the passage of the gas. Then anhydrous HCl, presaturated with SOCl, was passed through an 0.040 dm⁻³ sample of SOCl₂ for one hour and the mass gain determined.

The SOCl $_2$ had a specific conductivity of 5 x 10^{-7} (ohm cm) $^{-1}$ and no change in the value was noted upon saturating ESTIMATED ERROR: the solution with HCl. The IR absorption of the dissolved HCl is at 2800 cm⁻¹. On heating the HCl saturated solution to about 323 K the 2800 cm⁻¹ band disappears. Apparently the HCl is expelled from the solution.

There was no IR evidence of a reaction between HCl and AlCl3 in SOCl2. All operations were carried out in a dry box operating between 2 to 3 ppm water.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Matheson Co., Inc. Electronic grade.
- (2) Thionyl chloride. Mobay (?). Fractional distillation from Li metal in a dry room (3 % relative humidity). The material was devoid of IR absorptions above 2500 \mbox{cm}^{-1} using a 1 cm quartz cell.

 $\delta T/K = 2$ $\delta M/M = 0.025$ (Compiler)

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Quam, G. N. [7647-01-0] J. Am. Chem. Soc. 1925, 47, 103 - 8. (2) Hydrogen sulfide; H₂S; Quam, G. N.; Wilkinson, J. A. [7783-06-4] J. Am. Chem. Soc. 1925, 47, 989 - 94. VARIABLES: PREPARED BY: T/K = 194.7H. L. Clever p/kPa = 101.3(1 atm)

EXPERIMENTAL VALUES:

Temp	erature	Mol Fraction
t/°C	<i>T</i> /K	x_1
-78.5	194.7	0.432

The compiler estimated the temperature from the statement that the solubility was determined at the temperature of a diethylether + solid carbon dioxide bath.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS; Sealed tube. Solubility at temperature (1 Hydrogen chloride. No informaof ether + solid carbon dioxide tion. bath. (2) Hydrogen sulfide. Prepared by Since HCl boils about 6 degrees the action of hydrochloric acid lower temperature than the solubility on iron sulfide. Freed of HCl, experiment, it is assumed that the arsine, and moisture. result is for gaseous HCl. ESTIMATED ERROR: REFERENCES:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Sulfur dioxide; SO₂; [7446-09-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 218.15 - 253.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nSO2	Mol Fraction XHCl
218.15 223.15 228.15 233.15 243.15 248.15 253.15	0.365 0.293 0.234 0.185 0.096 0.057	0.267 0.227 0.190 0.156 0.0876 0.0539 0.0177

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HCl} = 501.382 - 620.308/(T/100) - 280.090 \ln (T/100)$

Standard Error About Regression Line = 2.42×10^{-2}

T/K	Mol Fraction XHCl
223.15	0.242
233.15	0.170
243.15	0.0747
253.15	0.0223

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the liquid sulfur dioxide to the saturation point, determined by repeated observations. The final liquid was quantitatively treated with water, and sulfurous acid and the total chloride were determined by titrations.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- The best specimen was passed through tubes at 263 K, and liquefied at the required temperature.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.07$

REFERENCES:

Ahmed, W.; Gerrard, W.;
 Maladkar, V. K.
 J. Appl. Chem. 1970, 20, 109.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Chesterman, D. R. [7647-01-0] J. Chem. Soc. 1935, 906 - 910. (2) Carbon disulfide; CS₂; [75-15-0] VARIABLES: PREPARED BY: T/K: 298.15 Total P/kPa: 101 (~1 atm) W. Gerrard EXPERIMENTAL VALUES: Solubility g HCL g⁻¹ Solution T/K Observed Mol Fraction Pressure x_1 p/mmHg 298.15 766 0.004 0.008 The mole fraction solubility value was calculated by the compiler. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The apparatus was that used for the (1) Hydrogen chloride. Prepared from conc. sulfuric acid and pure conductivity. A sample of the saturated solution was removed, sodium chloride. Passed through weighed, the hydrogen chloride was sulfuric acid and over P205. reacted with excess standard base (2) Carbon disulfide. which is back titrated with a Was stated to be the purest obtainable. Undried, b.p./°C (759 mmHg) = standard acid solution. 46 - 47.ESTIMATED ERROR: REFERENCES:

COMPONENTS:	EVALUATOR:
1. Hydrogen Chloride; HCl; [7647-01-0]	Peter G. T. Fogg Department of Applied Chemistry and Life Sciences,
2. Solvents Containing Boron	Polytechnic of North London, Holloway, London, N7 8DB, U.K.
	January 1989

CRITICAL EVALUATION:

Solubility of Hydrogen Chloride in Solvents Containing Boron.

Solubilities in various boron compounds over temperature ranges at barometric pressure have been measured by Gerrard and his co-workers (1-3). The data are self-consistent and likely to be reliable but there are no data by other workers for comparison.

Solubilities in the triethyl, tributyl and tripentyl esters of boric acid were investigated over a temperature range of 199.15 K to 321.15 K. As with many solvents containing oxygen, mole fraction solubilities are higher than reference line values corresponding to the Raoult's law equation i.e. ratio of partial pressure of hydrogen chloride to vapor pressure of liquid hydrogen chloride at the same temperature.

Mole fraction solubilities in dioxaboroles are lower than in the non-cyclic borates. The solubility increases with size of the substituent alkoxy group. The presence of a benzene ring lowers the solubility. Mole fraction solubilities at 101.3 kPa and 293.15 K are as follows:

(reference line value	0.024)
2-butoxy-1,3,2-dioxaborolane	0.123
2-methoxy -1,3,2-benzodioxaborole	0.0853
2-ethoxy-1,3,2-benzodioxaborole	0.109
2-propoxy-1,3,2-benzodioxaborole	0.115
2-butoxy-1,3,2-benzodioxaborole	0.118
2-pentoxy-1,3,2-benzodioxaborole	0.119

Mole fraction solubilities in solvents containing chlorine and boron, which were investigated, are appreciably lower. Values corresponding to 293.15 K are as follows:

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butoxydichloroborane 0.0213 dichlorophenylborane 0.0451 (extrapolated)
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Mole fraction solubilities in boron trichloride, at a partial pressure of hydrogen chloride of 101.3 kPa, fall below the reference line in the temperature range of 208.15 K to 263.15 K. Measurements have not been made outside this range.

- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. <u>1959</u>, 9, 89-93; <u>1960</u>, 10, 115-121.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109-115.
- 3. Ahmed, W. Thesis, 1970, University of London.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Gerrard, W.; Mincer, A. M. A.; [7647-01-0] Wyvill, P. L. (2) Boric acid triethyl ester or J. Appl. Chem. 1960, 10, 115-121. triethyl borate; C6H15BO3; [150-46-9] **VARIABLES:** PREPARED BY: T/K: 230.65 - 317.35 W. Gerrard Total P/kPa: 101.325 (1 atm)

EXPERIMENTAL VALUES:			
EXPERIMENTAL VALUES:	T/K	Mol Ratio	Mol Fraction
		n HC1 $^{/n}$ C $_{6}$ H $_{15}$ BO $_{3}$	x_1
	230.65	1.782	0.641
	273.95	0.454	0.312
	274.15	0.446	0.308
	278.55	0.388	0.280
	282.15	0.340	0.254
	286.15	0.287	0.223
	292.95	0.224	0.183
	302.75	0.156	0.135
	312.15	0.120	0.107
	317.35	0.0985	0.0897

The compiler calculated the mole fraction values.

 $\ln x_1 = 58.003 - 71.605/(T/100) - 32.786 \ln (T/100)$ Smoothed Data:

Standard error about the regression line is 3.72×10^{-3}

T/K	Mol Fraction
	x_1
233.15	0.630
243.15	0.562
253.15	0.480
263.15	0.395
273.15	0.315
283.15	0.244
293.15	0.185
303.15	0.138
313.15	0.101
323.15	0.0734

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

The hydrogen chloride absorbed at 230.65 K was determined by attaching the bubbler-tube to a flask containing water, and allowing the assembly to warm to room temperature, after which the chloride ion content was estimated ESTIMATED ERROR: by a Volhard titration.

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.

(smoothed data calculated by H.L. Clever)

(2) Boric acid triethyl ester. Carefully purified, and purity rigorously attested.

$$\delta x_1/x_1 = 0.02$$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Boric acid, tripentyl ester or tripentyl borate; C₁₅H₃₃BO₃; [621-78-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 273.15 - 321.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: -	T/K	Mol Ratio	Mol Fraction
	-,	ⁿ HC1 ^{/n} C ₁₅ H ₃₃ BO ₃	<i>x</i> ₁
	273.15	0.493	0.330
	278.75	0.413	0.292
1	283.65	0.355	0.262
Į	290.95	0.260	0.206
	301.95	0.183	0.155
	308.15	0.146	0.127
	314.25	0.122	0.109
i	321.15	0.108	0.0975

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 9.041 - 3.084/(T/100) - 8.950 \ln (T/100)$ Standard error about the regression line is 6.67×10^{-3}

T/K Mol Fraction

"1

273.15 0.339

283.15 0.256

293.15 0.195

303.15 0.149

313.15 0.115

323.15 0.0897

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Boric acid, tripentyl ester. Carefully purified and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.025$$

COMP	ONENTS:		
(1)	Hydrogen	chloride;	HCl;
	[7647-01-	-01	

(2) Organic derivatives of boric

acid.

VARIABLES:

T/K: See below Total P/kPa : 101.325 (1 atm) ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.;

J. Appl. Chem. 1959, 9, 89-93.

PREPARED BY:

Wyvill, P. L.

W. Gerrard

EXPERIMENTAL VALUES:	Т/К п	Mole ratio	Mole* fraction *HCl	Smoothed** mole fraction *HCl
Borıc acıd, tributyl ester,	199.15	7.805	0.886	
(tributy) borate.	203.15			0.850
tributoxyborane); C ₁₂ H ₂₇ BO ₃ ;	213.15			0.783
[688-74-4]	219.15	2.568	0.720	
•	223.15			0.709
	233.15			0.631
	239.65	1.339	0.572	
	243.15			0.549
	253.15			0.468
	255.15	0.850	0.459	
	263.15			0.390
		0.489	0.328	0.318
	281.55	0.377	0.274	
	283.15			0.253
	287.05		0.234	
		0.243	0.195	0.197
	298.75	0.196	0.164	
	303.15			0.150
	304.15		0.139	
	305.45		0.135	
	312.15		0.114	
	313.15			0.112
	319.35	0.109	0.0983	
	323.15			0.081

Smoothing equation: $\ln x_{HCl} = -29.9216 + 47.0282/(T/100)$

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determination at temperatures below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler was attached to a flask containing one \mbox{dm}^3 of water, and allowed to warm slowly to room temperature (12 hours). contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method. A low temperature, Teddington-type YM thermostat was used for temperatures below 273 K, the control being to ±2 K.

- SOURCE AND PURITY OF MATERIALS: (1) Hydrogen chloride: good
 - specimen from a commercial cylinder was dried.
- (2) Borates: carefully purified, and purity rigourously attested.

ESTIMATED ERROR:

 $\delta T/K = \pm 2 \text{ below } 273 \text{ K}$ $\delta x_{\text{HCl}} / x_{\text{HCl}} = \pm 0.005 \text{ to } 0.01$

NOTE: The smoothing equation for boric acid, tributyl ester deviates from the data. It is 4% low at 283 K, 5% high at 303 K, and 6.5% low at 320 K. Estimated error for this system: $\delta x_{\text{HCl}}/x_{\text{HCl}} = \pm 0.04$

```
COMPONENTS:
                                                  ORIGINAL MEASUREMENTS:
(1)
      Hydrogen chloride; HCl;
                                                  Gerrard, W.; Mincer, A. M. A.;
      [7647-01-0]
                                                  Wyvill, P. L.
                                                  J. Appl. Chem. 1959, 9, 89-93.
(2)
      Organic derivatives of boric
EXPERIMENTAL VALUES:
                                         T/K
                                                                  Mole*
                                                                                Smoothed**
                                                Mole ratio
                                                                 fraction mole fraction
                                              nHC1/nborate
                                                                   x<sub>HCl</sub>
                                                                                   x
HCl
                                        273.15
2-Butoxy-1,3,2-dioxaborolane,
                                                                                    0.206
                                                                  0.208
(cyclic ethylene butyl
                                        273.25
                                                   0.262
borate); C<sub>6</sub>H<sub>13</sub>BO<sub>3</sub>; [1124-68-1] 277.65
                                                   0.220
                                                                  0.180
                                        283.15
                                                                                    0.158
                                        283.95
                                                   0.184
                                                                  0.155
                                                                  0.144
                                        287.05
                                                   0.168
                                        290.15
                                                   0.150
                                                                  0.130
                                        293.15
                                                   0.141
                                                                  0.124
                                                                                    0.123
                                        297.55
                                                   0.124
                                                                  0.110
                                        303.15
                                                                                    0.0957
                                        308.45
                                                   0.0922
                                                                  0.0844
                                        313.15
                                                                                    0.0753
                                        313.75
                                                   0.0806
                                                                  0.0746
                                        318.65
                                                   0.0703
                                                                  0.0657
                                        323.15
                                                                                    0.0596
Smoothing equation: \ln x_{HCl} = 6.977 - 1.620/(T/100) \sim 7.925 \ln(T/100)
Standard error in x_{HCl} about the regression line = 1.78 × 10<sup>-3</sup>
                                       273.15
                                                                                    0.155
2-Methoxy-1,3,2-benzodioxa-
borole, (cyclic o-phenylene methyl borate); C<sub>7</sub>H<sub>7</sub>BO<sub>3</sub>;
                                       273.35
                                                  0.184
                                                                  0.155
                                       273.95
                                                  0.177
                                                                  0.150
[72035-41-7]
                                       277.65
                                                   0.153
                                                                  0.133
                                       281.15
                                                  0.135
                                                                  0.119
                                       283.15
                                                                                    0.114
                                       292.85
                                                   0.0967
                                                                  0.0882
                                       293.15
                                                                                    0.0853
                                       299.15
                                                   0.0819
                                                                  0.0757
                                       303.15
                                                                                    0.0651
                                       304.95
                                                   0.0647
                                                                  0.0608
                                       311.45
                                                  0.0572
                                                                  0.0541
                                       313.15
                                                                                    0.0505
                                       319.15
                                                   0.0438
                                                                  0.0420
                                       323.15
                                                                                    0.0399
Smoothing equation: \ln x_{HCl} = -10.652 + 24.009/(T/100)
Standard error in x_{HCl} about the regression line = 2.14 × 10<sup>-3</sup>
2-Ethoxy-1,3,2-benzodioxa-
                                       273.15
                                                                                    0.177
                                                  0.217
                                                                  0.178
borole, (cyclic o-phenylene
                                       273.45
ethyl borate); C8H9BO3;
                                       280.65
                                                  0.173
                                                                  0.147
[72035-40-6]
                                       283.15
                                                                                    0.139
                                                   0.141
                                       286.65
                                                                  0.124
                                       292.65
                                                  0.125
                                                                  0.111
                                       293.15
                                                                                    0.109
                                       303.15
                                                                                    0,0847
                                       303.65
                                                  0.0927
                                                                  0.0848
                                                   0.0718
                                                                  0.0670
                                       313.15
                                                                                    0.0655
                                       319.15
                                                  0.0580
                                                                  0.0548
                                       323.15
                                                                                    0.0505
Smoothing equation: \ln x_{HC1} = 31.213 - 36.129/(T/100) - 19.624 \ln(T/100)
Standard error in x_{HC1} about the regression line = 2.64 × 10<sup>-3</sup>
* calculated by the compiler
** smoothing equation and smoothed values were calculated by H.L. Clever
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ORIGINAL MEASUREMENTS:
COMPONENTS:

 Hydrogen chloride; HCl;

                                                   Gerrard, W.; Mincer, A. M. A.;
     [7647-01-0]
                                                   Wyvill, P. L.
                                                   J. Appl. Chem. 1959, 9, 89-93.
(2) Organic derivatives of boric acid
                                          T/K
                                                 Mole ratio
                                                                   Mole*
                                                                                  Smoothed**
EXPERIMENTAL VALUES:
                                               <sup>n</sup>HCl<sup>/n</sup>borate
                                                                   fraction mole fraction
                                                                    ^{x}HCl
                                                                                     ^{x}HCl
2-Propoxy-1,3,2-benzodioxa-
                                        273.15
                                                                                      0.183
borole, (cyclic o-phenylene
                                                    0.225
                                        273.65
                                                                    0.184
propyl borate); C9H11BO3;
                                        278.65
                                                    0.191
                                                                    0.160
[72035-39-3]
                                        283.15
                                                                                      0.145
                                        284.65
                                                    0.160
                                                                    0.138
                                        293.15
                                                                                      0.115
                                                                    0.107
                                        295.15
                                                    0.120
                                         298.45
                                                    0.115
                                                                    0.103
                                         303.15
                                                                                      0.0904
                                         308.15
                                                    0.0900
                                                                    0.0826
                                        313.15
                                                                                      0.0710
                                        319.65
                                                    0.0634
                                                                    0.0596
                                        323.15
                                                                                      0.0556
Smoothing equation: \ln x_{HC1} = 25.967 - 29.156/(T/100) - 16.909 \ln(T/100)
Standard error in x_{HC1} about the regression line = 2.86 × 10<sup>-3</sup>
2-Butoxy-1,3,2-benzodioxa-
                                        273.15
                                                    0.242
                                                                    0.195
                                                                                      0.195
                                        276.45
                                                    0.215
                                                                    0.177
borole, (cyclic o-phenylene
butyl borate); C<sub>10</sub>H<sub>13</sub>BO<sub>3</sub>;
                                        283.15
                                                                                      0.150
                                                    0.171
[3488-87-7]
                                                                    0.146
                                        283.65
                                        293.15
                                                                                      0.118
                                                                    0.117
                                                    0.132
                                        293.65
                                        300.75
                                                    0.110
                                                                    0.0991
                                        303.15
                                                                                      0.0937
                                        307.15
                                                    0.0981
                                                                    0.0893
                                        313.15
                                                                                      0.0758
                                        314.15
                                                                    0.0753
                                                    0.0814
                                        319.65
                                                    0.0679
                                                                    0.0636
                                                                                      0.0621
                                        323.15
Smoothing equation: \ln x_{HCl} = -9.027 + 20.188/(T/100)
Standard error in x_{HCl} about the regression line = 2.14 \times 10^{-3}
2-(Pentyloxy)-1,3,2-benzo-
                                        273.15
                                                                                      0.196
dioxaborole, (cyclic
                                        273.45
                                                    0.237
                                                                    0.192
o-phenylene pentyl borate); C_{11}^{H}_{15}^{BO}_{3}; [72035-38-2]
                                                                    0.158
                                        280.95
                                                    0.187
                                        283.15
                                                                                      0.151
                                        288.45
                                                    0.154
                                                                    0.133
                                        293.15
                                                                                      0.119
                                        299.95
                                                                    0.105
                                                    0.117
                                        303.15
                                                                                      0.0950
                                        308.55
                                                    0.0960
                                                                    0.0876
                                        313.15
                                                                                      0.0770
                                        319.15
                                                    0.0700
                                                                    0.0654
                                        323.15
                                                                                      0.0632
Smoothing equation: \ln x_{\rm HCl} = -8.928 + 19.929/(T/100)
Standard error in x_{\rm HCl} about the regression line = 2.90 × 10<sup>-3</sup>
2-(Octyloxy)-1,3,2-benzo-
                                        273.15
                                                                                      0.196
                                        275.15
                                                    0.232
dioxaborole, (cyclic
                                                                    0.188
o-phenylene octyl borate);
                                                    0.192
                                        282.65
                                                                    0.161
C<sub>14</sub>H<sub>21</sub>BO<sub>3</sub>; [72035-37-1]
                                        283.15
                                                                                      0.158
                                        290.65
                                                    0.153
                                                                    0.133
                                        293.15
                                                                                      0.127
                                        298.25
                                                    0.127
                                                                    0.113
                                        303.15
                                                                                      0.101
                                        305.85
                                                    0.1050
                                                                    0.0950
                                        310.75
                                                    0.0917
                                                                    0.0840
                                                                                      0.0785
                                        313.15
                                        319.65
                                                    0.0730
                                                                    0.0680
                                        323.15
                                                                                      0.0625
Smoothing equation: \ln x_{HCl} = 31.603 - 37.452/(T/100) - 19.426 \ln(T/100)
Standard error in x_{HCl} about the regression line = 7.57 × 10<sup>-4</sup>
  calculated by the compiler
   smoothing equation and smoothed values were calculated by H.L. Clever
```

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Butoxydichloroborane; C₄H₉BCl₂O; [16339-30-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
 Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 277.75 - 294.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

T/K	Mol Ratio nHC1/nC4H9BC120	Mol Fraction x1
277.75	0.0674	0.0631
284.35	0.0476	0.0454
294.15	0.0194	0.0190

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = -24.564 + 60.734/(T/100)$

Standard error about regression line is 6.53×10^{-3}

T/K	Mol Fraction
273.15	0.0974
283.15	0.0444
293.15	0.0214
303.15	0.0109

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Butoxydichloroborane. Carefully purified, and purity rigorously attested.

Solvent name is n-butyl dichloroboronite in paper.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.05$$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Dichlorophenylborane; C₆H₅BCl₂; [873-51-8]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 258.15 - 283.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC6H5BCl2	Mol Fraction XHCl
258.15	0.100	0.091
263.15	0.092	0.084
268.15	0.082	0.076
273.15	0.073	0.068
278.15	0.066	0.062
283.15	0.059	0.056

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_1 = 30.195 - 37.294/(T/100) - 19.128 \ln (T/100)$

The standard error about the regression line = 5.96×10^{-4}

T/K	Mol Fraction XHC1
253.15	0.0999
263.15	0.0834
273.15	0.0686
283.15	0.0559
293.15	0.0451

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a weighed amount of the borane in a bubbler tube as described in the main paper (1). For temperatures below 268 K the final mixture was quantitatively treated with water, and the total chloride determined by titration.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Dichlorophenylborane. The borane was an internal specimen, prepared by another group. It was rigorously purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.01$

REFERENCES:

COMPONENTS: 1. Hydrogen Chloride; HCl; [7647-01-0] 2. Trichloroborane; BCl ₃ ; [10294-34-5]	ORIGINAL MEASUREMENTS: Ahmed, W. Thesis, 1970 University of London
VARIABLES:	PREPARED BY:
T/K: 208.15 - 258.15 Total P/kPa: 101.325 (1 atm)	W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio nHCl/nBCl3	Mol Fraction XHCl
208.15 213.15 223.15 233.15 243.15 253.15 258.15	0.095 0.080 0.055 0.035 0.025 0.019 0.018	0.0868 0.0741 0.0521 0.0338 0.0244 0.0186 0.0177

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -20.864 + 30.290/(T/100) + 5.325 \ln (T/100)$

Standard Error About Regression Line = 2.47×10^{-3}

T/K	Mol Fraction XHCl
203.15	0.113
213.15	0.0726
223.15	0.0490
233.15	0.0346
243.15	0.0253
253.15	0.0192
263.15	0.0150

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Trichloroborane was distilled into the bubbler tube at low temperature. Hydrogen chloride was passed through for 2 hours. The final liquid was quantitatively treated with an aqueous solution of sodium hydroxide. Borate and total chloride were determined by titrations. See the main paper (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Good quality was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Trichloroborane. The purest obtainable specimen was obtained from a sealed ampoule at low temperature.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.02$

REFERENCES:

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. Trichloroborane; BCl₃;
 [10294-34-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 223.15 - 263.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/BCl	Mol Fraction XHCl
223.15	0.043	0.0412
233.15	0.0345	0.0333
243.15	0.0275	0.0268
253.15	0.022	0.0215
263.15	0.017	0.0167

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = 24.260 - 29.610/(T/100) - 17.669 \ln (T/100)$ Standard error about regression line 1.98 x 10^{-4}

T/K	Mol Fraction
	X _{HC1}
223.15	0.0411
233.15	0.0335
243.15	0.0269
253.15	0.0213
263.15	0.0168
273.15	0.0131

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1, 2).

The absorbed gas was determined by a chemical titration for boron and chloride.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commerical specimen. Was dried by passage through concentrated sulfuric acid.
- Trichloroborane. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.005$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. <u>1972</u>, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Phosphorus

EVALUATOR:

Peter G. T. Fogg Department of Applied Chemistry and Life Sciences, Polytechnic of North London, Holloway, London, N7 8DB, U.K.

January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Solvents Containing Phosphorus.

Solubilities in a variety of solvents containing phosphorus have been measured by Gerrard and his co-workers (1-4) over temperature ranges at barometric pressure. Data are self-consistent but, only in the case of tributyl phosphate can comparison be made with measurements by other workers. Borissov & Ionin (5) have published a small diagram showing a plot of the logarithm of the mole ratio solubility at 298.15 K and 101.3 kPa in five trialkyl esters against the carbon number of the alkyl group. In the case of tributyl ester the corresponding mole fraction solubility is about 0.6 which may be compared with a value of 0.684 by extrapolation of measurements by Gerrard et al.

- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89-93; 1960, 10, 115-121.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109-115.
- 3. Cook, T. M. Thesis, 1966, University of London.
- 4. Ahmed, Thesis, 1970, University of London.
- Borissov, R. S.; Ionin, M. V. Tr. Gor'k. Politekh. Inst. 1973, 29, 11-15.

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. Phosphorous trichloride; PCl₃;
 [7719-12-2]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 213.15 - 273.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	nHC1/nPC13	X _{HCl}
213.15 223.15 233.15 243.15 253.15 263.15 273.15	0.24 0.13 0.09 0.063 0.048 0.033	0.194 0.115 0.0826 0.0593 0.0458 0.0319

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HCl} = -24.930 + 37.360/(T/100) + 7.575 \ln (T/100)$

Standard error about regression line 4.54×10^{-3}

T/K	Mol Fraction
	XIICI
213.15	0.188
223.15	0.121
233.15	0.0826
243.15	0.0587
253.15	0.0434
263.15	0.0332
273.15	0.0262

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1, 2).

For temperatures below 253 K, a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- (2) Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/K = 0.02$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

COMPONENTS: 1. Hydrogen Chloride; HCl;

[7647-01-0]

2. Phosphoryl Chloride; Cl₃OP;
[10025-87-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 273.15 - 288.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio "HC1/"C13OP	Mol Fraction XHCl
273.15	0.320	0.242
278.15	0.208	0.172
283.15	0.137	0.120
288.15	0.125	0.111

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -17.064 + 42.613/(T/100)$

Standard Error About Regression Line = 1.1×10^{-2}

T/K	Mol Fraction XHCl
273.15	0.231
283.15	0.133
293.15	0.080

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a weighed amount of phosphoryl chloride in a bubbler tube as described in the main paper (1). The gas absorbed was weighed; and the result was checked by quantitative treatment with water followed by titrations of total chloride and acid.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Phosphoryl chloride. A good specimen was purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.02$

REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen Chloride; HCl; Ahmed, W. [7647-01-0] Thesis, 1970 University of London 2. Phenylphosphonous Dichloride; $C_6H_5Cl_2P; [644-97-3]$ **VARIABLES:** PREPARED BY: T/K: 268.15 - 283.15 W. Gerrard Total P/kPa: 101.325 (1 atm) (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC6H5Cl2P	Mol Fraction XHCl
268.15	0.143	0.125
273.15	0.125	0.111
278.15	0.111	0.100
283.15	0.100	0.091

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -59.555 + 86.494/(T/100) + 25.568 \ln (T/100)$

Standard error about regression line = 8.41×10^{-5}

T/K	Mol Fraction XHCl	
263.15	0.143	
273.15	0.111	
283.15	0.0910	
293.15	0.0780	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into the phosphine in a bubbler tube as described in the main paper (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen Chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Phenylphosphonous dichloride. The best specimen was rigorously purified and attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.005$$

REFERENCES:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Phenylphosphonic dichloride;
 C₆H₅Cl₂OP; [824-72-6]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 273.15 - 288.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction X _{HCl}
273.15 278.15	0.705 0.560	0.413
283.15 288.15	0.495 0.470	0.331 0.320

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_1 = -326.855 + 456.641/(T/100) + 158.028 \ln (T/100)$

The standard error about the regression line = 6.04×10^{-4}

T/K	Mol Fraction XHC1
273.15	0.413
283.15	0.331
293.15	0.325

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a weighed amount of the phosphorus compound in a bubbler tube, as described in the main paper (1).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Phenylphosphonic dichloride. The best quality specimen was purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.005$

REFERENCES:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Phenylphosphonothioic Dichloride; C₆H₅Cl₂PS; [3497-00-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 263.15 - 278.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC6H5Cl2PS	Mol Fraction XHCl
263.15	0.171	0.146
268.15	0.152	0.132
273.15	0.131	0.116
278.15	0.116	0.104

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = 42.041 - 51.456/(T/100) - 25.227 \ln (T/100)$

Standard Error About Regression Line = 1.33×10^{-3}

т/к	Mol Fraction XHC1
263.15	0.146
273.15	0.117
283.15	0.0918

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a weighed amount of the phosphorus compound in a bubbler tube as described in the main paper (1). For temperatures below 268 K the final mixture was quantitatively treated with water and the total chloride titrated.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good quality gas was obtained from a cylinder. It was passed through concentrated sulfuric acid and calcium chloride.
- Phenylphosphonothioic Dichloride.
 The best available specimen was rigorously purified and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.005$

REFERENCES:

358 Hydrogen Chloride in Non-Aqueous Solvents COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen chloride; HCl; Borissov, R. S.; Ionin, M. V. [7647-01-0] Tr. Gor'k. Politekh. Inst. 1973, (2) Phosphoric acid, trialkyl 29, 11 - 15. esters VARIABLES: PREPARED BY: T/K = 298.15p/kPa = 101.325W. Gerrard EXPERIMENTAL VALUES: Temperature Mol Ratio Mol Fraction T/K n_1/n_2 x_{7} Phosphoric acid, trimethyl ester; $C_3H_9O_4P$; [512-56-1] 298.15 0.66 0.398

Phosphoric acid, triethyl ester; $C_6H_{15}O_4P$; [78-40-0]

298.15

1.03

0.507

Phosphoric acid, tripropyl ester; $C_9H_{21}O_4P$; [513-08-6]

298.15

1.585

0.613

Phosphoric acid, tributyl ester; $C_{12}^{H}_{27}^{O}_{4}^{P}$; [126-73-8] 298.15

1.66

0.624

Phosphoric acid, tris(2-methylpropyl) ester; $c_{12}H_{27}O_4P$; [126-71-6]

298.15

1.66

0.624

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Not described.

Numerical data were not reported. The compiler has read the mole ratio values from a small diagram showing a carbonate in a vacuum. plot of log (mole ratio) vs. number of carbon atoms in R of (RO)₃PO. The corresponding mole fraction, x_1 , was calculated by the compiler.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Not stated.

ESTIMATED ERROR:

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Phosphoric acid tributyl ester; $C_{12}H_{27}O_4P$; [126-73-8]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 197.15 - 279.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

279.15 W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	n HC1 n C $_{12}^{H}_{27}^{O}_{4}^{P}$	Х _{НС1}
197.15	8.74	0.897
211.15	6.67	0.870
233.15	4.47	0.817
273.95	2.79	0.736
279.15	2.54	0.718

Smoothed Data: $\ln X_{HC1} = 2.051 - 2.169/(T/100) - 1.559 \ln (T/100)$

Standard Error About Regression Line = 4.39×10^{-3}

T/K	Mol Fraction
	X _{HC1}
193.15	0.906
203.15	0.885
213.15	0.864
200 15	0.010
223.15	0.842
233.15	0.820
243.15	0.798
253.15	0.776
263.15	0.755
273.15	0.734
283.15	0.713

At higher temperatures there is reaction between HCl and the ester.

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed at temperatures above 273 K was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determinations below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method.

A low temperature, Teddington type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

Other solvent name Tributyl phosphate

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Phosphoric acid tributyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 \text{ below 273 K} \\ \delta X_1/X_1 = 0.02$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Phosphorous acid di-2-propenyl ester or diallyl hydrogen phosphite; C₆H₁₁O₃P; [23679-20-1]

ORIGINAL MEASUREMENTS:

Cook, T. M.

Thesis, 1966 University of London

VARIABLES:

T/K: 277.95 - 287.15 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: -

т/к	Mol Ratio nHCl/nC6H11O3P	Mol Fraction X _{HCl}
277.95	1.594	0.614
281.15	1.535	0.606
282.65	1.495	0.599
282.75	1.492	0.599
283.15	1.478	0.596
287.15	1.384	0.581

The mole fraction values were calculated by the compiler.

Smoothed Data: $\ln X_{HC1} = 62.508 - 84.847/(T/100) - 31.762 \ln (T/100)$

Standard Error About Regression Line = 1.18×10^{-3}

T/K	Mol Fraction X _{HC1}
273.15	0.625
283.15	0.597
293.15	0.551

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The data were cited by Gerrard (1).

Hydrogen chloride was passed into a bubbler tube containing a weighed amount of solvent at the specified temperature until the increase in weight was constant at the barometric pressure (2).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Sample of best quality was self prepared, and was passed through concentrated sulfuric acid and calcium chloride.
- 2. Phosphorous acid, di-2-propenyl ester. Fractionally distilled, boiling point(10 mmHg)= $110-114^{\circ}$ C, and refractive index, $n_D^{25}=1.4443$, $d_A^{20}=1.0841$.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.005$$

- Gerrard, W.
 J. Chim. Phys. 1964, 61, 73;
 Solubility of Gases in Liquids,
 Plenum Press, New York, 1976.
- Ahmed, W.; Gerrard, W.;
 Maladkar, V. K. J. Appl. Chem. 1970, 20, 109.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Phosphorous acid triphenyl ester; $C_{18}H_{15}O_{3}P; [101-02-0]$

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 274.45 - 324.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:			
EXPERIMENTAL VALUES.	T/K	Mol Ratio	Mol Fraction
		ⁿ HC1/ ⁿ C ₁₈ H ₁₅ O ₃ P	X _{HC1}
	274.45	0.7969	0.443
	290.35	0.6083	0.378
	293.65	0.5749	0.365
	298.65	0.5279	0.346
ļ	304.15	0.4880	0.328
	310.95	0.4410	0.306
	313.15	0.4313	0.301
	324.15	0.3613	0.265

 $ln X_{HC1} = 12.012 - 13.851/(T/100) - 7.707 ln (T/100)$ Smoothed Data:

Standard Error about Regression Line = 1.30×10^{-3}

T/K	Mol Fraction
•	X _{HC1}
$\overline{273.15}$	0.448
283.15	0.406
293.15	0.367
303.15	0.331
313.15	0.299
323.15	0.269
333.15	0.242

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- 2. Phosphorous acid triphenyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

REFERENCES:

 $\delta x_1/x_1 = 0.005$

Other solvent name triphenyl phosphite (IUPAC)

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; Gerrard, W.; Mincer, A. M. A.; [7647-01-0] Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121. (2) Phosphorochloridic acid monophenyl ester; C6H6ClO3P or C6H5OP(0)Cl2; [13929-83-4] **VARIABLES:** PREPARED BY: T/K: 273.15 - 311.95 Total P/kPa: 101.325 (1 atm) 273.15 - 311.95 W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHCl/nC6H6ClO3P	Mol Fraction
273.15 282.15 291.75 298.05 303.45 311.95	0.488 0.372 0.293 0.251 0.210 0.163	0.328 0.271 0.227 0.201 0.174 0.140

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 58.681 - 75.268/(T/100) - 32.094 \ln (T/100)$

Standard error about the regression line is 4.19×10^{-3}

T/K	Mol Fraction
	1
273.15	0.325
283.15	0.271
293.15	0.220
303.15	0.175
313.15	0.137

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Phosphorochloridic acid, monophenyl ester. Carefully purified, and purity rigorously attested.

Solvent name is phenyl phosphorochloridate in paper, IUPAC name is phenyl hydrogen phosphorochloridate. ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Phosphorochloridic acid, diphenyl J. Appl. Chem. 1960, 10, 115-121. ester; C₁₂H₁₀ClO₃P or

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

 $(C_6H_5O)_2P(O)C1; [2524-64-3]$

VARIABLES:

T/K: 273.15 - 313.45 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: __

т/к	Mol Ratio nHCl/nC ₁₂ H ₁₀ ClO ₃ P	Mol Fraction ^x 1
273.15 279.15 285.15 290.25 298.15 307.55 313.45	0.773 0.665 0.588 0.513 0.409 0.300	0.436 0.399 0.370 0.339 0.290 0.231

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 94.089 - 125.672/(T/100) - 48.682 \ln (T/100)$

Standard error about the regression line is 3.08×10^{-3}

T/K	Mol Fraction "1
273.15	0.433
283.15	0.382
293.15	0.320
303.15	0.257
313.15	0.199

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Phosphorochloridic acid, diphenyl ester. Carefully purified, and purity rigorously attested.

Solvent IUPAC name in paper is diphenyl phosphorochloridate.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.005$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. 2,2,2-Trichloroethanol phosphite (3:1); $C_6H_6Cl_9O_3P$; [1069-93-8]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 273.35 - 313.95 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	nHC1/nC6H6C19O3P	X _{HCl}
273.35	0.5572	0.358
290.25	0.3940	0.283
294.05	0.3544	0.262
295.15	0.3489	0.259
300.65	0.3029	0.232
302.55	0.2892	0.224
306.15	0.2606	0.207
310.55	0.2542	0.203
313.95	0.2537	0.202

Smoothed Data:

 $\ln X_{HC1} = -5.817 + 13.129/(T/100)$

Standard Error About Regression Line = 6.58×10^{-3}

Mol Fraction
X _{HC1}
0.364
0.307
0.262
0.226
0.197
0.173

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- 2,2,2-Trichloroethanol phosphite (3:1). Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.02$$

Other solvent name
Tris(2,2,2-trichloroethyl) phosphite

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Silicon

EVALUATOR:

Peter G. T. Fogg
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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Solvents Containing Silicon.

Gerrard et al.(1) measured solubilities in four tetraalkyl esters of silicic acid over temperature ranges at a total pressure equal to 101.3 kPa. Solubility over a pressure and temperature range in one of these esters, the tetra(4-methyl-2-pentyl) ester, was reported by these authors in a later publication (2). Solubilities are very high under the conditions of measurement. The later measurements show that, at a total pressure of 101.3 kPa, mole fraction solubilities are not very sensitive to changes in pressure (see fig. 1). It follows that mole fraction solubilities at a total pressure of 101.3 kPa may be equated with mole fraction solubilities at a partial pressure of 101.3 kPa for the purpose of comparison of data with those for different systems.

Mole fraction solubilities at a total pressure of 101.3 kPa in the tetraethyl, tetrapropyl and tetra(4-methyl-2-pentyl) esters are close to each other over the temperature ranges in which comparison can be made. Mole fraction solubilities in the tetramethyl ester are close to those in the tetra(4-methyl-2-pentyl) ester at temperatures less than about 240 K. Solubilities in all four esters show a marked decrease with increase in temperature at temperatures above about 283.15 K but this decrease is especially marked in the case of the tetramethyl ester (see fig. 2).

Gerrard et al.(2) also measured solubilities in the tetrakis(2-chloroethyl) ester. Mole fraction solubilities at a total pressure of 101.3 kPa are again higher compared with the reference line based upon the Raoult's law equation but the presence of chlorine reduces solubility relative to the tetraethyl ester (see fig. 2).

Measurements of solubilities in the esters of silicic acid discussed above are consistent over wide temperature ranges. The only measurements available for comparison are those of the solubilities in the tetraethyl ester at three temperatures by Ditsent and co-workers which were cited by Gorshkov et al.(3). They correspond to lower solubilities than found by Gerrard et al. Details are not available. They should not be considered to cast serious doubt on the reliability of Gerrard's data.

Data published by Gorshkov et al.(3) show that the solubility of hydrogen chloride in triethoxy silane is also very high with a mole fraction solubility of about 0.6 at 293.15 K. The solubility was, however, found by an indirect method based upon kinetic measurements because of chemical reaction of hydrogen chloride with the solvent. This work must be considered to have only semi-quantitative significance.

Ahmed, Gerrard & Maladkar (4) measured solubilities in tetrachlorosilane over the temperature range 243.15 K to 293.15 K at a total pressure of 101.3 kPa. Solubilities are very low compared with those reported for dissolution in alkyl esters of silicic acid. The solvent is appreciably volatile at the higher temperatures of measurement (25.5 kPa at 293.15 K) and will make a significant contribution to the total pressure. The evaluator has estimated the mole fraction solubility at a partial pressure of 101.3 kPa from the solubility data at each temperature given by Ahmed et al. Rau (5) has measured solubilities in the same solvent over partial pressure ranges to a maximum of 0.298 kPa in the temperature range 290 K to 410.5 K. Mole fraction solubilities for a partial pressure of 101.3 kPa are inconsistent with solubilities for lower temperatures from data by Ahmed et al. Further work on this system is required.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Silicon

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

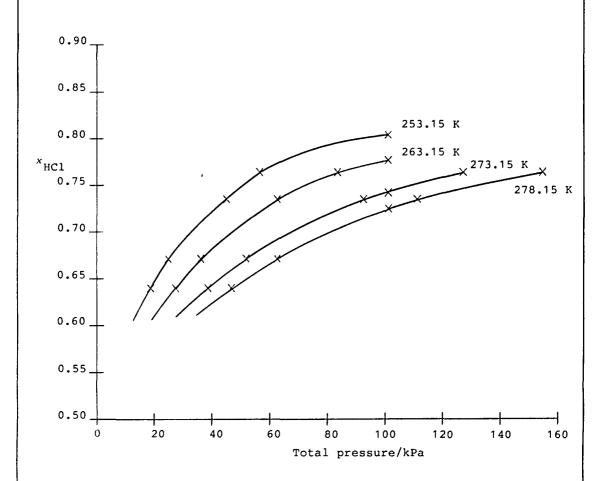


Figure 1

The dependence upon temperature and total pressure of the mole fraction solubility of hydrogen tetra(4-methyl-2-pentyl) ester.

(see ref. 2)

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Silicon

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

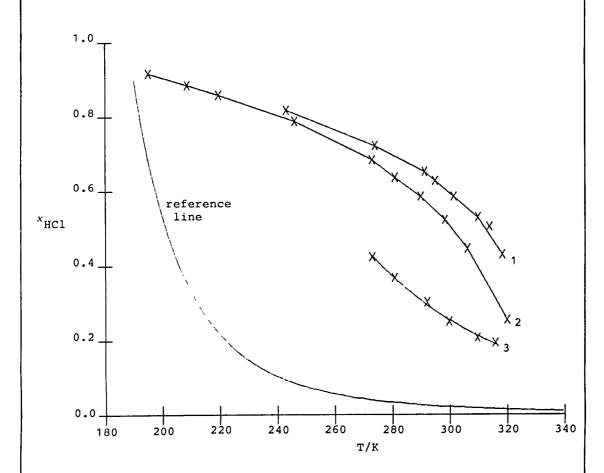


Figure 2

<u>Variation</u> with temperature of the mole fraction solubilities of hydrogen chloride in esters of silicic acid at a total pressure of 101.3 kPa.

- 1 Silicic acid, tetraethyl ester
- 2 Silicic acid, tetramethyl ester
- 3 Silicic acid, tetrakis(2-chloroethyl) ester.

The reference line corresponds to the variation in solubility given by the Raoult's law equation.

(see refs. 1 & 2)

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Solvents Containing Silicon

EVALUATOR:

Peter G. T. Fogg
Department of Applied Chemistry
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January 1989

CRITICAL EVALUATION:

- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1959, 9, 89-93.
- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121.
- Gorshkov, A. S.; Reibakh, M. S.; Tsirlin, A. M. Zh. Prikl. Khim. (Leningrad) 1967, 40, 151-155.
 J. Appl. Chem. USSR 1967, 40, 131-135.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109-115.
- 5. Rau, H. J. Chem. Thermodyn. 1982, 14, 77-82.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Silicic acid tetramethyl ester; $C_4H_{12}O_4Si$; [681-84-5]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 195.15 - 320.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES: _

T/K	Mol Ratio	Mol Fraction
	n HCl/ n C $_{4}$ H $_{12}$ O $_{4}$ Si	X _{HC1}
195.15	11.03	0.917
208.65	7.702	0.885
219.65	6.087	0.859
246.15	3.684	0.787
273.15	2.150	0.683
281.15	1.746	0.636
290.15	1.409	0.585
298.55	1.091	0.522
306.35	0.801	0.445
320.15	0.340	0.254

Smoothed Data: Neither the three nor the four constant smoothing equation fitted the data satisfactorily.

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed at temperatures above 273 K was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determinations below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method.

A low temperature, Teddington type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

Other solvent names are Tetramethyl orthosilicate Tetramethoxysilane

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Silicic acid tetramethyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 \text{ below 273 } K$ $\delta X_1/X_1 = 0.03$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- Silicic acid tetraethyl ester;
 C₈H₂₀O₄Si; [78-10-4]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 243.15 - 318.55 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	T/K	Mol Ratio	Mol Fraction
		n HCl/ n C $_{8}$ H $_{20}$ O $_{4}$ Si	X _{HC1}
	243.15	4.503	0.818
	274.15	2.590	0.721
	291.45	1.872	0.652
	295.15	1.683	0.627
	301.65	1.411	0.585
	310.05	1.123	0.529
	313.95	1.016	0.504
	318.55	0.750	0.429

Smoothed Data: $\ln x_1 = -394.5588 + 536.8451/(T/100K) + 402.1428 \ln (T/100K)$ -75.5649 (T/100K)

Standard error about regression line = 1.28×10^{-2}

T/K	Mol Fraction x1	T/K	Mol Fraction x_1
243.15 253.15 263.15 273.15 283.15	0.819 0.763 0.737 0.717 0.690	293.15 303.15 313.15 323.15	0.646 0.580 0.494 0.396

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed at temperatures above 273 K was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determinations below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing 1 dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method.

A low temperature, Teddington type YM thermostat was used for temperatures below 273 K, the control being within ± 2 K.

Other solvent names Tetraethyl orthosilicate Tetraethoxysilane

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Silicic acid tetraethyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta T/K = 2 \text{ below 273 K}$ $\delta X_1/X_1 = 0.025$

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Silicic acid tetrapropyl ester;
 C₁₂H₂₈O₄S; [682-01-9]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 273.15 - 331.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: -

T/K	Mol Ratio	Mol Fraction XHCl
273.15	2.646	0.726
283.15	2.212	0.689
298.15	1.601	0.616
311.15	1.150	0.535

Smoothed Data: $\ln X_{HC1} = 44.684 - 60.006/(T/100) - 22.925 \ln (T/100)$

Standard Error about Regression Line = 2.61×10^{-3}

T/K	Mol Fraction X _{HCl}
273.15	0.726
283.15	0.692
293.15	0.643
303.15	0.586
313.15	0.524

The mole fraction values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The solvent was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen Chloride. Good specimen from a commercial cylinder was dried.
- Silicic acid tetrapropyl ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.005$

Other solvent names tetrapropyl orthosilicate tetrapropoxysilane

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Silicic acid tetra(4-methyl-2pentyl) ester or tetra-(4-methylpent-2-yloxy)silane; C₂₄H₅₂O₄Si; [18765-36-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1959, 9, 89 - 93.

VARIABLES:

T/K: 211.15 - 321.55 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	ⁿ HC1 ^{/n} C ₂₄ H ₅₂ O ₄ Si	
211.15	8.230	0.892
222.15	6.754	0.871
229.85	5.928	0.856
248.15	4.862	0.829
259.15	3.772	0.790
275.15	2.810	0.738
280.65	2.500	0.714
289.15	2.100	0.677
291.65	1.970	0.663
299.65	1.691	0.628
314.05	1.080	0.519
320.55	0.882	0.469
321.55	0.844	0.458

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 21.804 - 27.452/(T/100K) - 11.990 \ln (T/100K)$ Standard error about the regression line is 2.55 x 10^{-2}

	T/K	Mol Fraction
The smoothed data		x_1
equation is for use	263.15	0.795
between the temper- atures of 263.15 and	273.15	0.745
323.15 K.	283.15	0.690
323.13 K.	293.15	0.634
	303.15	0.577
	313.15	0.523
	323.15	0.470

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

For determination at temperatures below 273 K, a chemical titration was carried out. After the maximum absorption at the stated temperature, the bubbler tube was attached to a flask containing one dm³ of water, and allowed to warm slowly (12 hours) to room temperature. The contents of the bubbler tube were then added to the water, and the total chloride ion was determined by the Volhard method. A low temperature, Teddington-type YM thermostat was used for temperatures below 273 K, the control being to ± 2 K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Silicic acid tetra(4-methyl-2pentyl)ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.03$$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Silicic acid tetra(4-methyl-2pentyl)ester or tetra-(4-methylpent-2-yloxy)silane; C₂₄H₅₂O₄Si; [18765-36-1]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A. Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115 - 121.

EXPERIMENTAL VALUES:

Variation of temperature and pressure at constant mole fraction.

sure at co	onstant mo	le fraction.
T/K	Pressure P1/mmHg	Mol Fraction
225.15 238.15 249.65 255.85 264.85 273.15 282.15 286.35 291.55 296.15 300.55 304.15 305.75 308.15	65 103 159 208 287 393 557 648 764 879 966 1046 1095	0.671
229.65 231.15 241.95 252.15 255.15 256.15 259.65 263.55 266.65 273.15 277.15	165 177 265 420 441 492 560 636 722 955	0.764
225.15 227.15 238.15 247.15 247.75 258.65 266.65 273.15 278.75 283.35 286.35 287.95 291.35	105 124 197 273 279 408 539 702 854 984 1080 1125 1231	0.735
224.65 230.65 243.15 248.65 256.15 261.75 269.75 272.65 278.15 283.65 290.95 296.55 300.75	57 64 101 121 158 200 255 285 353 458 600 746 856	0.640

METHOD/APPARATUS/PROCEDURE:

To measure the total pressure, taken to be p_1 , a weighed amount of silane was put into a flask fitted with a

Variation of pressure and mole fraction at constant temperature.

ressure M 1/mmHg	Mol Fraction *1
ı/mmHg	2°
	₩ 7
	
141	0.640
187	0.671
338	0.735
425	0.764
760	0.804
206	0.640
272	0.671
470	0.735
628	0.764
760	0.777
290	0.640
390	0.671
695	0.735
760	0.742
955	0.764
351	0.640
470	0.671
760	0.725
835	0.735
L162	0.764
	187 338 425 760 206 272 470 628 760 290 390 695 760 955 351 470 760

capillary bubbler tube through which the gas was passed into the liquid at room temperature (controlled). The flask was attached to the tapped end of a U-tube manometer containing Hg, the other limb being open to the atm; the pressure, p_1 , was measured to the nearest mmHg for the condition of equilibrium at each recorded temperature. From a plot of $p_1/\text{mmHg } vs.\ T/\text{K}$ the value of T/K for $p_1=1$ atm was read; and the separately determined x_1 for that T/K (1) was taken to be the x_1 value for the series. Data for 4 series were reported as above. From the set of $p_1 vs.\ T/\text{K}$ curves data given in the second table above were obtained.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. A good specimer was obtained from a cylinder and dried.
- (2) Silane. It was prepared and purified by a standard technique, and its purity was attested.

REFERENCES:

 Gerrard, W.; Mincer, A. M. A.: Wyvill, P. L. J. Appl. Chem. <u>1959</u>, 9, 89.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Silicic acid tetrakis(2-chloro ethyl) ester or tetra-(2-chloroethoxy)silane; C₈H₁₆Cl₄O₄Si;

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

[18290-84-1]

VARIABLES:

T/K: 273.15 - 316.05 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: __

T/K	Mol Ratio	Mol Fraction
****	$^{\text{n}}\text{HC1}^{/\text{n}}\text{C}_{8}^{\text{H}}_{16}^{\text{Cl}}_{4}^{\text{O}}_{4}^{\text{Si}}$	
273.15	0.734	0.423
280.95	0.580	0.367
292.25	0.432	0.302
299.85	0.333	0.250
309.75	0.259	0.206
316.05	0.239	0.193

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 9.293 - 6.404/(T/100) - 7.764 \ln (T/100)$

Standard error about the regression line is 7.06×10^{-3}

T/K	Mol Fraction
273.15	0.426
283.15	0.350
293.15	0.289
303.15	0.239
313.15	0.199
323.15	0.166

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Good specimen from a commercial cylinder was dried.
- (2) Silicic acid tetrakis (2-chloroethyl) ester. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.025$$

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Triethoxysilane; $C_6H_{16}O_3Si$ or $(C_2H_5O)_3SiH$; [998-30-1]
- (3) Silicic acid, tetraethyl ester; C₈H₂₀O₄Si; [78-10-4]

ORIGINAL MEASUREMENTS:

Gorshkov, A. S.; Reibakh, M. S.; Tsirlin, A. M.

Zh. Prikl. Khim. (Leningrad) 1967, 40, 151 - 155.

J. Appl. Chem. USSR (Engl. Transl.) 1967, 40, 131 - 135.

EXPERIMENTAL VALUES:

The objective of this work was to determine the solubility of HCl in component 2, Triethoxysilane. A kinetic method was used. The hydrogen chloride reacted with the solvent, which was initially 95.9 % triethoxysilane and 4.1 % silicic acid, tetraethyl ester or tetraethoxysilane, to form an intermediate chlorosilane. (chlorodiethoxysilane, C₄H₁₁ClO₂Si, [6485-91-2]),ethanol [64-17-5], and hydrogen [1333-74-0].

Tempe	nperature Mol Ratio Mol		Mol Fraction 1	Ratio of Mol Ratios ²
t/ºC	T/K	n_1/n_2	x_{1}	$(n_1/n_2)/(n_1/n_3)$
20	293.15	1.365	0.577	0.975
35	308.15	0.6785	0.404	0.715
60	333.15	0.1399	0.123	0.680

Mol fraction values calculated by the compiler. The hydrogen chloride partial pressure, p_1 , was stated to be 760 mmHg.

The conventional method of determination is frustrated by the occurrence of an irreversible conversion of the triethoxysilane into tetraethoxysilane and hydrogen, via an intermediate chlorosilane formulated as $(C_2H_5O)_2$ SiHCl. It was stated that the solubility was determined from kinetic curves, and the known solubility of HCl in ethanol (1) and in tetraethoxysilane (the citation being given merely as V. E. Ditsent and co-workers).

The solubility of HCl in monochloridiethoxysilane, $({\rm C_2H_5O})_2{\rm SiHCl}$ [6485-91-2], could not be determined from the kinetic curves; it was assumed to be half its solubility in triethoxysilane. It was stated that the data on the solubility of HCl in tetraethoxysilane for pressures below 760 mmHg (not recorded, but presumably those attributed to Ditsent, et al.) were used to convert the mole ratio values for 1 atm (Table above) to those for pressures below 1 atm by assuming that the solubility ratio, $(n_1/n_2)/(n_1/n_3)$, for 1 atm, at the chosen T/K remains constant at all partial pressures, p_1 , below 1 atm. These calculated data were presented as mole fractions, x_1 , for triethoxysilane, as shown on the next page.

The values are based on the solubility of HCl in silicic acid, tetraethyl ester at one atm HCl reported by V. E. Ditsent and co-workers.

- (1) Hydrogen chloride; HCl; [7647-01-[7647-01-0]
- (2) Triethoxysilane; $C_6H_{16}O_3Si$ or $(C_2H_5O)_3SiH$; [998-30-1]

ORIGINAL MEASUREMENTS:

Gorshkov, A. S.; Reibakh, M. S.; Tsirlin, A. M.

2h. Prikl. Khim. (Leningrad) <u>1967</u>, 40, 151 - 155.

J. Appl. Chem. USSR (Engl. Transl.) 1967, 40, 131 - 135.

VARIABLES:

T/K = 293.15 - 333.15 $p_1/kPa = 101.325$ (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

p ₁ /mmHg	T/K	Mol Fraction x_1	T/K	Mol Fraction x_I	T/K	Mol Fraction
25	293.15	0.077	308.15	0.0316	333.15	
50		0.143		0.0611		0.01525
100		0.247		0.1155		0.0301
200		0.371		0.209		0.0549
300		0.448		0.275		0.0720
400		0.498				0.0883
500		0.533		0.333		0.1005
600		0.555				0.1135
700		0.573		0.398		0.1225

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The amount of HCl absorbed was determined by titration by the Mohr's method. The amount of HCl absorbed was found by the difference between the amount passed through the initial flow meter, and that emerging from the absorption vessel as an effluent of HCl and H2, the former being absorbed in water, and the latter being collected over water in a buret. The volume of hydrogen was measured every 60 seconds.

Their Fig. 2 showed the variation of "chlorine" content in the solution with time, for each T/K. Their Fig. 3 showed the volume of hydrogen evolved from the reaction mixture with time.

The liquid phase contained monochlorodiethoxysilane, ethanol, tetraethoxysilane, triethoxysilane, and hydrogen chloride.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Obtained from aqueous hydrochloric acid and sulfuric acid (concentrated).
- (2) The initial liquid contained the triethoxysilane (95.9%) and tetraethoxysilane (4.1%).

ESTIMATED ERROR:

REFERENCES:

1. Technical Encyclopedia. Handbook of Chemical, Physical, and Technological Data (in Russian), 1930, 5, 422.

COMPONENTS: 1. Hydrogen chloride; HCl; Ahmed, W.; Gerrard, W.; Maladkar, V. K. 2. Tetrachlorosilane; SiCl₄; J. Appl. Chem. 1970, 20, 109 - 115. VARIABLES: T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm) PREPARED BY: W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	T/K	Mol Ratio "HC1/"SiC14	Mol Fraction XHCl
	243.15	0.086	0.0792
	253.15	0.068	0.0637
	263.15	0.0525	0.0499
	273.15	0.040	0.0385
	283.15	0.032	0.0310
	293.15	0.027	0.0263

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -2.881 + 7.722/(T/100) - 3.170 \ln (T/100)$

Standard error about regression line = 1.27×10^{-3}

T/K	Mol Fraction XHC1
243.15	0.0804
253.15	0.0624
263.15	0.0491
273.15	0.0392
283.15	0.0317
293.15	0.0258

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For the first three temperatures a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.
- Tetrachlorosilane. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.005$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen chloride; HCl; [7647-01-0] Rau. H. (2) Tetrachlorosilane or silicon J. Chem. Thermodyn. 1982, 14, 77 - 82 tetrachloride: SiCl,: [10026-04-7] VARIABLES: PREPARED BY: T/K = 290.0 - 410.53.1 - 298.0 $p_1/kPa =$ H. L. Clever

(0.031 - 2.94 atm)

EXPERIMENTAL VALUES:

Temperature	Pressure	Mol Fraction	Temperature	Pressure	Mol Fraction
T/K	p ₁ /kPa	10 ² x ₁	T/K	p ₁ /kPa	10 ² x ₁
290.0	46.4	0.869	364.0	3.1	0.066
290.5	84.8	1.380	364.0	97.6	0.866
293.0	124.4	2.054	364.0	165.8	1.367
295.5	30.8	0.456	364.0	243.3	2.162
296.0	5.3	0.057			
			376.5	56.0	0.473
315.5	159.7	2.055	377.0	11.3	0.055
318.5	42.3	0.453	377.5	111.2	0.872
320.0	7.2	0.055	378.0	183.7	1.378
320.5	69.4	0.857	378.0	271.0	2.128
320.5	116.0	1.365			
			389.5	74.4	0.475
333.0	47.1	0.455	390.0	298.0	2.154
333.5	134.9	1.351	392.0	13.0	0.055
334.0	10.0	0.051	392.0	123.3	0.883
334.0	193.1	2.062	392.0	208.3	1.389
348.0	49.1	0.463	404.0	81.7	0.487
349.0	148.1	1.360	406.5	152.7	0.896
349.0	219.6	2.078	406.5	233.3	1.407
349.5	9.1	0.055	408.0	94.2	0.490
349.5	87.4	0.860	408.5	4.0	0.067
347.3	0,.4	0.000	410.5	94.1	0.491
362.0	54.1	0.466	420.5	73.4	V. 471

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an all-silica Bourdon gage. A volume of HCl at a known pressure was condensed into the silca spiral. The SiCl₄ was added by breaking a glass ampule containing a known weight of the material.

The entire sealed apparatus was mounted in an autoclave with optical windows so that the pointer attached to the end of the spiral could be observed. The pointer was brought to its null position by a known pressure ESTIMATED ERROR: of argon gas.

The total pressure was measured as a function of temperature. The gas volume, the vapor composition, and

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Commercial cylinder. Condensed in a glass vessel, then vaporized to a predetermined pressure in a calibrated volume.
- (2) Tetrachlorosilane. Merck/Darmstadt Optipur. Distilled in high vacuum apparatus (all glass) and sealed in glass ampules.

 $\delta T/K = \pm 0.5$ $\delta p_t/p_t = \pm 0.001$ $\delta x_1/x_1 = \pm 0.10$

the HCl partial pressure are determined assuming that liquid HCl has a density of 0.8 g cm⁻³, the liquid SiCl₄ has the density of the pure liquid, the gas compression factors can be calculated from corresponding-state principle, HCl and SiCl4 do not interact in the gas phase, and HCl vapor behaves ideally. The author calculated Henry's constant in the form $C/Pa^{-1} = x_1/(p_1/Pa)$. A linear regression gave the equation $log(C/Pa^{-1}) = -8.279 + 437/(T/K)$. The author states that Henry's law is obeyed within experimental error.

- 1. Hydrogen Chloride; HCl; [7647-01-0]
- 2. Tetrachlorostannane; SnCl₄;
 [7646-78-8]
 Titanium Chloride; TiCl₄:
 [7550-45-0]

LVALUATOR:

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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Chloride in Tetrachlorostannane and in Titanium Chloride.

Ahmed et al.(1) have reported the solubility in tetrachlorostannane at a total pressure of 101.3 kPa over the temperature range 243.15 K to 293.15 K. The data are self-consistent and likely to be more reliable than the measurements at 273 K and 300 K reported by Howald & Willard (2) which correspond to lower solubilities. The mole fraction solubility at 273 K from Ahmed's data is 0.061 compared with 0.050 from Howald & Willard's data. The values for 300 K are 0.048 and 0.040 respectively.

Ahmed $et\ al.$ also reported solubility in titanium chloride at the same pressure over a temperature range of 243.15 K to 293.15 K. Measurements are self consistent and indicate mole fraction solubilities lower than for dissolution in tetrachlorostannane. The value of the mole fraction solubility at 273.15 K is 0.051.

- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109-115.
- Howald, R. A.; Willard, J. E. J. Am. Chem. Soc. 1955, 77, 2046-2049.

- (1) Hydrogen chloride; HCl; [7647-01-0]
- (2) Tetrachlorostannane; SnCl₄; [7646-78-8]

ORIGINAL MEASUREMENTS:

Howald, R. A.; Willard, J. E.

J. Am. Chem. Soc. 1955, 77, 2046 - 2049.

VARIABLES:

T/K: 273, 300 P/kPa: not given

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's Constant ¹ K x 10 ⁵	Mol Fraction ²
273	6.6 ± 0.5	0.050
300	5.2 ± 1.	0.040

 $x = x_1/(p_1/mmHg)$

The pressures of the measurements were not stated. They could have been as low as $40~\mathrm{mmHg}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility study was a very small part of the paper. The complete statement about the solubility measurement is as follows: "the solubility of HCl in SnCl4 was determined by measuring the pressure exerted by a known amount of HCl metered into a flask of known volume containing a known amount of SnCl4."

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen chloride. Matheson Co. Gas taken from cylinder.
- (2) Tetrachlorostannane. Source not given. Chemically pure, and analyzed anhydrous.

ESTIMATED ERROR:

Mol fraction solubility calculated for a partial pressure of HCl of 101.325 kPa (760mmHg). The compiler assumed a linear function of mole fraction vs. pressure up to 760 mmHg.

- 1. Hydrogen chloride; HCl; [7647-01-0]
- 2. Tetrachlorostannane; SnCl₄;
 [7646-78-8]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	$n_{\rm HCl}/n_{\rm SnCl}_4$	$x_{\sf HCl}$
243.15	0.115	0.103
253.15	0.092	0.0842
263.15	0.076	0.0706
273.15	0.065	0.0610
283.15	0.058	0.0548
293.15	0.053	0.0503

Smoothed Data: $\ln \chi_{HC1} = -34.460 + 47.835/(T/100) + 14.087 \ln (T/100)$

Standard error about regression line 3.49 \times 10⁻⁴

T/K	Mol Fraction
	X _{HC1}
243.15 253.15 263.15 273.15 283.15	0.103 0.0838 0.0705 0.0613 0.0548 0.0502
298.15	0.0485

The mole fraction solubilities were calculated from the mole ratio by the

compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen chloride was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

For the two lowest temperatures the gas absorbed was determined by a chemical titration.

The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. The HCl was dried by passage through concentrated sulfuric acid.
- Tetrachlorostannane. Best obtainable specimen was suitably purified, dried, fractionally distilled, and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2 \delta X/X = 0.005$$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

COMPONENTS: 1. Hydrogen chloride; HCl; [7647-01-0] 2. Titanium chloride; TiCl₄; [7550-45-0] VARIABLES: T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109 - 115. W. Gerrard

EXPERIMENTAL VALUES:	<u>T/K</u>	Mol Ratio	Mol Fraction XHC1
	243.15	0.105	0.0950
	253.15	0.080	0.0741
	263.15	0.064	0.0602
	273.15	0.054	0.0512
	283.15	0.047	0.0449
	293.15	0.040	0.0385

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HC1} = -28.984 + 41.417/(T/100) + 10.794 \ln (T/100)$

Standard error about regression line 7.31 \times 10⁻⁴

T/K	Mol Fraction
	XHCl
243.15	0.0945
253.15	0.0745
263.15	0.0608
273.15	0.0511
283.15	0.0441
293.15	0.0389
298.15	0.0368

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen chloride was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K. The procedure and apparatus are described by Gerrard (1,2).

For the first three temperatures a chemical titration was carried out.

SOURCE AND PURITY OF MATERIALS:

 Hydrogen chloride. Obtained from a cylinder containing a good commercial specimen. Was dried by passage through concentrated sulfuric acid.

(smoothed data calculated by H.L. Clever)

 Titanium chloride. Best obtainable specimen was suitably purified, dried, and fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- 1. Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

The Solubility of Hydrogen Bromide in Organic Solvents

Alkanes

Solubility in hexane was measured by Fontana & Herold (1) at 278.15 K and 293.15 K over the pressure range 41.4 kPa to 213.7 kPa and by Boedeker & Lynch (2) at 298.15 K, 308.15 K and 318.15 K over the pressure range 6.7 kPa to 93.3 kPa. Results were expressed as Henry's constants. Mole fraction solubilities at a partial pressure of 101.3 kPa from the sets of data may be fitted to the equation:

$$\ln x_{HBr} = -44.591 + 2912.4/(T/K) + 5.5481 \ln(T/K)$$

This equation is based upon data for the temperature range 278.15 K to 318.15 K. Extrapolation outside this range may lead to error. The standard deviation in values of $x_{\rm HBr}$ is 0.00089.

Solubility in decane at a total pressure of 101.3 kPa over the temperature range 243.15 K to 293.15 K has been measured by Ahmed et al.(3) and at 298.15 K to 319.15 K in the pressure range 6.7 kPa to 92.3 kPa by Boedeker & Lynch (2). The latter reported Henry's constants for three temperatures rather than measurements of solubility at individual pressures. Mole fraction solubilities at a partial pressure of 101.3 kPa from these Henry's constants show good consistency with values for lower temperature from Ahmed's data. The mole fraction solubility at 101.3 kPa by extrapolation of values based upon Ahmed's data is 0.0497 compared with the value of 0.0519 from the Henry's constant at this temperature published by Boedeker & Lynch. Mole fraction solubilities at 101.3 kPa from the two sources may be fitted to the equation:

```
\ln x_{HBr} = -73.774 + 4380.1/(T/K) + 9.8532 \ln(T/K)
```

The standard deviation in values of $x_{\rm HBr}$ is 0.0020.

Solubility in butane at 278.15 K and 298.15 K over a pressure range from 41.4 kPa to 213.7 kPa was measured by Fontana & Herold (1). Solubility in octane at partial pressures from 0.067 to 93.3 kPa at 298.15 K, 308.15 K and 318.15 K was measured by Boedeker & Lynch (2). In each case data were reported as Henry's constants from which mole fraction solubilities at a partial pressure of 101.3 kPa may be calculated.

Solubility in heptane at a total pressure of 101.3 kPa over a temperature range from 233.15 K to 293.15 K was measured by Ahmed et al.(3).

Mole fraction solubilities at $298.15~\mathrm{K}$ for a partial pressure of hydrogen bromide of 101.3 kPa, on the basis of the available data, are as follows:

```
butane 0.0332
hexane 0.0402
heptane 0.0446 (extrapolated and corrected to P<sub>HBr</sub> = 101.3 kPa)
octane 0.0448
decane 0.0527
(reference value from Raoult's law equation = 0.0410)
```

Mole fraction solubilities at this temperature are close to the reference value from the Raoult's law equation and show an increase in mole fraction solubility with increase in carbon number of the solvent. The solubilities of hydrogen chloride in alkanes are also close to reference line values but, in this case, the data do not clearly indicate an increase with carbon number of the alkane.

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

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January 1989

CRITICAL EVALUATION:

The available data for solubilities of hydrogen bromide in butane, heptane and octane are consistent with measurements of the solubilities of this gas in hexane and in decane which have been studied by more than one group. Solubilities in these three solvents may be accepted on a tentative basis.

Fontana & Herold (1) also showed that the mole fraction solubility in butane and in hexane are reduced in the presence of aluminium bromide under the conditions of their measurements. The accuracy of these additional measurements cannot be evaluated.

Aromatic hydrocarbons

Mole fraction solubilities in aromatic hydrocarbons at a partial pressure of gas of 101.3 kPa over the temperature range in which measurements are available lie above the reference line based upon the Raoult's law equation and increase in the order:

benzene < methylbenzene < 1,3-dimethylbenzene < 1,3,5-trimethylbenzene

Solubility in benzene in the range 263.15 K to 293.15 K at a total pressure of 101.3 kPa was measured by Ahmed et a1.(3). O'Brien & Bobalek (4) reported solubility at 298.15 K over the partial pressure range 0.111 kPa to 57.2 kPa, Kapustinskii & Mal'tsev (5) at 303.15 K & 323.15 K over the range 1.02 kPa to 84.35 kPa and Brown & Wallace (6) at 278.85 K at pressures to 20 kPa. Ahmed's data have been corrected to give values of the mole fraction solubility at a partial pressure of 101.3 kPa. Other data have been extrapolated to this pressure. The smoothing equation for mole fraction solubility at a partial pressure of 101.3 kPa based upon the data available for the temperature range 263.15 K to 323.15 K is:

 $\ln x_{\text{HD}} = 115.68 - 3357.2/(T/K) - 18.780 \ln(T/K)$

Values of $x_{\rm HBr}$ fit this equation with a standard deviation of 0.0054.

Ahmed et al.(3) have also reported the solubility in methylbenzene at a total pressure of 101.3 kPa in the temperature range 233.15 K to 293.15 K. O'Brien & Bobalek (4) measured the solubility at 298.15 K over a partial pressure range of 19.47 kPa to 47.73 kPa and Brown & Wallace (6) at 273.15 K and pressures to 18.7 kPa. Mole fraction solubilities by extrapolation or by correction to a partial pressure of 101.3 kPa may be fitted to the equation:

 $\ln x_{\text{HBr}} = 71.850 - 1427.6/(T/K) - 12.212 \ln(T/K)$

Values of $x_{\rm HBr}$ fit this equation with a standard deviation of 0.0091.

Ahmed et al.(3) measured the solubility in 1,3-dimethylbenzene at a total pressure of 101.3 kPa over the temperature range 233.15 K to 293.15 K. The difference between these measurements and the solubility at a partial pressure of gas of 101.3 kPa is likely to be less than experimental error. The mole fraction solubility for a partial pressure of 101.3 kPa at 273.15 K based upon these measurements is 0.134. This differs from the value of 0.204 corresponding to the Henry's constant from measurements to 15.3 kPa reported by Brown & Wallace (6) and based upon the assumption that the variation of mole fraction solubility with pressure is linear to 101.3 kPa. If the variation approximates to that expressed by the Margules equation then the mole fraction solubility at 101.325 kPa, corresponding to Brown & Wallace's measurement, would be about 0.16. This is closer to Ahmed's value.

Ahmed's data are likely to give a better measure of the solubility at a partial pressure of $101.3~\mathrm{kPa}$. They should be treated as tentative values until further measurements on the system are available.

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

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January 1989

CRITICAL EVALUATION:

Brown & Wallace (6) also measured the solubility in 1,3,5-trimethylbenzene at 273.15 K to 14.67 kPa. Measurements indicate that, to this pressure at least, solubility is greater than in 1,3-dimethylbenzene. Linear extrapolation to a partial pressure of 101.3 kPa gives a value of the mole fraction solubility of 0.226. If, however, the variation of mole fraction solubility with change of partial pressure approximates to the Margules equation then the mole fraction solubility at a partial pressure of 101.3 kPa would be about 0.17. These extrapolated values should be considered to be of semi-quantitative significance only.

Alkanols

Mole fraction solubilities in alkanols at a partial pressure of 101.3 kPa are appreciably higher than values represented by a reference line based upon the Raoult's law equation applied to hydrogen bromide. Mole fraction solubilities of hydrogen chloride show similar high values relative to the corresponding reference line for hydrogen chloride.

The mole fraction solubility in ethanol from data reported by Dorofeeva (7) is 0.285 at 298.15 K. It is not clear whether this corresponds to a total or to a partial pressure of 101.325 kPa as no details of the measurements were given. No other measurements of the solubility of hydrogen bromide in this solvent are available for comparison. The value is low in comparison with solubilities in higher alkanols and in chlorinated ethanols discussed below. Further measurements are needed.

Solubility in 1-octanol at a total pressure of 101.3 kPa was measured by Ahmed et al.(3) for the temperature range 213.15 K to 293.15 K. The partial pressure of the solvent makes insignificant contribution to the total pressure in this temperature range. Solubility at a partial pressure of 101.3 kPa in the range 288.15 K to 333.15 was measured by Fernandes (8). There is good agreement between solubilities over the few degrees in which the measurements overlap. At 288.15 K the interpolated value of mole fraction solubility from Ahmed's data is 0.530. The value given by Fernandes is 0.519. However the slopes of the curves of mole fraction solubility against temperature differ in the two cases so that extrapolated data from one source are not compatible with data from the other source. (fig. 1)

Mole fraction solubilities for a partial pressure of 101.3 kPa from the two sources may be represented by the equation :

 $\ln x_{HBr} = 31.5861 - 892.58/(T/K) - 5.1505 \ln(T/K)$

The standard deviation in values of $x_{\rm HBr}$ is 0.021.

In view of the differences between the two sets of data this equation is considered to be tentative. It should not be used to estimate solubilities outside the temperature range of $213.15~\rm{K}$ to $333.15~\rm{K}$.

Fernandes (7) also reported solubilities at a partial pressure of 101.3 kPa over temperature ranges of various extent in 1-pentanol, 1-hexanol, 1-heptanol, 1-nonanol, 1-decanol, 1-dodecanol. 1-tetradecanol and 1-hexadecanol. Variation of mole fraction solubility with chain length is rather irregular as may be seen below:

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

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January 1989

CRITICAL EVALUATION:

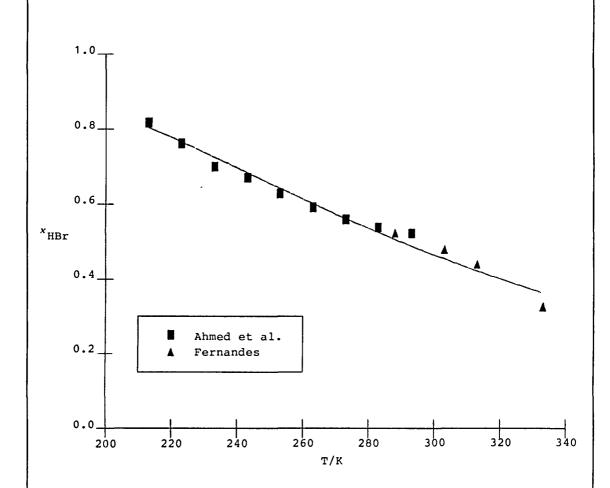


Figure 1

Variation with temperature of the mole fraction solubility in 1-octanol of hydrogen bromide at a partial pressure of 101.3 kPa.

(see refs. 3 & 8)

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

1-pentanol	0.334
1-hexanol	0.318
1-heptanol	0.305
1-octanol	0.322
1-nonanol	0.325
1-decanol	0.351
1-dodecanol	0.351
1-tetradecanol	0.301
1-hexadecanol	0.301

The solubility in 2,2-dimethyl-1-propanol at 268.15 K to 283.15 K was reported by Whitmore & Rothrock (9) as an incidental part of a study of chemical reaction. The pressure of hydrogen bromide was probably about 101.3 kPa. The mole fraction solubility at 283.15 K, calculated from these data, is 0.286. This may be compared with the value of 0.533 for the isomeric 1-pentanol, by extrapolation of Fernandes' data. Data for solubility of hydrogen chloride in 2,2-dimethyl-1-propanol are not available for comparison but the solubility of hydrogen chloride at a partial pressure of 101.3 kPa, at temperatures around 283.15 K, in the isomeric branched chain alcohol, 2-methyl-1-butanol, is close to that in 1-pentanol. Solubility of hydrogen chloride in 2-methyl-1-propanol is also close to that in 1-butanol. In the absence of any supporting evidence for low solubility of hydrogen halides in 2,2-dimethyl-1-propanol, compared with solubility in isomeric alcohols, the data reported by Whitmore and Rothrock should be rejected.

Substitution of chlorine into an alcohol lowers the solubility of hydrogen chloride in that alcohol. The solubility of hydrogen bromide in 2-chloroethanol, 2,2-dichloroethanol and in 2,2,2-trichloroethanol have been reported by Gerrard & co-workers for a pressure of 101.3 kPa within the temperature range of 253.15 K to 312.15 K. The work shows that mole fraction solubility decreases with increase in chlorine content. Data for solubility in 2,2,2-trichloroethanol are contained in two papers from the same laboratory with some disagreement between the two sets of data at the higher end of the temperature ranges. Mole fraction solubilities at 273.15 K, 283.15 K and 293.15 K from the earlier paper (10) are respectively 0.161, 0.130 and 0.0944. Values for these temperatures from the later paper (11) are, respectively, 0.149, 0.133 & 0.128.

The mole fraction solubility of hydrogen bromide in ethanol at 298.15 K and 101.325 kPa, from Dorofeeva's measurements discussed above, does not fit into the pattern. This value of 0.285 is less than the corresponding value of 0.377 for dissolution in 2-chloroethanol. The data for the chlorinated compound are likely to be the more reliable.

Ethers

The solubility in 1,1'-oxybisoctane was measured by Ahmed, Gerrard & Maladkar (11) at a total pressure of 101.3 kPa over the temperature range 223.15 K to 293.15 K. Data are self-consistent. Mole fraction solubility is very high, as is the solubility of hydrogen chloride in alkyl ethers under similar conditions. No other data for solubility of hydrogen bromide are available for comparison but these data may be accepted on a tentative basis.

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

Alkanoic acids

Ahmed, Gerrard & Maladkar (11) reported solubilities in acetic acid and in hexanoic acid at a total pressure of 101.3 kPa and over temperature ranges of 253.15 K to 293.15 K and 223.15 K to 293.15 K respectively. Mole fraction solubilities lie above the reference line corresponding to the Raoult's law equation. Values for hexanoic acid are greater than those for acetic acid. This is consistent with the observation that mole fraction solubilities of hydrogen chloride in alkanoic acids increase with chain length. At 293.15 K the value for acetic acid is 0.324 and that for hexanoic acid is 0.398. These data should be accepted on a tentative basis.

<u>Halogenated</u> alkanes

Howland $et\ al.(12)$ measured solubilities in trichloromethane over the temperature range 273.15 K to 298.15 K at partial pressures from 20.7 kPa to 88.5 kPa. They also measured solubilities in tetrachloromethane over this temperature range at pressures from 39.7 kPa to 74.0 kPa. The values of Henry's constant which were reported may be used to estimate mole fraction solubility at a partial pressure of 101.3 kPa.

Ahmed $et\ al.(11)$ measured solubilities in these two solvents at a total pressure equal to 101.3 kPa over the temperature range 233.15 K to 293.15 K. Values of mole fraction solubilities at a partial pressure of 101.3 kPa may be estimated from these data by allowing for the vapor pressure of the solvents.

Mole fraction solubilities at a partial pressure of 101.3 kPa from the two sources are in reasonably good agreement for trichloromethane over the temperature range in which measurements overlap. The value of the mole fraction solubility at 273.15 K under a partial pressure of hydrogen bromide of 101.3 kPa is 0.0734 from Howland's data and 0.077 from Ahmed's data. Mole fraction solubilities for the temperature range 233.15 K to 298.15 K may be represented by the equation:

 $\ln x_{HBr} = -58.395 + 3772.6/(T/K) + 7.4877 \ln(T/K)$

The standard deviation in values of $x_{\rm HBr}$ is 0.0015.

The agreement between mole fraction solubilities in tetrachloromethane at a partial pressure of 101.3 kPa and based upon data from the two sources is less satisfactory. Values from Howland's data are about 14% greater than values from Ahmed's data, extrapolated to 298.15 K. The two values for 273.15 K are 0.0628 and 0.054 respectively. The relative merits of the two sources of data cannot be judged. The available data may be represented by the equation:

 $\ln x_{HBr} = 17.294 + 684.90/(T/K) - 4.0365 \ln(T/K)$

Values of $x_{\rm HBr}$ fit this equation with a standard deviation of 0.0061.

Disparity between the data from the two sources should be borne in mind when this equation is used.

Ahmed et al.(11) also measured solubilities in dichloromethane at a total pressure of 101.3 kPa over the temperature range 233.15 K to 293.15 K. The pure solvent has a vapor pressure at 293.15 K of 46.8 kPa. Mole fraction solubilities at a partial pressure of 101.3 kPa lie close to values for trichloromethane at the same temperature but are higher than values for tetrachloromethane. Mole fraction solubilities at 273.15 K for

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

tetrachloromethane and for trichloromethane based upon the above equations and the value for dichloromethane based upon Ahmed's data are as follows:

tetrachloromethane 0.058
trichloromethane 0.076
dichloromethane 0.069
(reference value from the Raoult's law equation = 0.078)

Solubility in iodomethane at a total pressure of 101.3 kPa over the temperature range 254.65 K to 293.15 K was measured by Maladkar (13). The solubility at 273.15 K and a partial pressure of 101.3 kPa, obtained by correcting the measurements to allow for the partial pressure of the solvent, is 0.12. No other data on this system are available for comparison.

Solubility at a total pressure of 101.3 kPa was measured by Maladkar (13) in 1-bromopropane at 273.15 K to 293.15 K and in 1-bromobutane and 1-bromohexane at 273.15 K. Ahmed et al. (11) reported the solubility in 1-bromooctane also at a total pressure of 101.3 kPa over the range 233.15 K to 293.15 K. Maladkar also measured solubility in 1-iodopropane at this total pressure for the temperature range 253.15 K to 293.15 K. Mole fraction solubilities at 273.15 K and a partial pressure of hydrogen bromide of 101.3 kPa, based upon measurements on these solvents, are as follows:

1-bromopropane 0.139 1-bromobutane 0.153 1-bromohexane 0.170 1-bromooctane 0.141 1-lodopropane 0.141

These values are greater than values of mole fraction solubilities in alkanes of the same carbon number at this temperature. 1-Bromopropane is highly volatile at the highest temperature of measurement (vapor pressure 14.6 kPa at 293.15 K). The other three alkyl bromides are not appreciably volatile at the temperatures at which solubilities were determined. Measurements were made at three temperatures in the case of this solvent and at one temperature in the case of 1-bromobutane and of 1-bromohexane. Measurements were made at seven temperatures in the case of 1-bromooctane and are self-consistent over this range. Solubility data for this last solvent may therefore be more reliable than data for the other three solvents and may be accepted on a tentative basis. The data for the other 1-bromoalkanes should be considered to be of semi-quantitative significance until the measurements are confirmed by other workers. Solubility in 1-iodopropane was measured at five temperatures. The measurements are also self consistent and may be accepted on a tentative basis.

Solubilities in 1-chlorooctane and in 1-iodooctane were also reported by Ahmed et al.(11) for a total pressure of 101.3 kPa and a temperature range of 213.15 K to 293.15 K. Mole fraction solubilities in these two solvents are greater than in 1-bromooctane in the overlapping temperature range. At 273.15 K mole fraction solubilities from these measurements are:

1-bromooctane 0.141; 1-chlorooctane 0.194; 1-iodooctane 0.200.

The data for the chloro and the iodo compound are also self consistent and may be accepted on a tentative basis.

Maladkar (13) measured solubilities in 1,2-dibromoethane, 1,3-dibromopropane, 1,4-dibromobutane, and 1,6-dibromohexane at 273.15 K and a total pressure of 101.3 kPa. The partial pressures of the solvents were insignificant at this temperature. Mole fraction solubilities increase with carbon number of the solvent and may be accepted on a

COMPON	HENTS:	EVALUATOR:
1.	Hydrogen Bromide; HBr; [10035-10-6]	Peter G. Departme
2.	Organic Solvents	Polytech

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January 1989

CRITICAL EVALUATION:

tentative basis. Maladkar also measured the solubility in 1,2-dichloroethane at this pressure but over the temperature range 233.15 K to 273.15 K. These measurements may also be accepted on a tentative basis. The mole fraction solubility at 273.15 K in this solvent, corrected to give the value for a partial pressure of 101.3 kPa, is 0.114 compared with a value of 0.124 for solubility in 1,2-dibromoethane.

Halobenzenes

Ahmed $et\ al.$ (11) reported solubilities at a total pressure of 101.3 kPa in chlorobenzene, bromobenzene and iodobenzene for the temperature range 233.15 K to 293.15 K. Mole fraction solubilities increase under these conditions in the order:

chlorobenzene < bromobenzene < iodobenzene.

This is contrary to the trend indicated from data for solubility of hydrogen chloride in halobenzenes. However these data for hydrogen bromide solubilities are self consistent and may be accepted on a tentative basis.

Nitrogen compounds

Ahmed, Gerrard & Maladkar (11) measured the solubility of hydrogen bromide in nitrobenzene at a pressure of 101.3 kPa and at four temperatures from 263.15 K to 293.15 K. O'Brien & Bobalek (4) measured solubility in 1-methyl-2-nitrobenzene and 1-methyl-3-nitrobenzene at 298.15 K over pressure ranges below barometric pressure. The mole fraction solubility in nitrobenzene at 298.15 K by extrapolation of Gerrard's data is 0.0997 which is greater than the values for mole fraction solubility in 1-methyl-2-nitrobenzene and 1-methyl-3-nitrobenzene of 0.0941 and 0.0881 respectively. In the case of data for mole fraction solubilities of hydrogen chloride in these compounds the corresponding value for nitrobenzene is less than values for the methyl nitrobenzenes. Despite this apparent inconsistency these data for dissolution of hydrogen bromide may be accepted on a tentative basis.

Solvents containing sulfur

Frazer & Gerrard (14) reported solubilities at 273.15 K and a total pressure of 101.3 kPa in thiols and sulfides. Mole fraction solubilities were, in each case, above the reference values from the Raoult's law equation. The pattern of solubilities is similar to that for hydrogen chloride. Values for thiols are less than those for sulfides and values for aromatic compounds less than those for non-aromatic compound i.e.

Mole fraction solubilities at 273.15 K, corrected where necessary, at a partial pressure of 101.3 kPa

thiophene	0.126	
benzenethiol	0.153	
1,1'-thiobisbenzene	0.187	
2-propanethiol	0.248	
1-butaneth10l	0.261	
2,2'-thiobispropane	0.734	
1,1'-thiobisbutane	0.717	
(reference value from	the Raoult's law equation	0.078)

The overall pattern of these data is likely to be reliable but individual values for the different solvents must be considered to be tentative values.

Ahmed (15) measured the solubility of hydrogen bromide in liquid sulfur dioxide over the temperature range 228.15 K to 253.15 K in addition to measuring the solubility of hydrogen chloride in this solvent over a

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Organic Solvents

EVALUATOR:

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January 1989

CRITICAL EVALUATION:

similar temperature range. Despite liquid hydrogen bromide having a higher vapor pressure than hydrogen chloride at the same temperature the measurements indicate that hydrogen bromide has the lower mole fraction solubility. Further work on these two systems is desirable and these data should be considered to be of semi-quantitative significance until they can be verified by other workers.

Solvents containing boron

Gerrard et al.(10) measured the solubility of hydrogen bromide in tripentyl borate over a temperature range at a total pressure equal to barometric pressure in addition to measuring the solubility of hydrogen chloride in this solvent under similar conditions. Mole fractions solubilities are greater in the case of hydrogen bromide. This is to be expected because of the lower volatility of liquid hydrogen bromide at the same temperature. In each case experimental values are greater than those calculated from the Raoult's law equation. The variation of mole fraction solubility with variation of temperature shows a similar relationship to the reference line based upon the Raoult's law equation for hydrogen bromide as does the variation of mole fraction solubility of hydrogen chloride to the reference line for that gas. The measurements are likely to be reliable but no comparison with independent measurements on this system is possible.

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- 3. Ahmed, W.; Gerrard, W. J. Appl. Chem. 1970, 20, 109-115.
- 4. O'Brien S. J.; Bobalek, E. G. J. Am. Chem. Soc. 1940, 62, 3227-3230.
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- Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121.
- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109-115.
- Howland, J. J.; Miller, D. R.; Willard, J. E. J. Am. Chem. Soc. 1941, 63, 2807-2811.
- 13. Maladkar, V. K. Thesis, 1970, University of London.
- 14. Frazer, M. J.; Gerrard, W. Nature, 1964, 204, 1299-1300.
- 15. Ahmed, W. Thesis, 1970, University of London.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Butane; C_4H_{10} ; [106-97-8]

ORIGINAL MEASUREMENTS:

Fontana, C. M.; Herold, R. J.

J. Am. Chem. Soc. 1948, 70, 2881 - 2883.

VARIABLES:

T/K: 278.15, 298.15 P/kPa: 41.4 - 213.7 (6 - 31 psia)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's	Constants	Mol Ratio	Mol Fraction
	K/psia	K/atm	n_1/n_2	x_1
278.15	326	22.18	0.0472	0.0451
298.15	443	30.14	0.0343	0.0332

The Henry's constant, K/atm, the mole ratio and mole fraction values were calculated by the compiler. The mole ratio and mole fraction values are for a partial pressure of $101.325~\mathrm{kPa}$ (1 atm).

Henry's constants:

K/psia = $(p_1/psia)/x_1$ where psia is pounds per square inch absolute. K/atm = $(p_1/atm)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a stainless steel solubility bomb, 217.5 cm³ capacity, fitted with a charging and pressure measuring apparatus. A weighed amount of butane was added to the bomb and its vapor pressure was measured. Hydrogen bromide was added from a weighed container, a second weighing giving the amount added, and the pressure was measured

The solubility values at 298.15 K were shown on a graph. The Henry's constants were tabulated.

The heat of solution was stated to be $-2.51 \text{ kcal mol}^{-1} \text{ (-10.5 kJ mol}^{-1})$

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Dow Chemical Co. It was stored in a small stainless steel cylinder.
- (2) Butane. Purity 99⁺ percent. It was dried and degassed.

ESTIMATED ERROR:

COMPONENTS: (1) Hydrogen bromide; HBr;

[10035-10-6]

(2) Hexane; C_6H_{14} ; [110-54-3]

ORIGINAL MEASUREMENTS:

Fontana, C. M.; Herold, R. J.

J. Am. Chem. Soc. 1948, 70, 2881 - 2883.

VARIABLES:

278.15, 293.15 41.4 - 213.7 T/K: P/kPa:

(6 - 31 psia)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's	Constants	Mol Ratio	Mol Fraction
	K/psia	K/atm	ⁿ 1 ^{/n} 2	<i>x</i> ₁
278.15	265	18.03	0.0587	0.0555
293.15	348	23.67	0.0441	0.0422

The Henry's constant, K/atm, the mole ratio and mole fraction values were calculated by the compiler. The mole ratio and mole fraction values are for a partial pressure of 101.325 kPa (1 atm).

Henry's constants:

K/psia = $(p_1/psia)/x_1$ where psia is pounds per square inch absolute.

 $K/atm = (p_1/atm)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a stainless steel solubility bomb, 217.5 cm³ capacity, fitted with a charging and pressure measuring apparatus. weighed amount of solvent was added to the bomb and its vapor pressure was measured. Hydrogen bromide was added from a weighed container, a second weighing giving the amount added, and the pressure was measured.

The heat of solution was stated to be -3.05 kcal mol⁻¹ (-12.8 kJ mol⁻¹).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Dow Chemical Co. It was stored in a small stainless steel cylinder.
- (2) Hexane. The commercial specimen was rigorously purified and distilled; n_D^{25} , 1.3721.

ESTIMATED ERROR:

ORIGINAL MEASUREMENTS: COMPONENTS: Boedeker, E. R.; Lynch, C. C. (1) Hydrogen bromide; HBr; [10035-10-6] J. Am. Chem. Soc. 1950, 72, 3234 - 3236. (2) Hexane; C_6H_{14} ; [110-54-3] VARIABLES: PREPARED BY: T/K: 298.15 - 318.15 P/kPa: 6.67 - 93.33 W. Gerrard (50 - 700 mmHg)

EXPERIMENTAL VALUES:

T/K	Henry's Constant ¹ 10 ⁻³ K	Mol Ratio	Mol Fraction
298.15	1.64±0.02	0.0434	0.0416
308.15	1.97±0.08	0.0361	0.0349
318.15	2.20±0.08	0.0323	0.0313

¹ K/mmHg kg solution mol⁻¹. Note that the concentration of HBr is given as mol HBr per kg of solution.

The values of the mole ratio and the mole fraction at 101.325 (1 atm) HBr partial pressure were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was stated to be a modified form of that used by Howland, et al. (1). The solvent in the absorption flask was saturated with hydrogen bromide at a known pressure measured on a manometer. The hydrogen bromide in a known weight of a sample of the saturated solution was determined by a chemical titration.

be -2.62 kcal mol⁻¹ (-10.96 kJ mol⁻¹). ESTIMATED ERROR:

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Dow Chemical Co. Degassed by alternate freezing and thawing.
- (2) Hexane. Phillips Petroleum Co. b.p. at 1 atm T/K 341.9; $n_{\rm D}^{25}$ 1.3730.

 $\delta K/K = 0.05$

REFERENCES:

1. Howland, J. J.; Miller, D. R.; Willard, J. E. J. Am. Chem. Soc. 1941, 63, 2807.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109-115.

VARIABLES:

T/K: 233.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHBr/nC7H16	Mol Fraction X _{HBr}
233.15	0.220	0.180
243.15	0.148	0.129
253.15	0.108	0.0975
263.15	0.088	0.0809
273.15	0.070	0.0654
283.15	0.056	0.0530
293.15	0.047	0.0449

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HRr} = -22.304 + 34.013/(T/100) + 7.072 \ln (T/100)$

Standard Error about Regression Line = 2.42×10^{-3}

T/K	Mol Fraction
	X _{HBr}
233.15	0.177
243.15	0.131
253.15	0.100
263.15	0.0791
273.15	0.0642
283.15	0.0533
293.15	0.0452

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

For the four lowest temperatures the gas absorbed was determined by a chemical titration.

The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen bromide. High quality HBr was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide, dried by phosphorus pentoxide, and stored at 193 K.
- Heptane. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.02$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976.

COMPONENTS: (1) Hydrogen bromide; HBr; [10035-10-6] (2) Octane; C₈H₁₈; [111-65-9] VARIABLES: T/K: 298.15 - 318.15 P/kPa: 6.67 - 93.33 (50 - 700 mmHg) ORIGINAL MEASUREMENTS: Boedeker, E. R.; Lynch, C. C. J. Am. Chem. Soc. 1950, 72, 3234 - 3236. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

T/K	Henry's Constant ¹ 10 ⁻³ K	Mol Ratio	Mol Fraction
298.15	2.01 ± 0.05	0.0469	0.0448
308.15	2.33 ± 0.07	0.0404	0.0389
318.15	2.65 <u>+</u> 0.09	0.0356	0.0343

¹ K/mmHg kg solution mol⁻¹. Note that the concentration of HBr is given as mol HBr per kg of solution.

The values of the mole ratio and the mole fraction at 101.325 (1 atm) HBr partial pressure were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was stated to be a modified form of that used by Howland, et al. (1). The solvent in the absorption flask was saturated with hydrogen bromide at a known pressure measured on a manometer. The hydrogen bromide in a known weight of a sample of the saturated solution was determined by a chemical titration.

The heat of solution was stated to be $-2.49 \text{ kcal mol}^{-1} (-10.42 \text{ kJ mol}^{-1})$.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen bromide. Dow Chemical Co. Degassed by alternate freezing and thawing.
- (2) Octane. Connecticut Hard Rubber Co. Purified and distilled. B.p. at 1 atm T/K 398.15; n_D²⁵ 1.3952.

ESTIMATED ERROR:

 $\delta K/K = 0.05$

REFERENCES:

 Howland, J. J.; Miller, D. R.; Willard, J. E. J. Am. Chem. Soc. 1941, 63, 2807.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Decane; C₁₀H₂₂; [124-18-5]

ORIGINAL MEASUREMENTS:

Boedeker, E. R.; Lynch, C. C.

J. Am. Chem. Soc. 1950, 72, 3234 - 3236.

VARIABLES:

T/K: 298.15 - 318.15

P/kPa: 6.67 - 93.33 (50 - 700 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/ K	Henry's Constant ¹	Mol Ratio	Mol Fraction
298.15	2.15 ± 0.07	0.0548	0.0519
308.15	2.49 ± 0.07	0.0473	0.0452
318.15	2.75 ± 0.07	0.0428	0.0411

¹ K/mmHg kg solution mol⁻¹. Note that the concentration of HBr is given as mol HBr per kg of solution.

The values of the mole ratio and the mole fraction at 101.325 (1 atm) HBr partial pressure were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was stated to be a modified form of that used by Howland, et al. (1). The solvent in the absorption flask was saturated with hydrogen bromide at a known pressure measured on a manometer. The hydrogen bromide in a known weight of a sample of the saturated solution was determined by a chemical titration.

The heat of solution was stated to be $-2.34 \text{ kcal mol}^{-1} (-9.79 \text{ kJ mol}^{-1})$.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Dow Chemical Co. Degassed by alternate freezing and thawing.
- (2) Decane. Connecticut Hard Rubber Co. Purified and distilled. B.p. at 1 atm T/K 447.15; n_D²⁵ 1.4118.

ESTIMATED ERROR:

 $\delta K/K = 0.05$

REFERENCES:

 Howland, J. J.; Miller, D. R.; Willard, J. E. J. Am. Chem. Soc. 1941, 63, 2807.

COMPONENTS: 1. Hydrogen bromide; HBr; [10035-10-6]

2. Decane; C₁₀H₂₂; [124-18-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109-115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHBr/nC10H22	Mol Fraction X _{HBr}
243.15	0.243	0.195
253.15	0.173	0.147
263.15	0.123	0.110
273.15	0.090	0.0826
283.15	0.075	0.0698
293.15	0.059	0.0557

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HBr} = -9.021 + 17.947/(T/100)$

Standard Error about Regression Line = 2.31×10^{-3}

T/K	Mol Fraction
	X _{HBr}
243.1	5 0.194
253.1	5 0.145
263.1	5 0.111
273.1	5 0.0863
283.1	5 0.0684
293.1	5 0.0551

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

For the 3 lowest temperatures the gas absorbed was determined by a chemical titration.

The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide. High quality HBr was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide, dried by phosphorus pentoxide, and stored at 193 K.
- Decane. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.02$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Aluminum bromide; AlBr2; [7727-15-3]
- (3) Butane; C₄H₁₀; [106-97-8]

ORIGINAL MEASUREMENTS:

Fontana, C. M.; Herold, R. J.

J. Am. Chem. Soc. 1948, 70, 2881 - 2883.

VARIABLES:

278.15, 298.15 T/K: P/kPa: up to 241.3

(up to 35 psia)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Aluminum	Henry's Constants	
	Bromide Al ₂ Br ₆ mol per cent	K/psia	K/atm
278.15	0	326 346	22.18 25.54
298.15	0 2.80	443 479	30.14 32.59

Henry's constants:

 $K/psia = (p_1/psia)/x_1$ where psia is pounds per square inch absolute.

 $K/atm = (p_1/atm)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a stain-less steel solubility bomb, 217.5 cm³ capacity, fitted with a charging and pressure measuring apparatus. A weighed amount of solvent was added to the bomb and its vapor pressure was measured. Hydrogen bromide was added from a weighed container, a second weighing giving the amount added, and the pressure was measured.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Dow Chemical Co. It was stored in a small stainless steel cylinder.
- (2) Aluminum bromide. Doubly distilled from aluminum chips, sealed into ampoules under vacuum for storage until used.
- (3) Butane. Purity 99+ percent. It was dried and degassed.

ESTIMATED ERROR:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen bromide; HBr; Fontana, C. M.; Herold, R. J. [10035-10-6] J. Am. Chem. Soc. 1948, 70, 2881 - 2883. (2) Aluminum bromide; AlBr₃; [7727-15-3] (3) Hexane; C₆H₁₄; [110-54-3] **VARIABLES:** PREPARED BY: T/K: 278.15, 293.15 P/kPa: up to 241.3 W. Gerrard (up to 35 psia)

EXPERIMENTAL VALUES:

T/K	Aluminum Bromide	Henry's Constant	
	Al ₂ Br ₆ mol per cent	K/psia	K/atm
278.15	0 1.05	265 293	18.03 19.94
293.15	0 2.65	348 385	23.68 26.20

Henry's constants:

 ${\rm K/psia} = ({\rm p_1/psia})/x_1$ where psia is pounds per square inch absolute. $K/atm = (p_1/atm)/x_1$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a stainless steel solubility bomb, $217.5~{\rm cm}^3$ capacity, fitted with a charging and pressure measuring apparatus. weighed amount of solvent was added to the bomb and its vapor pressure was measured. Hydrogen bromide was added from a weighed container, a second weighing giving the amount added, and the pressure was measured. (3) Hexane. A commercial sample was

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Dow Chemical Co. It was stored in a small stainless steel cylinder.
- (2) Aluminum bromide. Doubly distilled from aluminum chips, sealed into ampoules under vacuum for storage until used.
- rigorously purified and distilled, $n_{\rm D}^{25}$, 1.3721.

ESTIMATED ERROR:

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Benzene; C₆H₆; [71-43-2]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Bobalek, E. G.

J. Am. Chem. Soc. 1940, 62, 3227 - 3230.

VARIABLES:

T/K: 298.15

11.11 - 57.20 P/kPa:

(83.3 - 429 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

т/к	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	83.3 125 128 170 233 429	0.097 0.162 0.167 0.226 0.302 0.477	1.13 1.01 1.01 0.99 1.02 1.18	0.00757 0.0126 0.0130 0.0176 0.0236 0.0372	0.00751 0.0125 0.0129 0.0173 0.0230 0.0359
	(760	0.971	1.03 av.	0.0757	0.0704)2

¹ k/atm mol -1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method and apparatus are those of Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HBr in the upper bulb is quantitatively removed and titrated with NaOH. The HBr partial pressure is calculated from the bulb volume and the number of moles of HBr assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

- SOURCE AND PURITY OF MATERIALS:
 (1) Hydrogen bromide. Prepared from bromine and tetralin, and passed successively over red phosphorus and phosphorus pentoxide.
- (2) Benzene. Stored over sodium and distilled, m.p. 278.63 K. Good quality.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0620 to 0.0730 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Benzene; C_6H_6 ; [71-43-2]

ORIGINAL MEASUREMENTS:

Kapustinskii, A. F.; Mal'tsev, B. A.
J. Phys. Chem. (USSR) 1940, 14,
105 - 109.

VARIABLES:

T/K: 303.15, 323.15 P/kPa: 1.016 - 84.353

(0.01003 - 0.8325 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure p ₁ /atm	Mol Fraction ^x l	Henry's Constant $K/atm = p_1/x_1$
303.15	0.01003	0.000612	16.3
	0.0835	0.005459	15.3
	0.2634	0.01649	16.0
	0.3953	0.02535	15.6
	0.4622	0.02913	15.9
	0.7455	0.04713	15.8
	[1.0	0.0633]¹	Mean: 15.8
323.15	0.1667	0.00686	24.3
	0.4243	0.01697	25.0
	.0.5339	0.02226	24.0
	0.8325	0.03418	24.4
	[1.0	0.0410 71	Mean: 24.4

¹ The 1 atm mole fraction value is based on a linear function of x_1 and p_1 .

The authors give the heat of solution of gaseous HBr in benzene as 4197 cal mol^{-1} (17.56 kJ mol^{-1}), and the heat of mixing of liquid HBr with benzene as 175 cal mol^{-1} (732 J mol^{-1})

AUXILIARY INFORMATION

METHOD 'APPARATUS/PROCEDURE:

An improved form of the apparatus described by Saylor (1) was used. Constant weight mixtures of dry hydrogen bromide and benzene were obtained after not less than five days. The weight of hydrogen bromide was determined separately in the gaseous and the liquid phases by a chemical titration.

The ICT (2) gives the vapor pressure of HBr as 26.1 atm at 303.15 K, and 40.2 atm at 323.15 K.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen bromide. Prepared by the action of water on phosphorus tribromide.
- (2) Benzene. Treated with sulfuric acid and water. Dried over sodium. Distilled, b.p./°C 80.1 - 80.3.

ESTIMATED ERROR:

- Saylor, J. H.
 J. Am. Chem. Soc. <u>1937</u>, 59, 1712.
- International Critical Tables, McGraw-Hill Co., New York, 1928, Vol. 3, p. 228.

COMPONENTS: (1) Hydrogen bromide; HBr; [10035-10-6] (2) Benzene; C₆H₆; [71-43-2] VARIABLES: P/kPa: up to 20 (150 mmHg) ORIGINAL MEASUREMENTS: Brown, H. C.; Wallace, W. J. J. Am. Chem. Soc. 1953, 75, 6268 - 6274. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES:

T/K	Highest Pressure Reported (graph) p ₁ /mmHg	Henry's Constant $K = p_1/x_1$		Mol Fraction at 101.325 kPa
	P1/mmarg	K/mmHg	K/atm	x_1
278.85	150	5920	7.79	0.128

The values of Henry's constant, K/atm, and the mole fraction solubility at one atm were calculated by the compiler.

The data were given simply as Henry's constant, K/mmHg, and as a straight line plot of x_1 and total pressure (4 points).

Henry's constant for an "ideal solution" was taken as the vapor pressure of pure liquid HBr (11850 mmHg or 15.59 atm) estimated from data reported by Bates, Halford and Anderson (1). The value from the International Critical Tables (2) is 14.3 atm.

The mole fraction solubility was calculated assuming Henry's law is obeyed up to a pressure of one atm, thus $x_1 = 1/(K/atm)$.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The amount of HBr absorbed at the observed total pressure was measured by the change in pressure in a calibrated bulb containing the gas. A high precision high vacuum apparatus was used.

The amount of solvent was probably about 0.03 mole.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Pure aluminium bromide was allowed to hydrate to approximately AlBr₃·H₂O, which was then heated in an evacuated tube. HBr was distilled from a bath at 193 K.
- (2) Benzene. The liquid may be taken as of high quality.

ESTIMATED ERROR:

- Bates, J. R.; Halford, J. O.; Anderson, L. C. J. Chem. Phys. <u>1935</u>, 3, 531.
- International Critical Tables, McGraw-Hill Co., New York, 1928, Vol. 3, p. 228.

COMPONENTS: ORIGINAL MEASUREMENTS: Ahmed, W.; Gerrard, W.; Hydrogen bromide; HBr; [10035-10-6] Maladkar, V. K. Benzene; C₆H₆; [71-43-2] J. Appl. Chem. 1970, 20, 109-115. 2. **VARIABLES:** PREPARED BY: W. Gerrard T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm) (smoothed data calculated by H.L. Clever) EXPERIMENTAL VALUES:

T/K	Mol Ratio nHBr/nC6H6	Mol Fraction X _{HBr}
263.15	0.210	0.174
273.15	0.150	0.130
283.15	0.119	0.106
293.15	0.095	0.0868

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HBr} = -55.228 + 81.862/(T/100) + 23.118 \ln (T/100)$

Standard error about regression line = 2.06×10^{-3}

T/K	Mol Fraction
	X _{HBr}
263.15	0.173
273.15	0.131
283.15	0.105
293.15	0.0872

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide. High quality
 HBr was obtained from a cylinder
 and passed through a tube at 223 K.
 For repeat runs it was prepared
 from phosphorus tribromide,
 dried by phosphorus pentoxide,
 and stored at 193 K.
- Benzene. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- Gerrard W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Methylbenzene or toluene; C7Hg; [108-88-3]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Bobalek, E. G.

J. Am. Chem. Soc. 1940, 62, 3227 - 3230.

VARIABLES: T/K: 298.15

19.47 - 47.73 P/kPa: (146 - 358 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES

т/к	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	146	0.185	1.03	0.0170	0.0167
	171	0.194	1.15	0.0178	0.0175
	210	0.286	0.97	0.0263	0.0256
	299	0.407	0.97	0.0374	0.0361
	335	0.446	0.97	0.0410	0.0394
	358	0.477	0.99	0.0439	0.0420
	(760	1.010	0.99 av.	0.0929	0.0850) ²

¹ k/atm mol-1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saylor (1) as modified by O'Brien et The main difference is the al. (2). use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HBr in the upper bulb is quantitatively removed and titrated with NaOH. The HBr partial pressure is calculated from the bulb volume and the number of moles of HBr assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- The method and apparatus are those of (1) Hydrogen bromide. Prepared from bromine and tetralin, and passed successively over red phosphorus and phosphorus pentoxide.
 - (2) Toluene. Good quality. Stored over sodium and distilled; $n_{\rm D}^{20}$, 1.4959.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0741 to 0.0866 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Methylbenzene or toluene; C₇H₈;
 [108-88-3]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Wallace, W. J.

J. Am. Chem. Soc. <u>1953</u>, 75, 6268 - 6274.

VARIABLES:

T/K: 273.15

P/kPa: up to 18.67 (140 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Highest Pressure Reported (graph)	Henry's (Mol Fraction at 101.325 kPa
	P ₁ /mmHg	K/mmHg	K/atm	$\frac{x_1}{x_1}$
273.15	140	4440	5.84	0.171

The values of Henry's constant, K/atm, and the mole fraction solubility at one atm were calculated by the compiler.

The data were given simply as Henry's constant, K/mmHg, and as a straight line plot of x_1 and total pressure (4 points).

Henry's constant for an "ideal solution" was taken as the vapor pressure of pure liquid HBr (10070 mmHg or 13.25 atm) estimated from data reported by Bates, Halford and Anderson (1). The value from the *International Critical Tables* (2) is 12.3 atm.

Note that the mole fraction solubility at 101.325 kPa (1 atm) is calculated with the assumption that Henry's law is obeyed up to a pressure of one atm, thus $x_1 = 1/(K/\text{atm})$.

For 194.65 K, the authors gave K/mmHg = 100 (0.132 atm, compiler), but they gave no information about the pressure range studied. The "ideal value" of Henry's constant was given as 404 mmHg.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

The amount of HBr absorbed at the observed total pressure was measured by the change in pressure in a calibrated bulb containing the gas. A high precision high vacuum apparatus was used.

The amount of solvent was probably about 0.03 mole.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Pure aluminum bromide was allowed to hydrate to approximately AlBr₃·H₂O, which was then heated in an evacuated tube. HBr was distilled from a bath at 193 K.
- (2) Methylbenzene. The liquid may be taken as of high quality.

ESTIMATED ERROR:

- Bates, J. R.; Halford, J. O.; Anderson, L. C. J. Chem. Phys. <u>1935</u>, 3, 531.
- International Critical Tables, McGraw-Hill Co., New York, 1928, Vol. 3, p. 228.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- Methylbenzene (toluene); C₇H_Q; [108-88-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109-115.

VARIABLES:

233.15 - 293.15

т/к: 101.325 (1 atm) Total P/kPa:

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHBr/nC7H8	Mol Fraction X _{HBr}
233.15	0.755	0.430
243.15	0.465	0.317
253.15	0.340	0.254
263.15	0.241	0.194
273.15	0.175	0.149
283.15	0.120	0.107
293.15	0.090	0.0826

The mole fraction solubilities were calculated from the mole ratio by the compiler.

 $\ln X_{HBr} = 22.521 - 22.991/(T/100) - 15.959 \ln (T/100)$ Smoothed Data: Standard Error about Regression Line = 5.45×10^{-3}

T/K	Mol Fraction X _{HBr}
233.15	0.428
243.15	0.328
253.15	0.251
263.15	0.191
273.15	0.145
283.15	0.110
293.15	0.0833

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by re-weighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

lowest temperatures the For the gas absorbed was determined by a chemical titration.

The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide. High quality HBr was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide, dried by phosphorus pentoxide, and stored at 193 K.
- 2. Methylbenzene. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.03$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976.

COMPONENTS: (1) Hydrogen bromide; HBr; [10035-10-6] (2) 1,3-Dimethylbenzene or m-xylene; C₈H₁₀; [108-38-3] | Components: | Brown, H. C.; Wallace, W. J. | | J. Am. Chem. Soc. 1953, 75, | | 6268 - 6274.

VARIABLES:

T/K: 273.15

P/kPa: up to 15.33 (115 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Highest Pressure Reported (graph)	Henry's K = p		Mol Fraction at 101.325 kPa
	p ₁ /mmHg	K/mmHg	K/atm	x_1
273.15	115	3730	4.908	0.204

The values of Henry's constant, K/atm, and the mole fraction solubility at one atm were calculated by the compiler.

The data were given simply as Henry's constant, K/mmHg, and as a straight line plot of x_1 and total pressure (4 points).

Henry's constant for an "ideal solution" was taken as the vapor pressure of pure liquid HBr (10070 mmHg or 13.25 atm) estimated from data reported by Bates, Halford and Anderson (1). The value from the *International Critical Tables* (2) is 12.3 atm.

Note that the mole fraction solubility at 101.325 kPa (1 atm) is calculated with the assumption that Henry's law is obeyed up to a pressure of one atm, thus $x_1 = 1/(K/atm)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The amount of HBr absorbed at the observed total pressure was measured by the change in pressure in a calibrated bulb containing the gas. A high precision high vacuum apparatus was used.

The amount of solvent was probably about 0.03 mole.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Pure aluminum bromide was allowed to hydrate to approximately AlBr₃·H₂O, which was then heated in an evacuated tube. HBr was distilled from a bath at 193 K.
- (2) 1,3-Dimethylbenzene. The liquid may be taken as of high quality.

ESTIMATED ERROR:

- Bates, J. R.; Halford, J. O.; Anderson, L. C. J. Chem. Phys. <u>1935</u>, 3, 531.
- International Critical Tables, McGraw-Hill Co., New York, 1928, Vol. 3, p. 228.

- 1. Hydrogen bromide; HBr; [10035-40-6]
- 1,3-Dimethylbenzene (m-xylene);
 C₈H₁₀; [108-38-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109-115.

VARIABLES:

T/K: 233.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Mol Ratio	Mol Fraction
nHBr/nC8H10	X _{HBr}
0.85	0.459
0.45	0.310
0.34	0.254
0.21	0.174
0.155	0.134
0.125	0.111
0.105	0.0950
	n _{HBr} /n _{C8} H ₁₀ 0.85 0.45 0.34 0.21 0.155 0.125

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HBr} = -27.542 + 43.370/(T/100) + 9.644 \ln (T/100)$ Standard error about regression line = 1.18 x 10⁻²

T/K	Mol Fraction
	X _{HBr}
233.15	0.460
243.15	0.321
253.15	0.234
263.15	0.177
273.15	0.139
283.15	0.112
293.15	0.0930

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

For the 4 lowest temperatures the gas absorbed was determined by a chemical titration.

The apparatus and procedure are described by Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen bromide. High quality
 HBr was obtained from a cylinder
 and passed through a tube at 223 K.
 For repeat runs it was prepared
 from phosphorus tribromide,
 dried by phosphorus pentoxide,
 and stored at 193 K.
- 1,3-Dimethylbenzene. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.03$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) 1,3,5-Trimethylbenzene or mesitylene; C₉H_{1,2}; [108-67-8]

ORIGINAL MEASUREMENTS:

Brown, H. C.; Wallace, W. J.

J. Am. Chem. Soc. 1953, 75, 6268 - 6274.

VARIABLES:

T/K: 273.15

P/kPa: up to 14.67 (110 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Highest Pressure Reported (graph)	Henry's (K = p		Mol Fraction at 101.325 kPa
	p ₁ /mmHg	K/mmHg	K/atm	$\frac{x_1}{}$
273.15	110	3370	4.434	0.226

The values of Henry's constant, K/atm, and the mole fraction solubility at one atm were calculated by the compiler.

The data were given simply as Henry's constant, K/mmHg, and as a straight line plot of x_1 and total pressure (4 points).

Henry's constant for an "ideal solution" was taken as the vapor pressure of pure liquid HBr (10070 mmHg or 13.25 atm) estimated from data reported by Bates, Halford and Anderson (1). The value from the *International Critical Tables* (2) is 12.3 atm.

Note that the mole fraction solubility at 101.325 kPa (1 atm) is calculated with the assumption that Henry's law is obeyed up to a pressure of 1 atm, thus $x_1 = 1/(K/atm)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The amount of HBr absorbed at the observed total pressure was measured by the change in pressure in a calibrated bulb containing the gas. A high precision high vacuum apparatus was used.

The amount of solvent was probably about 0.03 mole.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Pure aluminum bromide was allowed to hydrate to approximately AlBr₃·H₂O, which was then heated in an evacuated tube. HBr was distilled from a bath at 193 K.
- (2) 1,3,5-Trimethylbenzene. The liquid may be taken as of high quality.

ESTIMATED ERROR:

- Bates, J. R.; Halford, J. O.; Anderson, L. C. J. Chem. Phys. <u>1935</u>, 3, 531.
- International Critical Tables, McGraw-Hill Co., New York, 1928, Vol. 3, p. 228.

Trydrogen bronnuc in t	Ton-Aqueous corvents 471		
COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Hydrogen bromide; HBr; [10035-10-6]	Dorofeeva, N. G.		
(2) Ethanol; C ₂ H ₆ O; [64-17-5]	Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. <u>1962</u> , 5, 188-93.		
VARIABLES: $T/K = 298.15$ $p_1/kPa = 101.325$	PREPARED BY: H. L. Clever		
EXPERIMENTAL VALUES:	<u></u>		
Temperature Hydrogen Bromide $t/{}^0\mathrm{C}$ T/K /wt %	Mole Ratio Mol Fraction n_1/n_2 x_1		
25 298.15 41.2	0.399 0.285		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: No information on the solubility measurement.	SOURCE AND PURITY OF MATERIALS; ESTIMATED ERROR: REFERENCES:		

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) 2,2,-Dimethyl-1-propanol or neopentyl alcohol or t-butyl carbiol; C₅H₁₂O; [75-84-3]

ORIGINAL MEASUREMENTS:

Whitmore, F. C.; Rothrock, H. S.

J. Am. Chem. Soc. 1932, 54, 3431-5.

VARIABLES:

T/K = 268 - 283 $p_1/kPa = 101.3$

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature	2,2-Dimethy1-1-		Hydrogen bromide			
t/°C	T/K	propano wt/g	mol	wt/g	mol	Mole Ratio n_1/n_2	Mole Fraction x_1
-5	268	188	2.13	140	1.73	0.812	0.448
4	277	188	2.13	106	1.31	0.615	0.381
10	283	188	2.13	69	0.854	0.400	0.286

The compiler calculated the Kelvin temperatures, the moles of solute and solvent, the mole ratio and mole fraction solubilities. The compiler assumed a hydrogen bromide partial pressure of 101.3 kPa (1 atm).

An additional experiment at 263 K requiring 20 days resulted in a solution of mole ratio 1.03, mole fraction 0.507.

The saturated solution was heated to 65 $\,^{\circ}\mathrm{C}$ and maintained at that temperature for 20 days. Reactions took placewhich yielded several bromocompounds.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

This is not a well characterized measurement. The authors were not interested in solubility, but in obtaining the largest amount of HBr in the alcohol as possible to study the rearrangement reaction that take place at higher temperatures.

The alcohol melts at 52 °C. As HBr is passed over the alcohol a liquid forms which was cooled to 10 °C, and saturated with HBr by passing HBr through the liquid. Later the sample was cooled to 4 °C and resaturated, then to -5 °C, and saturated again. Thus all measurements were carried out on the same alcohol sample in the opposite order as presented in the table above.

The compiler assumed atmospheric pressure of the HBr as it bubbled from the solution.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. No information
- (2) 2,2,-Dimethyl-1-propanol. Prepared by reaction of t-butyl magnesium chloride plus formaldehyde. Melting point 52 °C. (ref 1).

ESTIMATED ERROR:

REFERENCES:

Beattie, R. W.
 Intermediate Laboratory of the Public Health Institute, Chicago, prepared the alcohol sample.

COMPONENTS:			ORIGINAL ME	ASUREMENTS	:
(1) Hydrogen bromide; [10035-10-6]	HBr;		Fernandes,	J. B.	
(2) Alkanols			J. Chem. En 377-379.	g. Data <u>19</u>	<u>72</u> , 17,
VARIABLES: T/K: See belo p ₁ /kPa : 101.325 (PREPARED BY	: Clever	
EXPERIMENTAL VALUES:	t/°C		Mole ratio HBr ^{/n} alcohol	Mole* fraction ^x HBr	Smoothed* mole fraction ^X HBr
1-Pentanol, (amyl alcohol); C ₅ H ₁₂ O; [71-41-0]	15 25 40 50 60 70 80	288.15 298.15 313.15 323.15 333.15 343.15 353.15	0.953 0.710 0.501	0.515 0.488 0.415 0.334 0.253	0.518 0.482 0.419 0.376 0.333 0.291 0.253
Smoothing equation for 1 1 x HBr = 38.4282 - 52 Standard error	use bet .0537/(in <i>x</i> HBr	ween 288 T/100) - about 1	8.15 K and 35 - 19.8635 ln(the regressio	3.15 K : T/100) in line = 5	.77 × 10 ⁻³
1-Hexanol; C ₆ H ₁₄ O; [111-27-3]	15 25 40 50 60 70 80	288.15 298.15 313.15 323.15 333.15 343.15 353.15	1.078 0.704 ¹ 0.4655 ¹ 0.34 ¹	0.519 0.413 0.318 0.254	0.521 0.475 0.407 0.364 0.324 0.286 0.252
Smoothing equation for ln x _{HBr} = 24.5414 - 31 Standard error	use bet .5332/(in x _{HBr}	ween 288 T/100) - about (3.15 K and 35 - 13.4652 ln(the regressio	3.15 K : T/100) n line = 8	.62 × 10 ⁻³
* calculated by the con The vapor pressure con method.			applied to th	e acid-bas	e titration
1					

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used:

Weight increase method. This method was used when the estimated vapor pressure of the alcohol was less than one mmHg. A 15-20 g sample of alcohol was placed in a clean, dry, weighed saturator and weiged. The saturator and contents were thermostatted. HBr gas was passed through the liquid for about one hour. The saturator and contents were weighed. The process was repeated until two successive readings agreed.

Acid-base titration method. The alcohol was saturated with HBr as in the weight increase method. A $1-2~{\rm cm}^3$ sample of the saturated solution was taken in a clean, dry and weighed sample tube; weighed and transferred to a flask containing a known amount of chilled standard NaOH solution. After reaction of the HBr and NaOH the excess base was titrated with a standard HCl solution.

The methods agreed within 1% by weight.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Matheson Co., Inc. Stated to be 99.8% pure. Used as received
- (2) Alkanols. K and K Labs. Reagent grade. Minimum purity 99%. Used as received.

ESTIMATED ERROR:

One percent by weight.

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COMPONENTS:
                                                       ORIGINAL MEASUREMENTS:
       Hydrogen bromide; HBr;
                                                       Fernandes, J. B.
(1)
       [10035-10-6]
                                                       J. Chem. Eng. Data 1972, 17,
                                                       377-379.
(2)
      Alkanols
EXPERIMENTAL VALUES:
                                   t/°C
                                             T/K
                                                     Mole ratio
                                                                         Mole*
                                                                                         Smoothed*
                                                                        fraction mole fraction
                                                   <sup>n</sup>HBr<sup>/n</sup>alcohol
                                                                         X
HBr
                                                                                            XHBr
1-Heptanol; C<sub>7</sub>H<sub>16</sub>O;
                                           288.15
                                    15
                                                       1.04
                                                                         0.510
                                                                                             0.513
[111-70-6]
                                     25
                                            298.15
                                                                                             0.497
                                            303.15
                                                                         0.491
                                     30
                                                        0.964
                                                                                             0.479
                                     40
                                            313.15
                                                        0.72
                                                                         0.419
                                                                                             0.429
                                     50
                                            323.15
                                                                                             0.368
                                     60
                                            333.15
                                                         0.438
                                                                         0.305
                                                                                             0.304
Smoothing equation for use between 288.15 K and 333.15 K: ln x_{\rm HBr} = 104.3866 - 146.933/(T/100) - 51.0831 ln(T/100) Standard error in x_{\rm HBr} about the regression line = 1.61 × 10<sup>-2</sup>
1-Octanol; C<sub>8</sub>H<sub>18</sub>O; [111-87-5]
                                     15
                                            288.15
                                                       1.08
                                                                        0.519
                                                                                             0.518
                                     25
                                            298.15
                                                                                             0.497
                                                       0.91
                                                                                             0.479
                                     30
                                            303.15
                                                                         0.476
                                     40
                                            313.15
                                                       0.772
                                                                         0.436
                                                                                             0.433
                                            323.15
                                     50
                                                                                             0.379
                                            333.15
                                                       0.474
                                                                         0.322
Smoothing equation for use between 288.15 K and 333.15 K: ln x_{\rm HBr} = 80.3287 - 112.5332/(T/100) - 39.6221 ln(T/100) Standard error in x_{\rm HBr} about the regression line = 4.23 × 10<sup>-3</sup>
1-Nonanol; C9H200;
                                                                                             0.511
                                            288.15
                                                        1.05
                                                                         0.512
                                                                                             0.508
[143-08-8]
                                            298.15
                                     30
                                            303.15
                                                                                             0.494
                                     40
                                            313.15
                                                        0.797
                                                                         0.444
                                                                                             0.449
                                                                                             0.388
                                     50
                                            323.15
                                     60
                                            333.15
                                                        0.481
                                                                         0.325
                                                                                             0.321
                                     70
                                           343.15
                                                                                             0.255
                                            353.15
                                                        0.242
                                                                         0.195
                                                                                             0.196
Smoothing equation for use between 288.15 K and 353.15 K: ln x_{\rm HBr} = 117.492 - 166.5975/(T/100) - 57.023 ln(T/100) Standard error in x_{\rm HBr} about the regression line = 6.80 \times 10<sup>-3</sup>
1-Decanol; C<sub>10</sub>H<sub>22</sub>O;
                                            288.15
                                                        1.06
                                                                         0.515
[112-30-1]
                                     25
                                           298.15
                                                       0.94
                                                                         0.485
                                                       0.89
                                                                         0.471
                                     30
                                           303.15
                                                                                             0.468
                                     40
                                            313.15
                                                       0.771
                                                                         0.435
                                                                                             0.434
                                                                                             0.398
                                     50
                                            323.15
                                     60
                                                                        0.351
                                                                                             0.359
                                            333.15
                                                       0.54
                                           343.15
                                     70
                                                                                             0.317
                                     80
                                            353.15
                                                        0.39
                                                                         0.281
                                                                                             0.273
                                     90
                                            363.15
                                                                                             0.229
                                   100
                                           373.15
                                                                                             0.186
                                                        0.303
                                                                        0.233
                                                                                             0.147
                                   110
                                            383.15
                                   120
                                            393.15
                                                        0.124
                                                                         0.110
                                                                                             0.112
                                   130
                                            403.15
                                                                                             0.082
                                   140
                                            413.15
                                                        0.063
                                                                         0.059
                                                                                             0.059
Smoothing equation for use between 298.15 K and 413.15 K:
\ln x_{\rm HBr} = -238.990 + 328.034/(T/100) + 220.254 \ln(T/100) - 37.688 (T/100 K)
Standard error in x_{\rm HBr} about the regression line = 6.73 × 10<sup>-3</sup>
The solubility values at 288.15 K and 373.15 K were omitted from the
smoothed data fit.
* calculated by the compiler.
```

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen bromide; HBr; Fernandes, J. B. (1)[10035-10-6] J. Chem. Eng. Data 1972, 17, (2) Alkanols 377-379. EXPERIMENTAL VALUES: t/°C T/K Mole ratio Mole* Smoothed* fraction mole fraction ⁿHBr^{/n}alcohol x HBr $x_{\mathtt{HBr}}$ 1-Dodecanol; C₁₂H₂₆O; 25 298.15 0.89 0.471 [112-53-8] 40 313.15 0.79 0.441 0.441 50 323.15 0.423 60 333.15 0.54 0.351 0.386 70 343.15 0.338 80 353.15 0.391 0.281 0.285 90 363.15 0.232 100 0.312 0.184 373.15 0.238 110 383.15 0.142 393.15 0.132 120 0.117 0.107 130 403.15 0.079 140 413.15 0.052 0.050 0.057 423.15 150 0.041 433.15 0.030 0.028 160 0.031 Smoothing equation for use between 313.15 K and 433.15 K: $\ln x_{\text{HBr}} = 116.623 - 170.943/(T/100) - 55.062 \ln(T/100)$ Standard error in x_{HBr} about the regression line = 3.64 × 10⁻² 1-Tetradecanol; C₁₄H₃₀O; 60 333.15 0.43 0.301 0.301 343.15 [112-72-1] 70 0.271 80 353.15 0.306 0.234 0.234 90 363.15 0.196 0.159 100 373.15 110 383.15 0.125 120 393.15 0.097 130 403.15 0.073 140 413.15 0.057 0.054 0.054 150 423.15 0.039 160 433.15 0.029 0.028 Smoothing equation for use between 333.15 K and 433.15 K: $\ln x_{\rm HBr} = 116.547 - 172.97/(T/100) - 54.702 \ln(T/100)$ Standard error in $x_{\rm HBr}$ about the regression line = 5.76 × 10⁻⁴ 1-Hexadecanol; C₁₆H₃₄O; 60 333.15 0.461 0.316 0.316 [36653-82-4] 70 343.15 0.245 80 0.236 0.191 353.15 0.191 90 363.15 0.150 100 373.15 0.119 110 383.15 0.094 120 393.15 0.075 130 403.15 0.061 140 413.15 0.051 0.049 0.049 Smoothing equation for use between 333.15 K and 413.15 K: $\ln x_{\rm HBr} = 9.991 - 1.153/(T/100) - 8.972 \ln(T/100)$ * calculated by the compiler.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. 1-Octanol; C₈H₁₈O; [111-87-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 213.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	T/K	Mol Ratio	Mol Fraction
		$^{\rm n}$ HBR/ $^{\rm n}$ C $_{8}$ H $_{18}$ O	$x_{\mathtt{HBr}}$
	$\overline{213.15}$	4.5	0.818
	223.15	3.20	0.762
	233.15	2.34	0.701
	243.15	2.04	0.671
	253.15	1.70	0.630
	263.15	1.45	0.592
	273.15	1.28	0.561
	283.15	1.17	0.539
	293.15	1.09	0.522

The mole fraction solubilities were calculated from the mole ratio by the compiler.

 $1n X_{HBr} = -2.427 + 4.288/(T/100) + 0.2867 ln(T/100)$ Smoothed Data: Standard error about regression line = 5.12×10^{-3}

T/K	Mol Fraction
	X
	^HBr
$\overline{213.15}$	0.820
223.15	0.759
233.15	0.708
243.15	0.664
253.15	0.627
263.15	0.594
273.15	0.566
283.15	0.541
293.15	0.519

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The gas absorbed was weighed by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For temperatures below about 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide of high quality was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide, and stored at 193 K.
- 2. 1-Octanol. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T = 0.2$ $\delta X/X = 0.01$

- Research, Lond. 1. Gerrard, W.
- 1954, 7. S20.
 2. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
 3. Gerrard, W. "Solubility of
- Gases and Liquids," Plenum Press, New York, 1976.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. 2,2-Dichloroethanol; C₂H₄OCl₂;
 [598-38-9]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. <u>1970</u>, 20, 109 - 115.

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHBr/nC2H4OCl2	Mol Fraction X _{HBr}
253.15	0.885	0.469
263.15	0.660	0.398
273.15	0.530	0.346
283.15	0.435	0.303
293.15	0.351	0.260

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HBr} = 4.027 - 1.506/(T/100) - 4.515 \ln (T/100)$

Standard error about regression line = 3.43×10^{-3}

T/K	Mol Fraction
	X _{HBr}
253.15	0.467
263.15	0.401
273.15	0.346
283.15	0.300
293.15	0.261

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The gas absorbed was weighed by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For the first two temperatures a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide of high quality was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide, and stored at 193 K.
- 2,2-Dichloroethanol.Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- 1. Gerrard, W. Research, Lond. 1954. 7. S20.
- 1954, 7, S20. 2. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
- Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1976.

COMPONENTS: (1) Hydrogen Bromide; HBr; [10035-10-6] (2) 2-Chloroethanol; C₂H₅ClO; [107-07-3] VARIABLES: T/K: 277.35 - 312.15 Total P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121. W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:			
	T/K	Mol Ratio nHBr nC2H5ClO	Mol Fraction x1
	277.35	0.776	0.437
	281.95	0.744	0.427
	285.15	0.715	0.417
	289.35	0.682	0.405
<u> </u>	294.35	0.638	0.389
	297.65	0.599	0.375
	307.15	0.541	0.351
	312.15	0.509	0.337

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 15.229 - 19.442/(T/100) - 8.864 \ln (T/100)$

Standard error about the regression line is 2.20×10^{-3}

T/K	Mol Fraction x_1
273.15	0.451
283.15	0.422
293.15	0.392
303.15	0.362
313.15	0.334

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Prepared by adding calculated amount of water to pure phosphorus tribromide (1). Dried over P2O5 and cooled to 243 K to remove traces of bromine.
- (2) 2-Chloroethanol. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.005$$

REFERENCES:

1. Gerrard, W. Research, London, 1954, 7, S20.

COMPONENTS: (1) Hydrogen bromide; HBr; Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. (2) 2,2,2-Trichloroethanol; C2H3Cl3O; [115-20-8] VARIABLES: T/K: 273.15 - 299.45 Total P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Gerrard, W.; Mincer, A. M. A.; Wyvill, P. L. J. Appl. Chem. 1960, 10, 115-121. PREPARED BY: W. Gerrard

EXPERIMENTAL VALUES: _

T/K	Mol Ratio nHBr/nC2H3Cl3O	Mol Fraction x1
273.15 275.15 279.35 285.95 291.95 299.45	0.192 0.186 0.163 0.140 0.107 0.0800	0.161 0.157 0.140 0.123 0.0967 0.0741

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 186.182 - 250.098/(T/100) - 95.980 \ln (T/100)$

Standard error about the regression line is 2.74×10^{-3}

T/K	Mol Fraction x 1
273.15	0.161
283.15	0.130
293.15	0.0944
303.15	0.0630

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen bromide. Prepared by adding calculated amount of water to pure phosphorus tribromide (1). Dried over P₂O₅ and cooled to 243 K to remove traces of bromine.

(smoothed data calculated by H.L. Clever)

(2) 2,2,2-Trichloroethanol. Carefully purified, and purity rigorously attested.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.02$$

REFERENCES:

 Gerrard, W. Research, London, <u>1954</u>, 7, S20.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. 2,2,2-Trichloroethanol;C₂H₃Cl₃O;
 [115-20-8]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

0.127

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: T/K Mol Ratio Mol Fraction n HBr/ n C₂H₃Cl₃O X_{HBr} 0.307 0.235 253.15 263.15 0.217 0.178 273.15 0.174 0.148 283.15 0.156 0.135

293.15

The mole fraction solubilities were calculated from the mole ratio by the compiler.

0.146

Smoothed Data: $\ln X_{HBr} = -101.97 + 141.75/(T/100) + 47.942 \ln (T/100)$

Standard error about regression line = 1.53×10^{-3}

T/K	Mol Fraction X _{HBr}
253.15	0.234
263.15	0.179
273.15	0.149
283.15	0.133
293.15	0.128

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen bromide was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The gas absorbed was weighed by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For the first two temperatures a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide of high quality was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide, and stored at 193 K.
- 2,2,2-Trichloroethanol. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.005$

- 1. Gerrard, W. Research, Lond. 1954, 7, S20.
- Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623.
 Gerrard, W. "Solubility of
- Gerrard, W. "Solubility of Gases and Liquids," Plenum Press, New York, 1976.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. 1,1'-Oxybisoctane or dioctyl ether; C₁₆H₃₄O; [629-82-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 223.15 - 293.15 101.325 (1 atm) Total P/kPa:

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

т/к	Mol Ratio	Mol Fraction
	ⁿ HBr/ ⁿ C ₁₆ H ₃₄ O	X _{HBr}
223.15	5.64	0.849
233.15	4.60	0.821
243.15	3.78	0.791
253.15	3.265	0.766
263.15	2.84	0.740
273.15	2.32	0.699
283.15	2.01	0.668
293.15	1.53	0.605

The mole fraction solubilities were calculated from the mole ratio by the compiler.

 $\ln X_{HBr} = 12.416 - 15.294/(T/100) - 7.145 \ln (T/100)$ Smoothed Data:

> Standard error about regression line 9.83 \times 10⁻³ T/K Mol Fraction

	X _{HBr}
223.15	0.841
233.15	0.825
243.15	0.801
252 15	0 770

253.15 0.770 263.15 0.734 0.696 273.15 283.15 0.656 293.15 0.615

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen bromide was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The gas absorbed was weighed by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For temperatures below about 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide of high quality was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide, and stored at 193 K.
- 2. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta x/x = 0.015$

- 1. Gerrard, W. Research, Lond.
- 1954, 7, S20.
 2. Gerrard, W. J. Appl. Chem.
 Biotechnol. 1972, 22, 623.
 3. Gerrard, W. "Solubility of
- Gases and Liquids," Plenum Press, New York, 1976.

- Hydrogen bromide; HBr; [10035-10-6]
- Acetic Acid; C2H4O2; [64-19-7]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 253.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction	
	$^{\mathrm{n}}$ HBR/ $^{\mathrm{n}}$ C $_{2}$ H $_{4}$ O $_{2}$	X _{HBr}	
253.15 263.15 273.15 283.15 293.15	1.14 0.87 0.73 0.60 0.48	0.533 0.465 0.422 0.375 0.324	

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln x_{HBr} = 16.788 - 19.505/(T/100) - 10.464 \ln (T/100)$

Standard error about regression line = 7.17×10^{-3}

T/K	Mol Fraction
	${}^{\mathrm{X}}{}_{\mathrm{HBr}}$
253.15	0.529
263.15	0.473
273.15	0.420
283.15	0.371
293.15	0.326

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen bromide was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The gas absorbed was weighed by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For the first two temperatures a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide of high quality was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide,
- and stored at 193 K.
 2. Acetic Acid. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.015$

- 1. Gerrard, W. Research, Lond.
- 1. Gerlaid, W. Research, Lond.

 1954, 7, S20.
 2. Gerrard, W. J. Appl. Chem.

 Biotechnol. 1972, 22, 623.
 3. Gerrard, W. "Solubility of

 Gases and Liquids," Plenum Press, New York, 1976.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. Hexanoic acid; $C_6H_{12}O_2$; [142-62-1]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 223.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

Mol Ratio	Mol Fraction
ⁿ HBr/ ⁿ C ₆ H ₁₂ O ₂	X _{HBr}
2.64	0.725
1.97	0.663
1.65	0.623
1.36	0.576
1.16	0.537
0.91	0.476
0.80	0.444
0.66	0.398
	n _{HBr} /n _{C6} H ₁₂ O ₂ 2.64 1.97 1.65 1.36 1.16 0.91 0.80

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HRr} = 11.677 - 13.476/(T/100) - 7.435 \ln (T/100)$

Standard error about regression line = 7.33×10^{-3}

Mol Fraction
X _{HBr}
0.719
0.672
0.624
0.576
0.528
0.483
0.440
0.400

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen bromide was passed into a known weight of liquid in a bubbler tube at a total pressure measured by a manometer assembly. The gas absorbed was weighed by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For the first 5 temperatures a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen bromide of high quality was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide, and stored at 193 K.
- 2. Hexanoic acid. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta x/x = 0.015$

- 1. Gerrard, W. Research, Lond.
- 1954, 7, S20.
 2. Gerrard, W. J. Appl. Chem.
 Biotechnol. 1972, 22, 623.
 3. Gerrard, W. "Solubility of
 - Gases and Liquids," Plenum Press, New York, 1976.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Haloalkanes

VARIABLES:

T/K: 233.15 - 293.15 Total P/kPa : 101.325 (1 atm)

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109-115.

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:		Mole ratio Br ^{/n} haloalk.	Mole* fraction ^x HBr	Smoothed** mole fraction *HBr
Dichloromethane, CH ₂ Cl ₂ ; [75-09-2]	233.15	0.338	0.253	0.262
	243.15	0.218	0.179	0.174
	253.15	0.142	0.124	0.119
	263.15	0.093	0.0851	0.0834
	273.15	0.060	0.0566	0.0598
	283.15	0.043	0.0412	0.0438
	293.15	0.036	0.0347	0.0327
Smoothing equation: ln $x_{ m HBr}$	= -7.132 + about the	17.892/(T/1	00) - 2.22	$14 \ln(T/100)$
Standard error in $x_{ m HBr}$		regression l	ine = 6.19	× 10^{-3}

Trichloromethane, CHCl2; 0.247 0.248 233.15 0.328 0.176 [67-66-3] 243.15 0.214 0.175 253.15 0.145 0.127 0.127 263.15 0.103 0.093 0.0937 273.15 0.078 0.072 0.0708 0.0544 283.15 0.056 0.053 293.15 0.045 0.043 0.0425

Smoothing equation: $\ln x_{\rm HBr} = -7.140 + 16.283/(T/100) - 1.462 \ln(T/100)$ Standard error in $x_{\rm HBr}$ about the regression line = 1.26 × 10⁻³

- * calculated by the compiler
- ** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K. For full description see Gerrard (2,3).

For temperatures below about 268 K a chemical titration was performed.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen bromide. High quality HBr was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide (1), dried by phosphorus pentoxide, and stored at 193 K.
- Haloalkanes. Best obtainable specimens were purified, fractionally distilled and attested.

ESTIMATED ERROR: $\delta T/K = 0.2$ $\delta x_{HBr}/x_{HBr} = 0.01-0.05$

- 1. Gerrard, W. Research, Lond. 1954, 7, S20.
- 2. Gerrard, W. J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976.

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COMPONENTS:
                                                    ORIGINAL MEASUREMENTS:
                                                    Ahmed, W.; Gerrard, W.;
(1) Hydrogen bromide; HBr;
       [10035-10-6]
                                                    Maladkar, V. K.
(2) Haloalkanes
                                                    J. Appl. Chem. 1970, 20, 109-115.
EXPERIMENTAL VALUES:
                                                                    Mole*
                                          T/K
                                                  Mole ratio
                                                                                 Smoothed**
                                               "HBr / "haloalk. fraction mole fraction
                                                                     x<sub>HBr</sub>
Tetrachloromethane; CCl<sub>4</sub>;
                                         233.15
                                                     0.19
                                                                     0.160
                                                                                      0.165
[56-23-5]
                                         243.15
                                                     0.155
                                                                     0.134
                                                                                     0.129
                                                    0.112
                                         253.15
                                                                    0.101
                                                                                     0.0991
                                         263.15
                                                    0.085
                                                                    0.078
                                                                                     0.0749
                                                                    0.052
                                         273.15 0.055
                                                                                     0.0560
                                         283.15
                                                                                      0.0415
                                                     0.042
                                                                     0.040
                                         293.15
                                                    0.033
                                                                     0.032
                                                                                      0.0305
Smoothing equation: \ln x_{\rm HBr} = 35.021 - 40.580/(T/100) - 22.935 \ln(T/100)
Standard error in x_{\rm HBr} about the regression line = 4.65 \times 10^{-3}
1,2-Dichloroethane; C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>;
                                         233.15
                                                     0.60
                                                                   0.375
[107-06-2]
                                         243.15
                                                     0.375
                                                                    0.273
                                                                                     0.274
                                                     0.250
0.180
                                         253.15
                                                                    0.200
                                                                                     0.202
                                         263.15
                                                                     0.153
                                                                                     0.150
                                                                     0.111
                                         273.15
                                                     0.125
                                                                                     0.112
Smoothing equation: \ln x_{\rm HBr} = 13.110 - 10.003/(T/100) - 11.581 \ln(T/100)
Standard error in x_{\rm HBr} about the regression line = 2.96 × 10<sup>-3</sup>
                                                  2.00
1-Chlorooctane; C<sub>8</sub>H<sub>17</sub>Cl;
                                         213.15
                                                                    0.667
                                                                                     0.704
[111-85-3]
                                         223.15
                                                     1.45
                                                                    0.592
                                                                                      0.558
                                                    0.85
                                         233.15
                                                                    0.459
                                                                                     0.448
                                                     0.58
                                         243.15
                                                                    0.367
                                                                                     0.363
                                         0.301
                                                                                     0.297
                                                                    0.237
                                                                                     0.245
                                                                    0.194
                                                                                     0.204
                                                                    0.167
                                                                                     0.171
                                         293.15
                                                 0.18
Smoothing equation: \ln x_{\rm HBr} = 2.176 + 1.598/(T/100) - 4.329 \ln(T/100) Standard error in x_{\rm HBr} about the regression line = 2.21 \times 10<sup>-2</sup>
                                         233.15
                                                    0.750
                                                                    0.429
                                                                                     0.432
1-Bromooctane; C<sub>8</sub>H<sub>17</sub>Br;
                                                    0.488
[111-83-1]
                                         243.15
                                                                    0.328
                                                                                     0.324
                                         253.15
                                                     0.330
                                                                    0.248
                                                                                     0.246
                                                                    0.188
                                         263.15
                                                    0.231
                                                                                     0.190
                                                     0.164
                                                                    0.141
                                         273.15
                                                                                     0.148
                                                                    0.127
                                         283.15
                                                     0.145
                                                                                      0.117
                                                                    0.0909
                                         293.15
                                                    0.100
                                                                                      0.094
Smoothing equation: \ln x_{\rm HBr} = 0.8425 + 5.261/(T/100) - 4.653 \ln(T/100)
Standard error in x_{\rm HBr} about the regression line = 6.91 \times 10<sup>-3</sup>
1-Iodooctane, C<sub>8</sub>H<sub>17</sub>I;
                                         213.15
                                                     2.4
                                                                   0.706
                                                                                     0.725
                                                    0.92
0.61
                                                    1.47
                                                                    0.595
[629-27-6]
                                         223.15
                                                                                     0.581
                                         233.15
                                                                    0.479
                                                                                      0.467
                                                                    0.379
                                                                                     0.377
                                         243.15
                                         253.15
                                                    0.43
                                                                   0.301
                                                                                     0.304
                                                   0.32
0.25
0.19
                                         263.15
                                                                   0.242
                                                                                     0.247
                                         273.15
                                                                    0.200
                                                                                     0.201
                                         283.15
                                                                    0.160
                                                                                     0.164
                                                  0.16
                                                                    0.138
Smoothing equation: \ln x_{\rm HBr} = 10.252 - 8.491/(T/100) - 8.707 \ln(T/100)
Standard error in x_{\rm HBr} about the regression line = 1.12 \times 10<sup>-2</sup>
 * calculated by the compiler
 ** smoothing equation and smoothed values were calculated by H.L. Clever
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- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Trichloromethane or chloroform; CHCl₂; [67-66-3]

ORIGINAL MEASUREMENTS:

Howland, J. J.; Miller, D. R. Willard, J. E.

J. Am. Chem. Soc. 1941, 63, 2807 - 2811.

VARIABLES: T/K: 273.15 - 298.15 P/kPa: 20.66 - 88.53

(155 - 664 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure Range p ₁ /mmHg	Number of Determinations	Henry's Constant ¹ 10 ⁵ K/(mmHg) ⁻¹	Mol Fraction ²
273.15	294 - 511	3	9.92 ± 0.03	0.0734
288.15	155 - 407	5	7.17 ± 0.03	0.0545
298.15	210 - 664	8	5.97 ± 0.03	0.0454

¹ Henry's constant, $K/(mmHg)^{-1} = x_1/(P_1/mmHg)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mercury manometer was attached to an absorption bulb. The solvent was added to the bulb, and the vapor pressure was determined. This pressure, p₂, was used to calculate the gas partial pressure, p1, from the total pressure, p_+ , measured by the manometer:

$$p_1 = p_t - p_2^0 (1 - x_1)$$
.

The amount of gas absorbed in a measured weight of solution withdrawn as a sample, was determined by a chemical titration.

The heat of solution was determined to be (-3.26 ± 0.30) kcal mol⁻¹ $(-13.64 \text{ kJ mol}^{-1})$.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Prepared by passing hydrogen and bromine over a hot spiral of platinum. Residual bromine was removed by mercury, and hydrogen by freezing the HBr in liquid air trap.
- (2) Trichloromethane. Merck and Co. Technical grade, purified and distilled.

ESTIMATED ERROR:

 $\delta K/K = 0.01$

² Values of the mole fraction solubility at 101.325 kPa (1 atm, 760 mmHg) calculated by the compiler.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Tetrachloromethane; CCl₄;
 [56-23-5]

ORIGINAL MEASUREMENTS:

Howland, J. J.; Miller, D. R. Willard, J. E.

J. Am. Chem. Soc. 1941, 63, 2807 - 2811.

VARIABLES:

T/K: 273.15 - 298.15 P/kPa: 39.73 - 73.99 (298 - 555 mmHg)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure Range P ₁ /mmHg	Number of Determinations	Henry's Constant ¹ 10 ⁵ K/(mmHg) ⁻¹	Mol Fraction ²
273.15	304 - 430	2	8.26 ± 0.01	0.0628
288.15	298 - 555	3	5.95 ± 0.02	0.0452
298.15	345 - 517	2	5.03 ± 0.02	0.0382

¹ Henry's constant, K/(mmHg) $^{-1} = x_1/(P_1/mmHg)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mercury manometer was attached to an absorption bulb. The solvent was added to the bulb, and the vapor pressure was determined. This pressure, p_2° , was used to calculate the gas partial pressure, p_1 , from the total pressure, p_t , measured by the manometer:

$$p_1 = p_t - p_2^0 (1 - x_1)$$
.

The amount of gas absorbed in a measured weight of solution with-drawn as a sample, was determined by a chemical titration.

The heat of solution was determined to be (-3.23 ± 0.30) kcal mol⁻¹ $(-13.51 \text{ kJ mol}^{-1})$.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Prepared by passing hydrogen and bromine over a hot spiral of platinum. Residual bromine was removed by mercury, and hydrogen by freezing the HBr in liquid air trap.
- (2) Tetrachloromethane. Merck and Co. Technical grade, purified and distilled.

ESTIMATED ERROR:

 $\delta K/K = 0.01$

 $^{^2}$ Values of the mole fraction solubility at 101.325 kPa (1 atm, 760 mmHg) calculated by the compiler.

COMPONENTS: (1) Hydrogen Bromide, HBr; [10035-10-6]		ORIGINAL ME Maladkar, V Thesis, 197	. K.	5:
		University		
(2) Alkyl halides				
VARIABLES: T/K: 253.15 - 293.15		PREPARED BY		
Total P/kPa : 101.325 (1 atm)	,	W. Ge	IIaid	
EXPERIMENTAL VALUES:	m/v	Mole ratio	Mole*	Cmoothod**
		HBr ^{/n} alk.hal.		Smoothed** mole fractio
		HBr alk.nal.	x _{HBr}	*HBr
1-Bromopropane; C ₃ H ₇ Br; [106-94-5]		0.153	0.133	0.129
[106-94-5]	283.15 293.15		0.068 0.043	0.0721 0.0418
Smoothing equation: $\ln x_{\text{HBr}} = $ Standard error in x_{HBr} about	-18.625 out the	+ 45.289/(T/ regression li	100) ne = 5.57	× 10 ⁻³
1-Bromobutane; C ₄ H ₉ Br; [109-65-9]	273.15		0.153	
1-Bromohexane; C ₆ H ₁₃ Br; [111-25-1]	273.15	0.205	0.170	
Iodomethane; CH3I; [74-88-4]	253.15			0.227
3	254.65	0.263	0.208	0 140
	263.15 273.15	0.180 0.111	0.153 0.100	0.148 0.099
	283.15	0.070	0.066	0.069
	293.15 303.15	0.0525	0.050	0.049
Smoothing equation: ln x _{HBr} = Standard error in x _{HBr} abo		+ 30.165/(T/ regression li	100) + 0.6 ne = 5.21	
1-Iodopropane; C ₃ H ₇ I:	253.15	0.325	0.245	0.250
[107-08-4]	263.15	0.242	0.195	0.187
	273.15		0.139	0.139
	283.15		0.097	0.102
	293.15 303.15	0.0825	0.076	0.074 0.054
Smoothing equation: ln x _{HBr} = Standard error in x _{HBr} abo	36.916 aut the s	- 41.575/(T/1 regression li	00) - 23.5 ne = 7.42	57 ln(T/100) × 10 ⁻³
* calculated by the compiler				

** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE
The gas was passed into a weighed amount of liquid in a bubbler tube as described by Ahmed et al.(1).
Temperature control was manual to within 0.5 K. Pressure control was within 1 mmHg. Because of the volatility of the alkyl halides, and especially for measurements at the low temperatures, the hydrogen bromide content was determined by quantitative addition of water to the bubbler assembly, and titration with silver nitrate.

The data were cited in reference (2)

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen bromide was of best quality, obtained from a cylinder, and passed through a tube at 223 K before use.
- Alkyl halides. Best specimens were dried over anhydrous calcium chloride, and freshly distilled. The purities were attested by the standard procedures.

ESTIMATED ERROR:

 $\delta x_{\rm HBr}/x_{\rm HBr} = 0.01 - 0.02$

- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109.
- Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York 1970.

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- Dibromoalkanes; C_nH_{2n}Br₂;

ORIGINAL MEASUREMENTS:

Maladkar, V. K.

Thesis, 1970 University of London

VARIABLES:

T/K: 273.15

Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

•	Nol Ratio	Mol Fraction X _{HBr}
1,2-Dibromoe	thane; C2H4	Br ₂ ; [106-93-4]
273.15	0.142	0.124
1,3-Dibromop	ropane; C ₃ H	6 ^{Br} 2; [109-64-8]
273.15	0.170	0.145
1,4-Dibromob	utane; C ₄ H ₈	Br ₂ ; [110-52-1]
273.15	0.199	0.166
1,6-Dibromoh	exane; C ₆ H ₁	2 ^{Br} 2; [629-03-8]

AUXILIARY INFORMATION

0.245

METHOD/APPARATUS/PROCEDURE:

The gas was passed into the weighed amount of liquid in a bubbler tube as described by Ahmed et al. (1). Temperature control was manual to within 0.2 K, and pressure control to within 1 mmHg.

273.15

The data were cited in reference 2.

SOURCE AND PURITY OF MATERIALS:

0.197

- Hydrogen bromide. Sample was of best quality, obtained from a cylinder, and passed through a tube at 233 K before use.
- Dibromoalkanes. The best specimens were washed and dried, and fractionally distilled under reduced pressure.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.005$$

- Ahmed, W.; Gerrard, W.;
 Maladkar, V. K.
 J. Appl. Chem. 1970, 20, 109.
- Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, <u>1976</u>.

COMPONENTS: (1) Hydrogen bromide; HBr; [10035-10-6]	ORIGINAL MEASUREMENTS: Ahmed, W.; Gerrard, W.; Maladkar, V. K.
(2) Halobenzenes	J. Appl. Chem. <u>1970</u> , 20, 109-115.
VARIABLES: T/K: 233.15 - 293.15 Total P/kPa : 101.325 (1 atm)	PREPARED BY: W. Gerrard
EXPERIMENTAL VALUES: T/K	Mole ratio Mole* Smoothed** $^{n}_{\mathrm{HBr}}/^{n}_{\mathrm{halobenz}}$ fraction mole fraction $^{x}_{\mathrm{HBr}}$ HBr
Chlorobenzene; C ₆ H ₅ Cl; 233.1 [108-90-7] 243.1 253.1 263.1 273.1 283.1 293.1	5 0.32 0.242 0.233 5 0.205 0.170 0.167 5 0.138 0.121 0.123 5 0.100 0.091 0.0930 5 0.077 0.0715 0.0715
Smoothing equation: $\ln x_{\text{HBr}} = -9.812$ Standard error in x_{HBr} about th	+ 20.312/(T/100) e regression line = 6.06×10^{-3}
Bromobenzene; C ₆ H ₅ Br; 233.1 [108-86-1] 243.1 253.1 263.1 273.1 283.1 293.1	5 0.356 0.263 0.258 5 0.230\$ 0.187 0.183 5 0.155 0.134 0.136 5 0.115 0.103 0.106 5 0.095 0.0868 0.0858
§ printed in error as 0.130 in origi Smoothing equation: $\ln x_{\rm HBr} = -41.07$ Standard error in $x_{\rm HBr}$ about th	nal paper. 6 + 61.493/($T/100$) + 16.240 ln($T/100$) e regression line = 5.10 × 10 ⁻³
Iodobenzene; C ₆ H ₅ I; 233.1 [591-50-4] 243.1 253.1 263.1 273.1 283.1 293.1	5 0.416 0.294 0.274 5 0.275 0.216 0.207 5 0.187 0.158 0.160 5 0.131 0.116 0.126 5 0.110 0.0991 0.101
Smoothing equation: $\ln x_{\text{HBr}} = -8.366$ Standard error in x_{HBr} about th	+ 17.189/(T/100) e regression line = 1.41 \times 10 ⁻²
* calculated by the compiler ** smoothing equation and smoothed	values were calculated by H.L. Clever
AUNTLTARY	INFORMATION

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K. For the four lowest temperatures the gas absorbed was determined by a chemical titration.

The apparatus and procedure are described by Gerrard (1,2).

- SOURCE AND PURITY OF MATERIALS: 1. Hydrogen bromide. High quality HBr was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide, dried by phosphorus pentoxide, and stored at 193 K.
- 2. Halobenzenes. Best obtainable specimens were purified, fractionally distilled and attested.

ESTIMATED ERROR: $\delta x_{\rm HBr}/x_{\rm HBr} = 0.02\text{-}0.05$ δT/K = 0.2

- Gerrard, W.
- J. Appl. Chem. Biotechnol. 1972, 22, 623-650. "Solubility of Gases and Liquids" Plenum Press, Gerrard, W. New York, 1976.

- 1. Hydrogen bromide; HBr; [10035-10-6]
- 2. Nitrobenzene; C₆H₅NO₂;
 [98-95-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W. Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109-115.

VARIABLES:

T/K: 263.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction X _{HBr}
263.15	0.252	0.201
273.15	0.171	0.146
283.15	0.130	0.115
293.15	0.115	0.103

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln x_{HBr} = -145.956 + 206.442/(T/100) + 68.114 \ln (T/100)$ Standard Error about Regression Line = 1.84×10^{-3}

T/K	Mol Fraction
	X _{HBr}
263.15	0.202
273.15	0.145
283.15	0.116
293.15	0.103
293.15	0.103

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen bromide was passed into a known weight of pure liquid in a bubbler tube at a total pressure measured by a manometer assembly. The absorbed gas was weighed by reweighing the bubbler tube. The temperature was manually controlled to within 0.2 K.

The apparatus and procedure are described by Gerrard (1,2).

- SOURCE AND PURITY OF MATERIALS:
- Hydrogen bromide. High quality HBr was obtained from a cylinder and passed through a tube at 223 K. For repeat runs it was prepared from phosphorus tribromide, dried by phosphorus pentoxide, and stored at 193 K.
- Nitrobenzene. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

$$\delta X/X = 0.01$$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623-650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) 1-Methyl-2-nitrobenzene or onitrotoluene; C7H7NO2; [88-72-2]

ORIGINAL MEASUREMENTS:

O'Brien, S. J., Bobalek, E. G.

J. Am. Chem. Soc. <u>1940</u>, 62, 3227 - 3230.

VARIABLES:

T/K: 298.15

2.93 - 44.40 (22.0 - 333 mmHg) P/kPa:

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES.

T/K	Pressure P1/mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction x1
298.15	22.0 28.6 43.9 60.5	0.0226 0.0300 0.0450 0.0632 0.147 0.323	1.27 1.25 1.28 1.26 1.31	0.00310 0.00411 0.00617 0.00867 0.0202 0.0443	0.00309 0.00410 0.00613 0.00859 0.0198 0.0424
	333 (760	0.758	1.32 av.		0.0941)2

 $^{^{1}}$ k/atm mol⁻¹ kg = $(p_{1}/atm)/(m_{1}/mol kg^{-1})$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saylor (1) as modified by O'Brien et al. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. The solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HBr in the upper bulb is quantitatively removed and titrated with NaOH. The HBr partial pressure is calculated from the bulb volume and the number of moles of HBr assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- The method and apparatus are those of (1) Hydrogen bromide. Prepared from bromine and tetralin, and passed over red phosphorus and then phosphorus pentoxide.
 - (2) o-Nitrotoluene. Stored over calcium oxide and distilled; $n_{\rm D}^{20}$, 1.5453.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0922 to 0.0988 for the mole fraction solubility at one atm (101.325 kPa).

- Hydrogen bromide; HBr; [10035-10-6]
- (2) 1-Methyl-3-nitrobenzene or mnitrotoluene; C7H7NO2; [99-08-1]

ORIGINAL MEASUREMENTS:

O'Brien, S. J.; Bobalek, E. G.

J. Am. Chem. Soc. 1940, 62, 3227 - 3230.

VARIABLES:

T/K: 298.15

4.29 - 65.73P/kPa: (32.2 - 493 mmHg) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Pressure P ₁ /mmHg	Molality m ₁ /mol kg ⁻¹	Henry's Constant k ¹	Mol Ratio	Mol Fraction
298.15	32.2 73.5 116	0.0315 0.0688 0.112	1.35 1.41 1.36	0.00432 0.00943 0.0154	0.00430 0.00935 0.0152
	402 493 (760	0.374 0.449 0.704	1.42 1.45	0.0513 0.0616 . 0.0966	0.0488 0.0580 0.0881) ²

¹ k/atm mol 1 kg

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saylor (1) as modified by O'Brien etal. (2). The main difference is the use of a 1 to 2 day instead of a 5 to 7 day equilibration time.

The apparatus consists of two bulbs which are separated by a tap. solvent is partially saturated with the gas, and the solution added to the lower bulb. The bulbs are partially evacuated, the tap opened, and the whole apparatus put in a thermostat from 1 to 2 days.

The tap is closed. The HBr in the upper bulb is quantitatively removed and titrated with NaOH. The HBr partial pressure is calculated from the bulb volume and the number of moles of HBr assuming ideal gas behavior. A weighed solution sample is removed from the lower bulb and titrated with NaOH.

SOURCE AND PURITY OF MATERIALS:

- The method and apparatus are those of |(1) Hydrogen bromide. Prepared from bromine and tetralin, and passed successively over red phosphorus and phosphorus pentoxide.
 - (2) m-Nitro toluene. Stored over calcium oxide, and distilled, m.p. 288.50 K, $n_{\rm D}^{20}$, 1.5460.

ESTIMATED ERROR:

 $\delta T/K = 0.02$

- 1. Saylor, J. H. J. Am. Chem. Soc. 1937, 59, 1712.
- 2. O'Brien, S. J.; Kenny, C. L. Zeurcher, R. A. J. Am. Chem. Soc. 1939, 61, 2504.

² Value calculated by the compiler from the average value of Henry's constant. Use of the high and low values of Henry's constant gives a range of 0.0864 to 0.0922 for the mole fraction solubility at one atm (101.325 kPa).

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Thiols, thioethers, thiophene and tetrahydrothiophene

VARIABLES:

T/K: 273.15

Total P/kPa : 101.3 (barometric, nearly 1 atm)

EXPERIMENTAL VALUES:

ORIGINAL MEASUREMENTS:

Frazer, M. J.; Gerrard, W.

Nature 1964, 204, 1299 - 1300

PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES;			
	т/к	Mole ratio	Mole fraction* ^X HBr
2-Propanethiol, (2-propy1mercaptan); C ₃ H ₈ S; [75-33-2]	273.15	0.29	0.225
1-Butanethiol, (<i>l-butylmercaptan</i>); C ₄ H ₁₀ S; [109-79-5]	273.15	0.35	0.259
Benzenethiol, (thiophenol, mercaptobenzene); C ₆ H ₆ S; [108-98-5]	273.15	0.18	0.153
2,2'-Thiobispropane, (d11sopropyl sulfide); C ₆ H ₁₄ S; [625-80-9]	273.15	2.76	0.734
1,1'-Thiobisbutane, (dibutyl sulfide); C ₈ H ₁₈ S; [544-40-1]	273.15	2.53	0.717
1,1'-Thiobisbenzene, (diphenyl sulfide); C ₁₂ H ₁₀ S; [139-66-2]	273.15	0.23	0.187
Thiophene, (thiofuran); C ₄ H ₄ S; [110-02-1]	273.15	0.14	0.123
Tetrahydrothiophene; C ₄ H ₈ S; [110-01-0]	273.15	1.0 (white solid	formed)

^{*} calculated by the compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

The gas was passed into a weighed amount of solvent (about 2 g) in a U-tube kept at 273.15 K. The pressure was atmospheric, approximately 1 atm. The maximum amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen bromide. Self made and carefully purifed.
- 2. Sulfur compounds. The purities were checked by boiling points and gas-liquid chromatography. After each measurement of solubility the gas was removed by treatment with water, the liquid was recovered and identified with the original compound.

ESTIMATED ERROR:

- 1. Hydrogen Bromide; HBr; [10035-10-6]
- 2. Sulfur dioxide; SO₂; [7446-09-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 228.15 - 253.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHBr/nSO2	Mol Fraction X _{HBr}
228.15 233.15 243.15 248.15 253.15	0.255 0.225 0.130 0.090 0.057	0.203 0.184 0.115 0.0826 0.0539

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HBr} = 374.219 - 467.346/(T/100) - 207.280 \ln (T/100)$

Standard Error About Regression Line = 8.03×10^{-4}

T/K	Mol Fraction X _{HBr}
223.15	0.204
233.15	0.184
243.15	0.116
253.15	0.0541

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen bromide was passed into the liquid sulfur dioxide to saturation, as determined by repeated observations. The final liquid was quantitatively treated with water, and the sulfurous acid and total bromide was determined by titrations.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen Bromide. Good quality gas was obtained from a cylinder. It was passed through a tube at 223 K before use.
- Sulfur dioxide. The best specimen was passed through tubes at 263 K, and liquefied at the required temperature.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.005$

REFERENCES:

 Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109.

- (1) Hydrogen bromide; HBr; [10035-10-6]
- (2) Boric acid, tripentyl ester or tripentyl borate; C₁₅H₃₃BO₃; [621-78-3]

ORIGINAL MEASUREMENTS:

Gerrard, W.; Mincer, A. M. A.;
 Wyvill, P. L.

J. Appl. Chem. 1960, 10, 115-121.

VARIABLES:

T/K: 273.15 - 307.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES: _

T/K	Mol Ratio HBr ^{/n} C ₁₅ H ₃₃ B	Mol Fraction x_1
273.15 280.45 285.95 288.15 290.65 298.35 306.05	0.714 0.614 0.527 0.498 0.462 0.393 0.317	0.417 0.380 0.345 0.332 0.316 0.282 0.241
307.15	0.300	0.231

The compiler calculated the mole fraction values.

Smoothed Data: $\ln x_1 = 51.682 - 66.722/(T/100) - 27.993 \ln (T/100)$

Standard error about the regression line is 3.26×10^{-3}

т/к	Mol Fraction x_1
273.15	0.417
283.15	0.362
293.15	0.307
303.15	0.253
313.15	0.206

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The liquid component was weighed in a bubbler tube. The amount of gas absorbed was determined by reweighing to constant weight. The total pressure was barometric, very nearly 1 atm (101.325 kPa).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen bromide. Prepared by adding calculated amount of water to pure phosphorus tribromide (1). Dried over P₂O₅ and cooled to 243 K to remove traces of bromine.
- (2) Boric acid, tripentyl ester. Carefully purified, and purity rigorously attested.

I STIMATED ERROR:

$$\delta x_1/x_1 = 0.01$$

REFERENCES:

 Gerrard, W. Research, London, <u>1954</u>, 7, S20.

- 1. Hydrogen Iodide; HI; [10034-85-2]
- 2. Organic Solvents

EVALUATOR.

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January 1989

CRITICAL EVALUATION

The Solubility of Hydrogen Iodide in Organic Solvents.

Alkyl halides

Ahmed, Gerrard & Maladkar (1) reported the solubility at a total pressure of 101.3 kPa over the temperature range 243.15 K to 293.15 K in 1-chlorooctane, 1-bromooctane and 1-iodooctane. Solubility in lower 1-haloalkanes at this total pressure in the range 273.15 K to 303.15 K were also reported by Maladkar (2). The lower alkyl halides which were investigated are: 1-chloropropane, 1-chlorobutane, bromoethane, 1-bromopropane, 1-bromobutane, iodomethane, iodoethane, 1-iodopropane. Mole fraction solubilities at a total pressure of 101.3 kPa show an almost consistent pattern with values increasing with chain length for each series of halides and with values increasing from chloride to bromide to iodide for a fixed alkyl group. 1-Iodopropane spoils the pattern, however, as the mole fraction solubility in this solvent is less than in iodoethane.

Under the experimental conditions the difference between solubility at 101.3 kPa total pressure and solubility at 101.3 kPa partial pressure of hydrogen iodide can be neglected in the case of the 1-halocatanes. The lower halides have, however, significant vapor pressure at the temperatures of measurement. The vapor pressure of iodomethane at 303.15 K, the highest temperature of measurement, is 64.0 kPa. That of 1-bromoethane is 53.3 kPa at 294.15 K. Other alkyl halides have lower vapor pressures at the highest temperature of the measurement of solubility. Estimation of mole fraction solubility at a partial pressure of 101.3 kPa from the value of the mole fraction solubility at a total pressure of 101.3 kPa becomes more unreliable the greater the vapor pressure of the solvent. The evaluator has used two approximate methods to correct the measurements to give solubility at a partial pressure of 101.3 kPa. One method makes use of the relationship:

$$x_{\text{HI}} = \frac{101.3 \text{ x}'_{\text{HI}}}{101.3 - (1-x'_{\text{HI}})P'_{\text{S}}/\text{kPa}}$$

 $x_{\rm HI}$ is the mole fraction solubility at a partial pressure of 101.3 kPa. $x_{\rm HI}^{\dagger}$ is the mole fraction solubility at a total pressure of 101.3 kPa. $P_{\rm S}^{\circ}$ is the vapor pressure of pure solvent at the temperature of the solubility measurement.

The other method is based upon the assumption that partial vapor pressures of solute and solvent, s, change with composition of solution according to the Margules relationships. 1.e.

$$P_{\text{HI}} = P_{\text{HI}}^{\circ} x_{\text{HI}} \exp(\alpha x_{\text{S}}^{2})$$

$$P_{\text{S}} = P_{\text{S}}^{\circ} x_{\text{S}} \exp(\alpha x_{\text{HI}}^{2})$$

$$P_{\text{total}} = P_{\text{HI}} + P_{\text{S}}$$

 ${\tt P_{HT}^{\,\circ}}$ is the vapor pressure of pure liquid hydrogen iodide.

In the case of the systems under consideration the two methods of correction give very similar values of mole fraction solubility when the vapor pressure of pure solvent is less than about 13.3 kPa (100 mmHg). The vapor pressure of pure 1-chlorobutane is 11.1 kPa (83.5 mmHg) at 293.15 K. The mole fraction solubility at a total pressure of 101.3 kPa from Maladkar's measurements is 0.160. The corrected value for a partial pressure of 101.3 kPa according to the first method of correction is 0.218. The second method gives a value of 0.217.

- 1. Hydrogen Iodide; HI; [10034-85-2]
- 2. Organic Solvents

EVALUATOR.

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January 1989

CRITICAL EVALUATION:

Corrected values obtained by either method maintain a similar pattern to the uncorrected values in cases in which the vapor pressure of pure solvent is less than 13.3 kPa (100 mmHg). The mole fraction solubility usually increases with carbon number for a particular temperature and halide series and also from chloride to iodide for a fixed carbon number. The order of the 1-10dopropane and 10doethane is, however, again inverted. pattern does not persist with the corrected values of the more volatile solvents.

The data for the 1-halooctanes published by Ahmed $et\ al.$ and measured at six temperatures are self-consistent and may be accepted on a tentative basis. The data for the more volatile solvents, obtained at three temperatures in each case, may be accepted as approximating to a general pattern for these solvents but individual measurements should be used with caution.

Solvents containing oxygen

The solubility in 1-octanol was measured by Ahmed, Gerrard & Maladkar (1) at a total pressure of 101.3 kPa in range 243.15 K to 293.15 K. Mole fraction solubility is high in this solvent which has a vapor pressure of less than 1 mmHg under the conditions of measurement. The pattern of data is similar to that for hydrogen chloride and bromide in this solvent. Measurements may be accepted on a tentative basis.

Ahmed, Gerrard & Maladkar (1) also measured the solubility of hydrogen iodide in 1,1'-oxybisoctane at a total pressure of 101.3 kPa over a
temperature range of 243.15 K to 283.15 K. Measured values are very high
relative to a reference line based upon the Raoult's law equation. The variation in mole fraction solubility over the temperature range is small and almost linear with change in temperature. The value is 0.868 at 243.15 K and 0.723 at 283.15 K. The reference value for hydrogen iodide at 283.15 K from the Raoult's law equation is 0.138. The behaviour of hydrogen chloride and bromide in dialkyl ethers is similar. Other measurements of solubilities of hydrogen iodide in ethers are not available for comparison. The data should be accepted on a tentative basis.

Ahmed, Gerrard & Maladkar (1) published solubilities at a total pressure of 101.3 kPa in acetic acid over the range 259.15 K to 283.15 K and in hexanoic acid over the range 243.15 K to 293.15 K. In common with dissolution of hydrogen halides in other solvents containing oxygen, solubility of hydrogen iodide in these two acids is high relative to the reference line based on the Raoult's law equation. The mole fraction solubility of hydrogen iodide in acetic acid, as well as that of hydrogen chloride and bromide, is less than that in hexanoic acid. These measurements may be accepted on a tentative basis.

Solvents containing sulfur

Frazer & Gerrard (3) reported solubilities in thiols and sulfides at 273.15 K and a total pressure of 101.3 kPa. Solubilities at a partial pressure of 101.3 kPa are likely to be close to the measured solubilities. Mole fraction solubilities are above the value from the Raoult's law equation and increase in the order:
 benzenethiol < 1,1'-thiobisbenzene = 2-propanethiol < 1-butanethiol</pre>

< 1,1'-thiobisbutane < 2,2'-thiobispropane.

Solubilities in the last named solvents are very high with mole fraction solubilities of 0.743 and 0.761 respectively. Frazer & Gerrard reported a similar pattern of solubilities of hydrogen chloride and of hydrogen bromide in thiols and sulfides. These data may be accepted on a tentative basis.

- 1. Hydrogen Iodide; HI; [10034-85-2]
- 2. Organic Solvents

EVALUATOR.

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Department of Applied Chemistry
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January 1989

CRITICAL EVALUATION.

Solvents containing boron

Ahmed (*) reported the solubility in trichloroborane at 273.15 K and 256.15 K at a total pressure of 101.3 kPa. Values of the mole fraction solubility, corrected to a partial pressure of 101.3 kPa, are relatively low and fall below the reference line based upon Raoult's law. According to data reported by Ahmed, the pattern of behaviour of hydrogen chloride in this solvent is similar. The general pattern of solubility of hydrogen lodide is likely to be reliable but the two individual measurements should be considered to be semi-quantitative until they are supported by other measurements on the system.

- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. <u>1970</u>, 20, 109-115.
- 2. Maladkar, V. R. Thesis, 1970, University of London.
- Frazer, M. J.; Gerrard, W. Nature, 1964, 204, 1299-1300.
- 4. Ahmed, W. Thesis, 1970, University of London.

- 1. Hydrogen iodide; HI; [10034-85-2]
- 2. 1-Octanol; C₃H₁₈O; [111-87-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard (smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	"HI/"C8H18O	x _{HI}
243.15	4.65	0.823
253.15	2.65	0.726
263.15	1.98	0.664
273.15	1.625	0.619
283.15	1.38	0.580
293.15	1.20	0.545

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HT} = -15.376 + 22.953/(T/100) + 6.456 \ln (T/100)$

Standard error about regression line = 5.15×10^{-3}

T/K	Mol Fraction
	xHI
243.15	0.819
253.15 263.15	0.732 0.666
273.15	0.616
283.15	0.577
293.15	0.548

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

For temperatures below 268 K a chemical titration was performed.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen iodide. Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus triiodide.
- 1-Octanol. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

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- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- 2. Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

- 1. Hydrogen iodide; HI; [10034-85-2]
- 2. 1,1'-Oxybisoctane or Dioctylether; $C_{16}^{H}_{34}^{O}$; [629-82-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 283.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHI/nC16H34O	Mol Fraction
242 15		
243.15 253.15	6.56 5.20	0.868 0.839
263.15 273.15	3.93 2.97	0.797 0.748
283.15	2.61	0.748

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HI} = 6.355 - 7.162/(T/100) - 3.993 \ln (T/100)$ Standard error about regression line = 8.32×10^{-3}

T/K	Mol Fraction
	X _{HI}
243.15	0.871
253.15	0.833
263.15	0.795
273.15	0.757
283.15	0.719

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

For temperatures below 268 K a chemical titration was performed.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen iodide. Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus triiodide.
- 1,1'-Oxybisoctane or Dioctylether. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen iodide; HI; [10034-85-2]
- Acetic Acid; C₂H₄O; [64-19-7]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 259.15 - 283.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	n HI/ n C2 $^{H}_{4}$ O	X _{HI}
259.15	0.78	0.438
273.15	0.625	0.385
283.15	0.61	0.379

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HT} = -2.6106 + 4.598/(T/100)$

Standard error about regression line = 1.32×10^{-2}

T/K	Mol Fraction
	XHI
263.15	0.422
273.15	0.396
283.15	0.373
293.15	0.353

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen Iodide. Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus trilodide.
- Acetic Acid. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.03$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. <u>1972</u>, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen iodide; HI; [10034-85-2]
- Hexanoic acid; C₆^H₁₂O₂; [142-62-1]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	ⁿ HI/ ⁿ C6 ^H 12	o ₂ X _{HI}
243.15	2.70	0.730
253.15	2.02	0.669
263.15	1.40	0.583
273.15	1.04	0.510
283.15	0.78	0.438
293.15	0.60	0.375

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HI} = 30.616 - 37.236/(T/100) - 17.571 \ln (T/100)$

Standard error about regression line = 5.11×10^{-3}

T/K	Mol Fraction
	XHI
243.15 253.15 263.15 273.15 283.15 293.15	0.734 0.662 0.586 0.511 0.439 0.374

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

For temperatures less than 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen iodide. Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus triiodide.
- Hexanoic acid. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

$$\delta X/X = 0.01$$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972,
 22, 623 650.
- 2. Gerrard. W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976

COMPONENTS:

ORIGINAL MEASUREMENTS:

(1) Hydrogen Iodide; HI; [10034-85-2]		Maladkar, V. K. Thesis, 1970, University of London.		
(2) Alkyl halides				
VARIABLES: T/K: 243.15 - 303.15 Total P/kPa : 101.325 (1 atm)		PREPARED BY W. Ge	: rrard	
EXPERIMENTAL VALUES:		Mole ratio	Mole* fraction *HI	
1-Chloropropane; C ₃ H ₇ Cl; [340-54-5]	283.15	0.38 0.25 0.18	0.275 0.200 0.153	0.274 0.202 0.152
Smoothing equation: $\ln x_{\text{HI}}$ Standard error $\ln x_{\text{HI}}$	= -9.895 + about the r	23.489/(T/10 regression li	0) ne = 2.52	× 10 ⁻³
1-Chlorobutane; C ₄ H ₉ Cl; [109-69-3]	283.15	0.42 0.26 0.19		0.292 0.212 0.158
Smoothing equation: ln x _{HI} Standard error in x _{HI}	= -10.244 + about the r	24.672/(T/1 regression li	00) ne = 7.79	× 10 ⁻³
Bromoethane; C ₂ H ₅ Br; [74-96-4]		0.24	0.286 0.194 0.138	0.283 0.198 0.141 0.103
Smoothing equation: $\ln x_{\rm HI}$ Standard error $\ln x_{\rm HI}$	= -11.466 about the r	+ 27.874/(T/1 regression li	00) ne = 4.65	× 10 ⁻³

** smoothing equation and smoothed values were calculated by H.L. Clever

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE The gas was passed into a weighed amount of liquid in a bubbler tube as described by Ahmed et al.(1). Temperature control was manual to within about 0.5 K. Pressure control was within 1 mmHg. In addition to direct weighing of the gas absorbed, hydrogen lodide was quantitatively absorbed in water and titrated by silver nitrate.

* calculated by the compiler

The data were cited in reference (2)

- SOURCE AND PURITY OF MATERIALS: 1. Hydrogen iodide was prepared from self prepared phosphorus triiodide, and dried by phosphorus pentoxide. It was passed through a tube at 243 K, and then frozen to a white solid, from which it was obtained by temperature control.
- 2. Alkyl halides: Best specimens were dried over anhydrous calcium chloride, and freshly distilled. The purities were attested by the standard procedures.

ESTIMATED ERROR: $\delta x_{\rm HI} / x_{\rm HI} = 0.005 - 0.02$

- Ahmed, W.; Gerrard, W.; Maladkar, V. K. J. Appl. Chem. 1970, 20, 109.
- Gerrard, W. "Solubility of Gases and Liquids" Plenum Press, New York, 1976.

Hydrogen	lodide in No	n-Aqueous Sol	vents	44!
COMPONENTS:		ORIGINAL ME	ASUREMENTS	:
(1) Hydrogen Iodide; HI; [10034-85-2]		Maladkar, V Thesis, 197 University	0,	
(2) Alkyl halides		oniversity	01 20	
EXPERIMENTAL VALUES:	m / v	Mole ratio	M-1-*	Cmaathad**
		I ^{/n} alk.hal.		Smoothed** mole fraction
		i aik.nai.	*HI	×HI
1-Bromopropane; C ₃ H ₇ Br; [106-94-5]	283.15	0.47 0.29 0.19	0.320 0.225 0.160	0.321 0.224 0.160 0.117
Smoothing equation: $\ln x_{\text{HI}} = \text{Standard error in } x_{\text{HI}}$ at	-11.294 +	27.745/(T/1	00)	- 2
			ne = 1.25	× 10 ⁻³
1-Bromobutane; C ₄ H ₅ Br; [109-65-9]	273.15	0.495 0.30 0.23	0.331 0.231	0.324 0.241
[109-03-9]	293.15	0.23	0.187	0.183
Smoothing equation: $\ln x_{\text{HI}} = \text{Standard error in } x_{\text{HI}}$ at	-9.518 + cout the r	22.922/(T/10 egression li	0) ne = 1.28	× 10 ⁻²
<pre>Iodomethane; CH₃I; [74-88-4]</pre>	283.15 293.15	0.46 0.27	0.315 0.213	0.313 0.215
	303.15	0.18		0.152
Smoothing equation: $\ln x_{\text{HI}} = \text{Standard error in } x_{\text{HI}}$ as	-12.113 + bout the r	31.010/(T/1 egression li	00) ne = 3.27	× 10 ⁻³
Iodoethane; C ₂ H ₅ I;	273.15	0.46	0 315	0.442
[75-03-6]	283.15	0.46 0.33	0.315 0.248	0.320 0.237
	299.15 303.15	0.24	0.194	0.179
Smoothing equation: $\ln x_{\text{HI}} = \text{Standard error in } x_{\text{HI}}$ at	-9.967 + oout the r	24.997/(T/10 egression li	0) ne = 1.35	× 10 ⁻²
1-Iodopropane; C ₃ H ₇ I:	273.15	0.573 0.375	0.364	0.369
[107-08-4]		0.375 0.238		0.265 0.195
Smoothing equation: $\ln x_{\text{HI}} = \text{Standard error in } x_{\text{HI}}$	-10.357 + out the re	25.569/(T/1 gression lin	00) e = 9.76 ×	10-3
<pre>* calculated by the compile: ** smoothing equation and sr</pre>	r noothed va	lues were ca	lculated b	y H.L. Clever

- 1. Hydrogen iodide; HI; [10034-85-2]
- 2. 1-Chlorooctane; C₈H₁₇Cl;
 [111-85-3]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:	<u> T/K</u>	Mol Ratio nHI/nC8H17C1	Mol Fraction X _{HI}
	243.15	5.0	0.833
	253.15	1.75	0.636
	263.15	1.00	0.500
	273.15	0.65	0.394
	283.15	0.50	0.333
	293.15	0.375	0.273

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HT} = -15.978 + 28.304/(T/100) + 4.676 \ln (T/100)$

Standard error about regression line = 4.66×10^{-3}

T/K	Mol Fraction
	X _{HI}
243.15	0.833
253.15	0.635
263.15	0.498
273.15	0.400
283.15	0.328
293.15	0.274

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

For temperatures below 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen iodide. Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus triiodide.
- 1-Chlorooctane. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen iodide; HI; [10034-85-2]
- 2. 1-Bromooctane; C₈H₁₇Br;
 [111-83-1]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard
(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction	
	$^{\rm n}$ HI/ $^{\rm n}$ C $_{8}$ H $_{17}$ Br	x_{HI}	
243.15	5.75	0.852	
253.15	1.85	0.649	
263.15	1.10	0.524	
273.15	0.68	0.405	
283.15	0.49	0.329	
293.15	0.37	0.270	

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HT} = -2.514 + 10.499/(T/100) - 2.213 \ln (T/100)$

Standard error about regression line = 7.40×10^{-3}

T/K	Mol Fraction
	XHI
243.15 253.15 263.15 273.15 283.15 293.15	0.850 0.656 0.514 0.409 0.330 0.269

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

For temperatures below 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen iodide. Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus triiodide.
- 1-Bromooctane. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.015$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972,
 22, 623 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

- 1. Hydrogen iodide; HI; [10034-85-2]
- 2. 1-Iodooctane; C₉H₁₇I; [629-27-6]

ORIGINAL MEASUREMENTS:

Ahmed, W.; Gerrard, W.; Maladkar, V. K.

J. Appl. Chem. 1970, 20, 109 - 115.

VARIABLES:

T/K: 243.15 - 293.15 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

W. Gerrard

(smoothed data calculated by H.L. Clever)

EXPERIMENTAL VALUES:

T/K	Mol Ratio	Mol Fraction
	ⁿ HI/ ⁿ C ₈ H ₁₇ I	x^{HI}
243.15	5.8	0.853
253,15	2.03	0.670
263.15	1.13	0.531
273.15	0.73	0.422
233.15	0.53	0.346
293.15	0.425	0.298

The mole fraction solubilities were calculated from the mole ratio by the compiler.

Smoothed Data: $\ln X_{HI} = -13.267 + 24.441/(T/100) + 3.447 \ln (T/100)$ Standard error about regression line = 7.19 x 10⁻³

T/K	Mol Fraction
	$^{\mathrm{X}}$ HI
243.15	0.859
253.15	0.664
263.15	0.526
273.15	0.425
283.15	0.351
293.15	0.295

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

Hydrogen iodide was passed into a bubbler tube at a total pressure measured by a manometer assembly. The weight of the gas absorbed was determined by re-weighing the tube. The temperature was manually controlled to within 0.2 K. For full description, see Gerrard (1,2).

For temperatures below 268 K a chemical titration was conducted.

SOURCE AND PURITY OF MATERIALS:

- Good quality hydrogen iodide was obtained from a cylinder, and passed through a tube at 243 K. Check measurements were made by using gas obtained from freshly prepared phosphorus triiodide.
- 1-Iodooctane. Best obtainable specimen was purified, fractionally distilled, and attested.

ESTIMATED ERROR:

 $\delta T/K = 0.2$ $\delta X/X = 0.01$

- Gerrard, W.
 J. Appl. Chem. Biotechnol. 1972, 22, 623 - 650.
- Gerrard, W.
 "Solubility of Gases and Liquids"
 Plenum Press, New York, 1976

0.761

0.743

0.333

Hydrogen lodide in No	on-Aqueous So	lvents	449
COMPONENTS:	ORIGINAL M	EASUREMENTS:	
(1) Hydrogen iodide; HI; [10034-85-2](2) Thiols, thioethers, thiophene and tetrahydrothiophene	Frazer, M. J.; Gerrard, W. Nature 1964, 204, 1299 - 1300		
VARIABLES:	PREPARED B	Y:	
T/K: 273.15 Total P/kPa : 101.3 (barometric, nearly 1 atm)	W. Gerrard		
EXPERIMENTAL VALUES:	·		
	T/K	Mole ratio	
2-Propanethiol, (2-propylmercaptan); C ₃ H ₈ S; [75-33-2]	273.15	0.45	0.310
1-Butanethiol, (1-butylmercaptan); C ₄ H ₁₀ S; [109-79-5]	273.15	0.67	0.401
Benzenethiol, (thiophenol, mercaptobenzene); C ₆ H ₆ S; [108-98-5]	273.15	0.39	0.281

2,2'-Thiobispropane, (d11sopropy1 273.15 3.18 sulfide); C₆H₁₄S; [625-80-9]

* calculated by the compiler

Thiophene, (thiofuran); C4H4S;

C₈H₁₈S; [544-40-1]

 $C_{12}H_{10}S$; [139-66-2]

[110-02-1]

1,1'-Thiobisbutane, (dibutyl sulfide);

1,1'-Thiobisbenzene, (diphenyl sulfide); 273.15

Tetrahydrothiophene; C₄H₈S; [110-01-0] 273.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

The gas was passed into a weighed amount of solvent (about 2 g) in a U-tube kept at 273.15 K. The pressure was atmospheric, approximately 1 atm. The maximum amount of gas absorbed was determined by weighing.

SOURCE AND PURITY OF MATERIALS:

1. Hydrogen iodide. Self made and carefully purifed.

2.89

0.50

(reacts further)

(white solid formed)

1.0

273.15

273.15

2. Sulfur compounds. The purities were checked by boiling points and gas-liquid chromatography. After each measurement of solubility the gas was removed by treatment with water, the liquid was recovered and identified with the original compound.

ESTIMATED ERROR:

- 1. Hydrogen Iodide; HI; [10034-85-2]
- 2. Trichloroborane; BCl₃;
 [10294-34-5]

ORIGINAL MEASUREMENTS:

Ahmed, W.

Thesis, 1970 University of London

VARIABLES:

T/K: 256.15 - 273.15 Total P/kPa: 101.325 (1 atm) PREPARED BY:

W. Gerrard

EXPERIMENTAL VALUES:

T/K	Mol Ratio nHI/nBCl3	Mol Fraction X _{HI}	
273.15	0.086	0.0792	
256.15	0.176	0.150	

The mole fraction solubilities were calculated from the mole ratio by the compiler.

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Trichloroborane was distilled into the bubbler tube at low temperature. Hydrogen iodide was passed through for two hours. The final liquid was quantitatively treated with an aqueous solution of sodium hydroxide. Borate and total halide were then determined by titrations.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen iodide was prepared from self prepared phosphorus triiodide, and dried by phosphorus pentoxide. It was passed through a tube at 243 K, and frozen to a white solid, from which it was obtained by temperature control.
- Trichloroborane. The purest obtainable specimen was used.

ESTIMATED ERROR:

$$\delta T/K = 0.2$$

 $\delta X_1/X_1 = 0.02$

REFERENCES:

Ahmed, W.; Gerrard, W.;
 Maladkar, V. K.
 J. Appl. Chem. 1970, 20, 109.

(1) Hydrogen fluoride; HF;
 [7664-39-3]
 Hydrogen chloride; HCl;
 [7647-01-0]
 Hydrogen bromide; HBr;
 [10035-10-6]
 Hydrogen iodide; HI;[10034-85-2]

Appendix I

Some Physical Properties of the Hydrogen Halides.

Appendix I summarizes some physical property values of the hydrogen halides which will be of interest to the users of the solubility data. The property values are based on data in the International Critical Tables (ref 1), NBS Circular 500 (ref 2), The Handbook of Chemistry and Physics, 64th Ed. (ref 3), and recent measurements of Henderson at al. (ref 4) on hydrogen chloride. The data were evaluated at time of publication, but the user should be alert for more up to date values in future publications. The data given here are believed to be adequate for most applications related to the solubility of the hydrogen halides.

Below are values of the enthalpy, entropy and heat capacity changes on fusion and on vaporization at atmospheric pressure. The values have been recalculated in kJ and J from values given in NBS Circular 500. The temperatures for fusion and vaporization from Circular 500 are given in Table I on the following page.

Substance	∆H/kJ mol-1		$\Delta S/J$ K ⁻¹ mol ⁻¹		$\Delta C_p/J$ K ⁻¹ mol ⁻¹	
	Fusion	Vaporization	Fusion	Vaporization	Fusion	Vaporization
HF HCl HBr HI	4.58 1.99 2.41 2.87	7.5 16.2 17.6 19.8	24.1 12.5 12.9 12.9	25.5 85.8 85.3 83.1	10.7 8.8 6.9 4.6	-46 -29.9 -30.8 -29.9

The enthalpy change on vaporization of HCl is $16.194 \text{ kJ mol}^{-1}$ at the normal boiling point according to Henderson $et \ al.$ (ref 4).

Table I gives the fusion and normal boiling point temperatures, the critical temperatures and pressures, and the ideal mole fraction solubility at a number of temperatures at a gas partial pressure of one atmosphere.

The fusion and normal boiling point temperatures of HF, HBr and HI were taken from Circular 500, the values of HCl are from Henderson et al. The critical property values were taken from the compilation of R. Loebel in the Handbook of Chemistry and Physics. The critical temperature and pressure of HCl are from Henderson et al. The critical values differ by only about one percent from values given in the International Critical Tables which were compiled from data taken before 1928.

The ideal mole fraction solubilities are based on Raoults law. The values are for a gas partial pressure of one atm. For HF the required vapor pressures were calculated from the equation given in the <code>Handbook</code> of <code>Chemistry</code> and <code>Physics</code>. For HCl, HBr and HI the vapor pressures were taken from the <code>International Critical Tables</code>. The ideal mole fraction solubility values are useful in discussions about the departure of solubility from ideal behavior and the <code>Gerrard Reference Line</code>.

- International Critical Tables, E. W. Washburn, Editor, McGraw-Hill Book Co., New York, 1928, Volume III, p. 228.
- Selected Values of Chemical Thermodynamic Properties [NBS Circular 500] Rossini, F.D.; Wagman, D.D.; Evans, W.H.; Levine, S.; Jaffe, I. U. S. Government Printing Office, Washington, DC 1952 (reprinted 1961), Part I, Series II, pp. 548-551.
- 3. Handbook of Chemistry and Physics, Weast, R. C., Editor, CRC Press, Inc., Boca Raton, FL, 1983, 64th. Edition.
- 4. Henderson, C.; Lewis, D.G.; Prichard, P.C.; Staveley, L.A.K.; Fonseca, I.M. A.; Lobo, L.Q. J. Chem. Thermodynam. 1986, 18, 1077-1088.

(1) Hydrogen fluoride; HF;
[7664-39-3]
Hydrogen chloride; HC1;
[7647-01-0]
Hydrogen bromide; HBr;
[10035-10-6]
Hydrogen iodide; HI; [10034-85-2]

Appendix I (continued)

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1983, July; revised 1986, Nov

Table 1. Some physical properties of the hydrogen halides. Melting, normal boiling, and critical temperatures. Estimated "ideal" solubilities.

		icies.			
Tempera	ture	Hydrogen Fluoride	Hydrogen Chloride	Hydrogen Bromide	Hydrogen Iodide
t/°C	T/K				-
-114.10	159.05	_	Fusion(t.p.)	_	_
- 86.82	186.28	-		Fusion	-
- 84.95 - 83.07	188.20 190.09	- Fusion	n.b.p.	-	-
- 80 - 70	193.15 203.15		0.75 0.46		
- 66.73	206.43	-	-	n.b.p.	-
- 60	213.15	•	0.29	0.71	
- 50.8	222.36	-	-	-	Fusion
- 50 - 40	223.15 233.15		0.19 0.13	0.46 0.30	
- 35.36	237.80	-	-	-	n.b.p.
- 30 - 20 - 10 0	243.15 253.15 263.15 273.15 283.15		0.094 0.069 0.052 0.039 0.031	0.21 0.15 0.11 0.081 0.063	0.79 0.54 0.38 0.27 0.20
19.9	293.05	n.b.p.	-	-	-
20 25 30 40 50	293.15 298.15 303.15 313.15 323.15	0.995 0.84 0.71 0.51 0.38	0.024 0.021 0.019 0.016 0.013	0.049 0.043 0.038 0.031 0.025	0.15 0.13 0.12 0.090 0.072
51.53	324.68	-	[p _c /MPa = 8.256]	-	-
60 70 80	333.15 343.15 353.15		0.2301	0.020 0.017 0.014	0.058 0.047 0.039
90	363.2	-	~	$[p_o/MPa =$	
90 100 110 120 130 140	363.15 373.15 383.15 393.15 403.15 413.15 423.15			8,56]	0.032 0.027 0.023 0.019 0.017
150	423	-	-	-	[p _c /MPa = 8.30]
188	461	[p _c /MPa = 6.48]	-	-	- 0.301
190	463.15	6.48]			

SYSTEM INDEX

Page numbers preceded by E refer to evaluation texts. Substances are indexed in the same manner as in Chemical Abstracts, e.g. toluene appears as benzene, methyl-; boron truchloride as borane, trichloro- etc.

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