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SOLUBILITY DATA SERIES

Volume 5/6

HYDROGEN AND DEUTERIUM

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Volume 5/6

HYDROGEN AND DEUTERIUM

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FOREWORD

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

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

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

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

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

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

With the status of current secondary and tertiary services being as briefly stated above, the innovative approach of the *Solubility Data Project* is that its compilation and critical evaluation work involve consolidation and reprocessing services when both activities are based on intellectual and scholarly reworking of information from primary sources. It comprises compact compilation, rationalization and simplification, and the fitting of isolated numerical data into a critically evaluated general framework.

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

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

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

The Critical Evaluation part gives the following information: (i) a verbal text of evaluation which discusses the numerical solubility information appearing in the primary sources located in the literature. The evaluation text concerns primarily the quality of data after consideration of the purity of the materials and their characterization, the experimental method employed and the uncertainties in control of physical parameters, the reproducibility of the data, the agreement of the worker's results on accepted test systems with standard values, and finally, the fitting of data, with suitable statistical tests, to mathematical functions; (ii) a set of recommended numerical data. Whenever possible, the set

of recommended data includes weighted average and standard deviations, and a set of smoothing equations derived from the experimental data endorsed by the evaluator;

(iii) a graphical plot of recommended data.

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

The typical data sheet carries the following information:
(i) components - definition of the system - their names, formulas and Chemical Abstracts registry numbers;

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

(iii) experimental variables;

(iv) identification of the compiler;

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

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

(vi) experimental method used for the generation of data;

(vii) type of apparatus and procedure employed; (viii) source and purity of materials;

(ix) estimated error;

(x) references relevant to the generation of experimental data as cited in the primary source.

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

Finally, the role of education is more than corollary to the efforts we are seeking. The scientific standards advocated here are necessary to strengthen science and technology, and should be regarded as a major effort in the training and formation of the next generation of scientists and engineers. Specifically, we believe that there is going to be an impact of our project on scientific-communication practices. The quality of consolidation adopted by this program offers down-to-earth guidelines, concrete examples which are bound to make primary publication services more responsive than ever before to the needs of users. The self-regulatory message to scientists of 15 years ago to refrain from unnecessary publication has not achieved much. The literature is still, in 1980, cluttered with poor-quality articles. The Weinberg report (in "Reader in Science Information", Eds. J. Sherrod and A. Hodina, Microcard Editions Books, Indian Head, Inc., 1973, p.292) states that "admonition to authors to restrain themselves from premature, unnecessary publication can have little effect unless the climate of the entire technical and scholarly community encourages restraint...". We think that projects of this kind translate the climate into operational terms by exerting pressure on authors to avoid submitting low-grade material. The type of our output, we hope, will encourage attention to quality as authors will increasingly realize that their work will not be suited for permanent retrievability unless it meets the standards adopted in this It should help to dispel confusion in the minds of many authors of what represents a permanently useful bit of information of an archival value, and what does not.

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

A. S. Kertes

PREFACE

The users of this volume will find (1) the experimental solubility data of hydrogen, hydrogen deuteride and deuterium gas in liquids as reported in the scientific literature (2) evaluations and tables of tentative or recommended solubility data when two or more laboratories have reported consistent solubility data over the same range of temperature and pressure for a system. (3) general evaluations of groups of related systems when more detailed comments on individual systems are not possible. In some instances users have the option of using the experimental values, either directly, or in their own smoothing equations, or of using the smoothed values prepared by the compilers and evaluators.

A fairly liberal interpretation of the terms, "gas", "liquid" and "solubility" has been taken. In particular virtually all two phase equilibria have been considered as "solubility" when one component is hydrogen even at high pressures. The "gas" being the less dense phase and the "liquid" being the more dense phase. The two phase equilibria between isotopes of hydrogen has been excluded. The helium and hydrogen mixtures are considered in the volume on helium.

The literature has been, in general, covered up until the end of 1979 although some papers published during 1979 in journals not readily available may have been omitted. Some 1980 papers are cited.

Some words of explanation are required with respect to units, smoothing equations, auxiliary data and data sources, and other points. In general the experimental data are presented in the units found in the original paper. In addition, the original data are often converted to other units.

Only in the past 15 years have experimental methods for the determination of the solubility of gases in liquids developed to the point where 0.5 per cent or better accuracy is attained. For hydrogen the corrections for non-ideal behaviour and for expansion of the liquid phase on dissolution of the gas are small for pressures below 200 kPa and well within the normal experimental error. Thus such corrections were not made for the gas solubility of hydrogen at low pressures.

Most gas solubility measurements carried out near armospheric conditions are measured at a total pressure near one atmosphere with the gas saturated with the solvent vapor. Usually the actual partial pressure of the gas is not known. In most cases the Ostwald coefficient is the directly measured coefficient. The Bunsen coefficient and the mole fraction gas solubility at one atmosphere gas partial pressure are calculated from the Ostwald coefficient assuming the Ostwald coefficient is independent of pressure. The assumption may not be true, especially if the gas is at a partial pressure well below atmospheric, if the solvent has a high vapor pressure or if the gas is soluble enough to change the solvent properties measureably from their pure liquid properties. This problem, which becomes important for more soluble gases, is one which evaluators will need to pay more attention to as the precision of solubility measurements increases in the future. The Bunsen coefficients and mole fraction solubility values calculated from Ostwald coefficients in this volume need to be used with the above caution in mind.

The lack of high accuracy is also the reason that only a two-constant equation is used to smooth and evaluate most of the gas solubility data. A Gibbs energy of solution equation linear in temperature is used

$$\Delta G^{O}/J \text{ mol}^{-1} = -RT \text{ ln } x_1 = A + BT$$

or in alternative form

$$\ln x_1 = -\Delta G^{O}/RT = -A/RT - B/R$$

where A is ΔH° , B is $-\Delta \text{S}^{\circ}$, x_1 is the mole fraction solubility at a gas partial pressure of 101.325 kPa (1 atm) and R is 8.31441 J K⁻¹ mol⁻¹. The constants A and B require five digits to reproduce the mole fraction solubility to three significant figures. Although the constants are given to five digits it is not intended to imply that the values of the changes in enthalpy and entropy of solution are significant to more than two or three digits.

An inconsistency, which we believe is justified, is found with respect to the solubility data in water. A recommended equation and table of values is given for the solubility of hydrogen in water. However, for systems which contain water and other solvent compounds such as electrolytes or water miscible polar organic compounds, the experimental gas solubility in water from the paper is given, even when it is at variance with the recommended values. These data are presented because the author's ratio of gas solubility in water to the solubility in the aqueous solution may be more accurate than the solubility itself.

Solvent density data were often required in making conversions from Ostwald coefficients to mole fraction solubilities. Where the density data were not referenced, as in other volumes in this series, the main sources of density data were:

Circular 461 of the U.S. National Bureau of Standards American Petroleum Research Project 44 Publications The International Critical Tables, Volume III (E.W. Washburn, Editor) McGraw-Hill Co., 1931 Smow Table, Pure and Applied Chemistry, 1976, 45, 1-9. Thermodynamic Properties of Aliphatic Alcohols, R.C. Wilhoit and B.J. Zwolinski, J. Phys. Chem. Ref. Data, 1972, 2, Supplement No.1. Organic Solvents, J.A. Riddick and W.B. Bunger, Technique of Chemistry, Volume II, A. Weissberger, Editor, Wiley-Interscience, New York, 1970, 3rd Edn.

Chemical Abstracts recommended names and registry numbers were used throughout. Common names are cross referenced to Chemical Abstracts recommended names in the Index. There is a registry number index.

The Editor would appreciate users calling errors and omissions to his attention.

The Editor gratefully acknowledges the advice and comments of members of the IUPAC Commission on Solubility Data, the help and hard work of Professor Larry Clever and the efforts of the typist, Carolyn Dowie, Lesley Flanagan, Peggy Tyler and Joy Wall. The help of Kerri Hubbard in Obtaining copies of papers not available in Melbourne was appreciated.

Acknowledgement is made to the University of Melbourne for a Travel Grant for Research which considerably aided the completion of this volume.

Colin L. Young

Melbourne, Victoria

THE SOLUBILITY OF GASES IN LIQUIDS

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

INTRODUCTION

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

DEFINITION OF GAS SOLUBILITY

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

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

UNITS AND QUANTITIES

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

.EVALUATION AND COMPILATION

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

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

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

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

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

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

PURITY OF MATERIALS

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

APPARATUS AND PROCEDURES

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

METHODS OF EXPRESSING GAS SOLUBILITIES

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

The Mole Fraction, x(g)

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

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

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

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

The Weight Per Cent Solubility, wt%

For a binary system this is given by

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

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

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

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

The weight solubility is the number of moles of dissolved gas per gram of solvent when the partial pressure of gas is 1 atmosphere. The weight solubility is related to the mole fraction solubility at one atmosphere partial pressure by

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

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

The Moles Per Unit Volume Solubility, n

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

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

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 x is related to the Bunsen coefficient by

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

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,

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

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:

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

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

$$x = \left[\frac{RT}{P(g) L v^{\circ}(1)} + 1 \right]^{-1}$$

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

$$P(g) = K_H x$$

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

$$C(g) = K_CC(1)$$

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

The Mole Ratio, N

The mole ratio, N, is defined by

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

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

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

where v is the molal volume of the gas in $\text{cm}^3\text{mol}^{-1}$ 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 the molal volume of the gas (cm $^3\text{mol}^{-1}$) at the temperature of the measurement.

SALT EFFECTS

The effect of a dissolved salt in the solvent on the solubility of a gas is often studied. The activity coefficient of a dissolved gas is a function of the concentration of all solute species (see ref. 8). At a given temperature and pressure the logarithm of the dissolved gas activity coefficient can be represented by a power series in $\mathbf{C}_{\mathtt{S}}$, the electrolyte concentration, and $\mathbf{C}_{\mathtt{I}}$, the nonelectrolyte solute gas concentration

$$\log f_{i} = \sum_{m,n} k_{mn} C_{s}^{n} C_{i}^{m}$$

It is usually assumed that only the linear terms are important for low $C_{\rm s}$ and $C_{\rm i}$ values when there is negligible chemical interaction between solute species.

$$\log f_i = k_s C_s + k_i C_i$$

where k_s is the salt effect parameter and k_s is the solute-solute gas interaction parameter. The dissolved gas activity is the same in the pure solvent and a salt solution in that solvent for a given partial pressure and temperature

$$a_i = f_i S_i = f_i^{\circ} S_i^{\circ}$$
 and $f_i = f_i^{\circ} \frac{S_i^{\circ}}{S_i}$

where S_i and S_i^{O} are the gas solubility in the salt solution and in the pure solvent, respectively, and the f's are the corresponding activity coefficients. If follows that $\log f_i/f_O = \log S_i^{O}/S_i = k_S C_S + k_i^{O}(S_i-S_i^{O})$. When the

quantity (S; - S; $^{\rm O}$) is small the second term is negligible even though k and k; may be of similar magnitude. This is generally the case for gas solubilities and the equation reduces to

$$\log \frac{f_{i}}{f_{i}^{o}} = \log \frac{s_{i}^{o}}{s_{i}} = k_{s}C_{s}$$

which is the form of the empirical Setschenow equation in use since the 1880's. A salt that increases the activity coefficient of the dissolved gas is said to salt-out and a salt that decreases the activity coefficient of the dissolved gas is said to salt-in.

Although salt effect studies have been carried out for many years, there appears to be no common agreement of the units for either the gas solubility or the salt concentration. Both molar (mol dm 3) and molal (mol kg 1) are used for the salt concentration. The gas solubility ratio S $_{\bf i}$ /S $_{\bf i}$ is given as Bunsen coefficient ratio and Ostwald coefficient ratio,

which would be the same as a molar ratio; Kueunen coefficient ratio, volume dissolved in 1 g or 1 kg of solvent which would be a molal ratio; and mole fraction ratio. Recent theoretical treatments use salt concentration in mol dm $^{-3}$ and S_{i} $^{0}/S_{i}$ ratio as mole fraction ratio with each salt ion acting as a mole. Evaluations which compare the results of several workers are made in the units most compatible with present theory.

TEMPERATURE DEPENDENCE OF GAS SOLUBILITY

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

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

It is then possible to write the thermodynamic functions $\Delta \overline{G}^{\,0}$, $\Delta \overline{H}^{\,0}$, $\Delta \overline{S}^{\,0}$ and $\Delta \overline{C}^{\,0}$ for the transfer of the gas from the vapor phase at 101.325 Pa partial pressure to the (hypothetical) solution phase of unit mole fraction

$$\Delta \overline{G}_1^0 = -RAT - 100 RB - RCT ln (T/100)$$

$$\Delta \overline{S}_1^0 = RA + RC \ln (T/100) + RC$$

$$\Delta \overline{H}_{1}^{0} = -100 \text{ RB} + \text{RCT}$$

$$\Delta \overline{C}^{0}_{p_1} = RC$$

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

$$\Delta \overline{G}_1^0 = - RT \ln x = A + BT$$

in which case $A = \Delta \overline{H}_{1}^{0}$ and $-B = \Delta \overline{S}_{1}^{0}$.

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- 8. Long, F.A.; McDevit, W.F. Chem. Rev. 1952, 51, 119.

Water 1

COMPONENTS:

EVALUATOR:

(1) Hydrogen; H₂; [1333-74-0]

Rubin Battino and Emmerich Wilhelm Department of Chemistry Wright State University Dayton, OH 45435 USA

(2) Water; H₂O; [7732-18-5]

July 1977, revised May 1980

CRITICAL EVALUATION:

The solubility of hydrogen in water has been studied by many workers. We found the experimental work of ten to be of sufficient reliability to use in the smoothing equation. In the process of fitting the data to the smoothing equation any data points which differed from the smooth equation by about two standard deviations or more were rejected. The 75 points used for the final smoothing were obtained as follows (reference number - number of data points taken from that reference): 1-11; 2-2; 3-1; 4-3; 5-5; 6-2; 7-3; 8-1; 9-41; 10-6. The fitting equation used was

$$\ln x_1 = A + B/(T/100K) + C \ln (T/100K) + D(T/100K) + E(T/100K)^2$$
 (1)

Using T/100K as the variable rather than T/K gives coefficients of approximately equal magnitude. The best fit for the 75 data points was

$$\ln x_1 = -48.1611 + 55.2845/(T/100K) + 16.8893ln (T/100K)$$
 (2)

where \mathbf{x}_1 is the mole fraction solubility at 101.325 Pa partial pressure of gas. The fit in $\ln \mathbf{x}_1$ gave a standard deviation of 0.52% taken at the middle of the temperature range. Table 1 gives smoothed values of the mole fraction solubility and the Ostwald coefficient at 5K intervals.

Table 1 also gives the thermodynamic functions $\Delta \overline{G}_1^{\circ}$, $\Delta \overline{H}_1^{\circ}$, $\Delta \overline{S}_1^{\circ}$, and $\Delta \overline{C}_{P_1}^{\circ}$ for the transfer of gas from the vapor phase at 101.325 Pa partial gas pressure to the (hypothetical) solution phase of unit mole fraction. These thermodynamic properties were calculated from the smoothing equation according to the following equations with R = 8.3144 J K⁻¹ mol⁻¹:

$$\Delta \overline{G}_1^{\circ}/RT = -\ln x_1 \tag{3}$$

$$\Delta \overline{H}_{1}^{\circ}/RT = -B(100K/T) + C + D(T/100K) + 2E(T/100K)^{2}$$
 (4)

$$\Delta \overline{S}_{1}^{\circ}/R = A + C(\ln (T/100K) + 1) + 2D(T/100K) + 3E(T/100K)^{2}$$
 (5)

$$\Delta \overline{C}_{p_3}^{\circ}/R = C + 2D(T/100K) + 6E(T/100K)^2$$
 (6)

The experimental work of ten other workers was not compiled or used for the smoothing equation for a variety of reasons. Müller's two data points (11) were about 2% high. Symons (12) measured solubility by gas chromatography and his duplicate values at 25°C were 3% high. Braun's measurements (13) were 12% high at his lower temperatures and came down to reasonable values at 25°C. Bunsen's measurements (14) were erratically high and low indicating a poor precision. Christoff's single value (15) was 7% high; and Drucker's single value (16) was 2% high. Findlay's measurement at 25°C was 3% high (17): Just's two measurements (18) were 3-4% high. Knopp's (19) single value at 20°C was 4% high. Milligan's (20) single value at 25°C was about 3% low. Gereche and Bittrich's (21) value at 25°C is 1% high. A data sheet is included.

The curve obtained from the smoothing equation shows a distinct minimum at 327 K.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

Rubin Battino and Emmerich Wilhelm Department of Chemistry Wright State University

Dayton, OH 45435 USA

July 1977, revised May 1980

CRITICAL EVALUATION:

Table 1. Recommended values of the solubility and thermodynamic functions^{1,2} at 5K intervals for hydrogen in water at a hydrogen partial pressure of 101.325 kPa (1 atm). Calculations based on equations 2 to 6.

T/K	Mol Fraction $x_1 \times 10^5$	Ostwald Coefficient L x 10 ²	$\Delta \overline{G}_{l}^{ob}/k \; J \; mol^{-l}$	$\Delta \overline{H}_1^{\circ}/k \text{ J mol}^{-1}$	∆\$°/J K ⁻¹ mol ⁻¹
273.15	1.755	2.184	24.87	-7.61	-118.9
278.15	1.657	2.010	25.46	-6.91	-116.4
283.15	1.576	2.032	26.03	-6.20	-113.8
288.15	1.510	1.980	26.60	-5.50	-111.4
293.15	1.455	1.940	27.15	-4.80	-109.0
298.15	1.411	1.911	27.69	-4.10	-106.6
303.15	1.377	1.893	28.21	-3.40	-104.3
308.15	1.350	1.883	28.73	-2.69	-102.0
313.15	1.330	1.883	29.23	-1.99	-99.7
318.15	1.317	1.890	29.73	-1.290	-97.5
323.15	1.310	1.905	30.21	-0.588	-95.3
328.15	1.308	1.927	30.68	+0.114	-93.1
333.15	1.312	1.957	31.14	0.816	-91.0
338.15	1.320	1.993	31.59	1.518	-88.9
343.15	1.333	2.037	32.03	2.22	-86.9
348.15	1.350	2.087	32.46	2.92	-84.8
353.15	1.371	2.144	32.88	3.62	-82.8

^{1.} The heat capacity change, $\Delta C_{\rm p}^{\circ}$, is independent of temperature and has a value of 140.4 J K $^{-1}$ mol $^{-1}$.

^{2.} cal_{th} = 4.184 Joules

Water 3

COMPONENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

Rubin Battino and Emmerich Wilhelm Department of Chemistry Wright State University Dayton, OH 45435 USA

July 1977, revised May 1980

CRITICAL EVALUATION:

References

- 1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819.
- 2. Geffcken, G. Z. Physik. Chem. 1904, 49, 257.
- 3. Hüfner, G. Z. Physik. Chem. 1907, 57, 611.
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- 20. Milligan, L. H. J. Phys. Chem. 1924, 28, 494.
- 21. Gerecke, J.; Bittrich, H. J. Wiss. Zeitschrift (Leuna-Merseburg)
 1971, 13, 115.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Timofejew, W.

Z. Physik. Chem. 1890, 6, 141-152.

VARIABLES:

T/K: 274.55 - 298.85 H₂ P/kPa: 101.325 (1 atm) PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^5$	Bunsen Coefficient a x 10 ²
274.55 281.50 286.15 291.60 298.85	1.712 ¹ 1.611 ¹ 1.542 ¹ 1.500 1.434	2.1295 2.0044 1.9174 1.8629 1.7789

The Bunsen coefficients are average values of several measurements.

The mole fraction solubility values were calculated by the compiler.

Mole fraction values which were used in the final smoothing equation for the recommended solubility equation given in the critical evaluation

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: An absorption vessel of 110 cm³ or

300 cm³ is used for the measurements. The volume of gas absorbed is measured on a gas buret. Also measured the solubility of hydrogen in alcohol (ethanol).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. No comment by author.
- (2) Water. No comment by author.

ESTIMATED ERROR:

REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Winkler, L. W.

Ber. 1891, 24, 89-101.

VARIABLES:

T/K: 273.65 - 323.15 H₂ P/kPa: 101.325 (1 atm)

PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

		_		
T/K	Bunsen Coefficient a x 10 ²		T/K	Bunsen Coefficient $\alpha \times 10^2$
273.65	2.141		303.15	1.706
273.73	2.134		313.11	1.649
273.77	2.132		313.04	1.639
283.22	1.956		313.03	1.636
283.00	1.961		313.15	1.644
283.15	1.948		313.15	1.645
293.15	1.828		313.15	1.648
293.18	1.815		323.17	1.603
293.15	1.815		323.00	1.609
303.16	1.692		323.13	1.609
303.15	1.696		323.25	1.616
303.12	1.671		323.18	1.607
303.15	1.712		323.05	1.606
303.15	1.714	•		

Average values calculated by the compiler.

T/K	Mol Fraction $x_1 \times 10^5$	Bunsen Coefficient
273.72		$\frac{\alpha \times 10^2}{2.333}$
	1.714	2.131
283.12	1.5721	1.955
293.16	1.465¹	1.819
303.15	1.372 ¹	1.699
313.11	1.332 ¹	1.644
323.13	1.308 ¹	1.608

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas is introduced over degassed water (1) Hydrogen. Made from zinc and in an absorption vessel in a thermostat. The volume of gas absorbed is measured on a thermostated gas buret. (2) Water. Distilled.

SOURCE AND PURITY OF MATERIALS:

- dilute sulfuric acid.
- Mole fraction solubility values which were used to obtain thefinal smoothing equation given in the critical evaluation.

ESTIMATED ERROR:

REFERENCES:

ORIGINAL MEASUREMENTS: COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Geffcken, G. (2) Water; H₂O; [7732-18-5] Z. Physik. Chem. 1904, 49, 257-302. VARIABLES: PREPARED BY: T/K: 288.15 - 298.15 H_2 P/kPa: 101.325 (1 atm) R. Battino

EXPERIMENTAL	WAT HEC.		
EMERIFICATAL	VALIUES:	T/K	Ostwald
			Coefficient
			1×10^{2}
		288.15	1,973
		200.13	1.7/3
		288.15	1.979
		288.15	1.992
		288.15	1.984
		298.15	1.935
		298.15	1.911
		298.15	1.932
		298.15	1.936
		298.15	1.922
		298.15	1.921
		298.15	1.924

Average values calculated by the compiler.

Mol Fraction	Ostwald
v 10 ⁵	Coefficient
x1 x 10	$L \times 10^2$
	
1.5111	1.982
1.4221	1.926
	$\frac{x_1 \times 10^5}{1.511^1}$

¹ Mole fraction values which were used to obtain the recommended smoothing equation which was given in the critical evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Amount of gas dissolved is determined (1) Hydrogen. No comment by author. in a thermostated gas buret system. Details given in original paper. (2) Water. No comment by author. Solubilities also determined in aqueous solutions of acetic acid, monochloracetic acid, nitric acid, hydrochloric acid, sulfuric acid, sodium hydroxide, and potassium hydroxide. ESTIMATED ERROR: REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Hüfner, G.

Z. Physik. Chem. 1907, 57, 611-624.

VARIABLES:

T/K: 293 H₂ P/kPa: 103

293.15 - 293.34 101.325 (1 atm) PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^5$	Bunsen Coefficient $\alpha \times 10^2$
293.34		1.812
293.26		1.805
293.15		1.812
293.25	1.4571	1.810

The mole fraction value was calculated by the compiler.

¹ Mole fraction value which was used to obtain the recommended smoothing equation which was given in the critical evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Apparatus described in reference 1. An absorption type using gas burets and an absorption flask. Solubilities also determined in several other solvents and solutions.

- SOURCE AND PURITY OF MATERIALS:
- (1) Hydrogen. No comment by author.
- (2) Water. Pure.

ESTIMATED ERROR:

REFERENCES:

Hüfner, G.
 Archiv. F. Anatomie und
 Physiologie, Physiolog. Abtly.
 1894, 5, 191.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Morrison, T. J.; Billett, F.

J. Chem. Soc. 1952, 3819-3822.

VARIABLES:

PREPARED BY:

T/K: 285.45 - 344.85 H₂ P/kPa: 101.325 (1 atm)

R. Battino

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^5$	Solubility cm ³ (STP)H ₂
		1.0000 kg ⁻¹ H ₂ O
285.45	1.5461	19.23
289.25	1.5051	18.71
290.45	1.492^{1}	18.54
296.15	1.439¹	17.86
298.15	1.427	17.70
306.35	1.372 ¹	16.98
318.15	1.329¹	16.37
320.45	1.3241	16.29
327.55	1.319 ¹	16.18
333.45	1.3141	16.07
338.65	1.323 ¹	16.14
344.85	1.3281	16.14

The authors smoothing equation is $log_{10} S_o = -36.250 + 1847/(T/K)$

 $+ 12.65 \log_{10} (T/K)$

The compiler calculated the mole fraction solubility values.

Mole fraction values which were used to obtain the recommended smoothing equation which is given in the critical evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Used the apparatus of Morrison and Billett (1) but with improvements described in the current paper in the degassing procedure and the absorption spirals. Degassed liquid is flowed slowly down a spiral containing the gas. The amount of gas absorbed is determined by using the liquid as its own gas buret. Volumes are determined in the burets and/or by weighing.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared from pure zinc and hydrochloric acid.
- (2) Water. No comment by authors.

ESTIMATED ERROR:

REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033. Water 9

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Water; H₂O; [7732-18-5] VARIABLES: T/K: 291.65 - 304.55 H₂ P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: de Wet, W. J. J. S. Afr. Chem. Inst. 1964, 17, 9-17. PREPARED BY: R. Battino

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^5$	Bunsen Coefficient $lpha imes 10^2$
291.65	1.497	1.86
298.85	1.411 ¹	1.75
304.55	1.365 ¹	1.69

The mole fraction solubility values were calculated by the compiler.

Mole fraction values which were used to obtain the recommended smoothing equation which is given in the critical evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Degassed liquid is flowed in a thin film through a spiral containing the gas. Volumes are determined via calibrated burets.

Used modification of Morrison and Billett apparatus (1). Degassing as modified by Clever, et al. (2).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. From commercial cylinders. Purified over activated charcoal at liquid nitrogen temperatures. Less than 0.3% impurities.
- (2) Water. Distilled.

ESTIMATED ERROR:

REFERENCES:

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033; ibid., 1952, 3819.
- Clever, H. L.; Battino, R.; Saylor, J. H.; Gross, P. M. J. Phys. Chem. <u>1957</u>, 61, 1078.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Ruetschi, P.; Amlie, R. F.

J. Phys. Chem. 1966, 70, 718-723.

VARIABLES:

T/K: 303.15 H₂ P/kPa: 101.325 (1 atm) PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^5$	Bunsen Coefficient $\alpha \times 10^2$
303.15 303.15 303.15 303.15	1.375 ¹ 1.365 1.381 ¹ 1.367 ¹	1.703 1.690 1.710 1.693

The mole fraction solubility values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

They used the apparatus of Ben-Naim and Baer (1). A calibrated dissolution vessel contains degassed water. Gas is introduced wet from a calibrated gas buret system. Stirring the liquid forces it up sidearms attached to the top of the flask and the liquid returns via a central The amount of gas dissolved is determined via the gas burets. The gas burets and dissolution vessel are thermostated in a water bath. The original paper contains a diagram ESTIMATED ERROR: and a description of operation. The solubility of H2 was also determined in KOH and H2SO4 solutions at 303.15K.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Prepurified grade (99.5% min purity).
- (2) Water. No comment by author.

 $\delta \alpha / \alpha = 0.005$

REFERENCES:

 Ben-Naim, A.; Baer, S. Trans. Faraday Soc. 1963, 59, 2735.

¹ Mole fraction values which were used to obtain the recommended smoothing equation which is given in the critical evaluation.

Water 11

COMPONENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Shoor, S. K.; Walker, R. D.; Gubbins, K. E.

J. Phys. Chem. 1969, 73, 312-317.

VARIABLES:

T/K: 298.15 - 333.15 H₂ P/kPa: 101.325 (1 atm) PREPARED BY:

R. Battino

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x \times 10^5$	$\frac{C_{\text{H}}/\text{mol dm}^{-3}}{c \times 10^3}$		
298.15	1.431	0.792		
313.15	1.295	0.713		
333.15	1.3051	0.712		

The mole fraction solubility values were calculated by the compiler.

Mole fraction values which was used to obtain the recommended smoothing equation which is given in the critical evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solutions are saturated by bubbling. After equilibration, samples are removed and analyzed by gas chromatography. Details are given by Gubbins, et al. (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Purity 99.9 per cent.
- (2) Water. Distilled from an allglass and teflon still.

ESTIMATED ERROR:

REFERENCES:

 Gubbins, K. E.; Carden, S. N.; Walker, R. D. J. Gas Chromatog. 1965, 3, 98.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
(1) Hydrogen; H ₂ ; [1333-74-0]	Gerecke, J.; Bittrich, H. J.		
(2) Water; H ₂ O; [7732-18-5]	Wiss. Zeitschrift (Leuna-Merseburg) 1971, 13, 115-122.		
	Chem. Abstr. <u>1972</u> , 76, 77239m.		
VARIABLES:	PREPARED BY:		
T/K: 298.15 H ₂ P/kPa: 101.325 (1 atm)	R. Battino		
EXPERIMENTAL VALUES:			
T/K Mol Frac $x_1 \times 1$			
298.15 1.42	7 1.77		
The mole fraction solubility value wa	s calculated by the compiler.		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE: Absorbed gas is measured in a gas buret using mercury manometers. Only written description of apparatus given. Also measured solubilities in many aqueous salt solutions.	SOURCE AND PURITY OF MATERIALS: (1) Hydrogen. No comment by authors.		
	ESTIMATED ERROR:		
	REFERENCES:		

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Crozier, T. E.; Yamamoto, S.

J. Chem. Eng. Data 1974, 19, 242-244.

VARIABLES:

PREPARED BY:

T/K: 274.60 - 302.47 P/kPa: 101.325 (1 atm) R. Battino

EXPERIMENTAL VALUES:

EXPERIMENTAL	VALUES:				
T/K	Mol Fraction1	Bunsen	T/K	Mol Fraction:	Bunsen
	5	Coefficient		5	Coefficient
	$x_1 \times 10^5$	$\frac{\alpha \times 10^2}{3.150}$		$x_1 \times 10^5$	$\frac{\alpha \times 10^2}{1.871}$
274.60	1.728	2.150	287.85	1.505	1.871
274.63	1.727	2.148	287.91	1.514	1.882
274.64	1.730	2.152	287.92	1.503	1.869
277.54	1.672	2.080	287.94	1.505	1.871
277.70	1.667	2.074	287.94	1.520	1.890
277.70	1.661	2.067	287.94	1.516	1.885
277.73	1.665	2.072	287.95	1.512	1.880
277.74	1.671	2.079	293.01	1.454	1.806
282.98	1.571	1.954	293.01	1.459	1.812
282.99	1.579	1.964	293.02	1.458	1.811
282.99	1.567	1.949	293.03	1.453	1.804
283.00	1.565	1.947	293.03	1.453	1.805
283.00	1.567	1.949	297.85	1.403	1.740
283.00	1.572	1.955	297.85	1.414	1.754
283.01	1.576	1.960	297.88	1.408	1.747
283.01	1.573	1.957	297.88	1.403	1.741
283.02	1.573	1.957	297.92	1.404	1.742
283.03	1.576	1.960	301.99	1.369	1.696
287.77	1.514	1.882	302.17	1.379	1.709
287.80	1.509	1.876	302.31	1.377	1.706
287.82	1.507	1.873	302.47	1.382	1.712

All of the mole fraction values above except the one at 301.99 K were used in the computer fit to obtain the recommended smoothing equation which is given in the critical evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubility measurements were made by the Scholander micro-gasometric technique (1) as modified by Douglas (2). Equilibration is with 6cm³ of gasfree water. All volumes are read on a micrometer which adjusts the amount of mercury in the system.

The authors also report the solubility of hydrogen in seawater and NaCl solutions.

The authors smoothing equation for their data is

 $\ln \alpha = -39.9611 + 5393.81/(T/K)$

+ 16.3135 ln (T/100K)

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Linde Specialty Gas. 99.9995% purity.
- (2) Water. Glass distilled water.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta \alpha/\alpha = 0.003$

REFERENCES:

- Scholander, P. F.
 J. Biol. Chem. 1947, 167, 235.
- Douglas, E.
 J. Phys. Chem. <u>1964</u>, 68, 169.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Gordon, L. I.; Cohen, Y.; Standley, D. R.

Deep-Sea Res. 1977, 24, 937 - 941.

VARIABLES:

T/K: 273.29 - 302.40 P/kPa: 101.325 (1 atm)

PREPARED BY:

EXPERIMENTAL VALUES:

Temperature		Mol Fraction	Bunsen	Ostwald	
t/ºC	T/K	$x_1 \times 10^5$	Coefficient $\alpha \times 10^3$	Coefficient L x 10 ³	
0.14	273.29	1.7821	22.17	22.18	
5.04	278.19	1.6581	20.63	21.01	
.0.00 .6.67	283.15 289.82	1.581 ¹ 1.501 ¹	19.66 18.66	20.38 19.80	
3.63	296.78	1.4201	17.62	19.80	
9.25	302.40	1.3871	17.18	19.02	

The mole fraction and Ostwald coefficient solubility values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

The method of Ben-Naim and Baer (1) as modified by Murray, Riley, and Wilson (2) was used with slightly further modifications.

The Bunsen coefficients were corrected for the change in volume of the solution upon dissolution of the hydrogen using a partial molal volume of 26 cm³ mol⁻¹. The correction increased the Bunsen coefficient about 0.12 per cent.

The results above average approximately 0.5 per cent higher than the results of Crozier and Yamamoto (3).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Ultra-pure electrolytically generated gas (Elhygen R generator).
- (2) Water. Doubly distilled.

ESTIMATED ERROR:

Root mean square deviation from authors fitted equation is 0.7 per cent. Equation fitted to water and sea water data above and ref 3.

REFERENCES:

- Ben-Naim, A.; Baer, S. Trans. Faraday Soc. 1963, 59,2735.
- Murray, C. N.; Riley, J. P.; Wilson, T. R. S. Deep-Sea Res. <u>1969</u>, 16, 297.
- Crozier, T. E.; Yamamoto, S.
 J. Chem. Eng. Data 1974, 19, 242.

Mole fraction solubility values which were used to obtain the recommended smoothing equation which is given in the critical evaluation.

Water 15

Wa	ater
COMPONENTS: 1. Hydrogen; H ₂ ; [1333-74-0] 2. Water; H ₂ O; [7732-18-5]	ORIGINAL MEASUREMENTS: Longo, L. D.; Delivoria- Papadopoulos, M.; Power, G. G.; Hill, E. P.; Forster, R. E., Am. J. Physiology, 1970, 219, 561-569.
VARIABLES:	PREPARED BY: + C. L. Young
EXPERIMENTAL VALUES:	<u> </u>
T/K Bunsen coeffi	cient, a S.D.*
310.15 0.01629	0.0001
than that derived from recomm	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Liquid samples were equilibrated with gas and then the dissolved gas was stripped out under vacuum and measured in a manometric Van Slyke apparatus. Some details in ref. 1.	No details given.
	ESTIMATED ERROR: $\delta T/K = \pm 0.03.$ REFERENCES:
	1. Power, G. G., J. Appl. Physiology, 1968, 24, 468.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Power, G.G.; Stegall, H. 2. Water; H₂O; [7732-18-5] J. Appl. Physiology, 1970, 29,145-9 VARIABLES: PREPARED BY: C.L. Young + EXPERIMENTAL VALUES: Bunsen coefficient, S.D. * No. of measurements T/K 310.15 0.01629 0.00011 * Standard deviation. + added by editor. Bunsen coefficient is about 1.5% lower than that derived from recommended smoothing equation AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 5 to 12 ${\rm cm}^{-3}$ samples placed in a stirrer cell and gas, saturated Matheson sample, purity better than 99.7 mole per cent. with water vapor passed through water for 30-60 mins. Samples of saturated liquid withdrawn and transferred to Van Slyke apparatus. Dissolved gas removed under reduced pressure. ESTIMATED ERROR: $\delta T/K = \pm 0.1$ REFERENCES:

- 1. Hydrogen; H₂; 1333-74-0
- 2. Sea Water

EVALUATOR:

Denis A. Wiesenburg Department of Oceanography Texas A&M University College Station, Texas 77843 USA June 1980

CRITICAL EVALUATION:

There are two reports of the solubility of hydrogen in sea water $(1,\,2)$. It is fortunate that these two reports cover both a wide range of temperatures and salinities, use different experimental techniques, and obtain results in good agreement. Crozier and Yamamoto (1) report 222 solubility measurements for distilled water and three salinities $(27.665,\,33.680,\,39.927\%_{\circ})$ for many different temperatures between 274.60 and 303.48° K. Their solubility measurements are estimated to have an accuracy of $0.5\%_{\circ}$. Gordon et al. (2) report 39 solubility values over the temperature range 272.80 to $\overline{302.41^{\circ}}$ K for distilled water and sea water to $39.096\%_{\circ}$. The data of Gordon et al. (2) average about $0.5\%_{\circ}$ higher than those of Crozier and Yamamoto $\overline{(1)}$, but differences are never greater than $1\%_{\circ}$. Both of these studies measured Bunsen solubility coefficients by equilibrating sea water with pure hydrogen at 1 atm total pressure. The volumes of sea water equilibrated in each study were quite different, however, 6 ml (1) vs. 1000 ml (2).

The solubility data of Crozier and Yamamoto (1) and Gordon et al. (2) are similar in precision and thus are combined to form the data base for this evaluation. Gordon et al. (2) also combined the two data sets and determined a smoothing equation, but they weighted each data set equally. Since the data of Crozier and Yamamoto (1) are not statistically different from those of Gordon et al. (2), the data used here are combined without weighting. The combined data sets have been fitted (3) by the method of least squares to an equation developed by Weiss (4) which expresses solubility as the natural logarithm of the Bunsen coefficient, α , and is consistent with both the integrated form of the van't Hoff equation and the Setchenow salt effect relation. The equation for hydrogen is valid from 273.15 to 303.15°K and a salinity range, S, of 0 to 40%. The smooth equation reproduced the combined hydrogen data with a root-mean-square deviation of 7.8 x 10-5 units (\sim 0.46%). The equation is

```
\ln \alpha = -47.9848 + 65.0368 (100/T) + 20.1709 \ln (T/100) 
+ S[-0.082225 + 0.049564 (T/100) - 0.0078689 (T/100)^2]
```

where S is the salinity in parts per thousand. Wiesenburg and Guinasso (3) give an extensive table of hydrogen Bunsen coefficients calculated from the above equation.

Although the Bunsen solubility coefficients are well defined by the above equation, for practical purposes, oceanographers require the atmospheric equilibrium solubility values in their work. Weiss (4) has proposed an equation similar to the above which expresses the atmospheric equilibrium solubility from moist air at 1 atm total pressure, in units of Volume (STP) dm-3, as a function of salinity and temperature. In working with samples from the depths of the ocean, it is also advantageous to express atmospheric solubilities in terms of mol kg-1, which are pressure and temperature independent (4, 5). Weiss' atmospheric solubility equation is based on the assumption of a constant atmospheric concentration of hydrogen. Since hydrogen is variable in the atmosphere, Weiss' (4) equation has been modified (3) to include the atmospheric concentration as a variable. The combined data sets for hydrogen (1, 2) have been fitted (3) to the equations

- Hydrogen; H₂; 1333-74-0
- 2. Sea Water

EVALUATOR:

Denis A. Wiesenburg Department of Oceanography Texas A&M University College Station, Texas 77843 USA June 1980

CRITICAL EVALUATION:

$$\ln \text{ m/nmol kg}^{-1} = f_g - 320.3079 + 459.7398 (100/T)$$

$$+ 299.2600 \ln (T/100) - 49.3946 (T/100)$$

$$+ S \left[-0.074474 + 0.043363 (T/100) - 0.0067420 (T/100)^2 \right]$$

where f_g is the mole fraction of hydrogen in dry air. In these calculations hydrogen was assumed to be an ideal gas. Vapor pressure for pure water was calculated using the equation of Bridgeman and Aldrich (6) and corrected for salinity effects using the expression of Robinson (7). Knudsen's (8) formula was used to calculate densities. These two equations can be used to calculate the atmospheric equilibrium solubility of hydrogen under any given conditions of temperature, salinity, and atmospheric concentration. Using an atmospheric hydrogen mole fraction of 0.58 x 10^{-6} (9), the equations reproduce the individual calculated atmospheric solubilities with a root-mean-square deviation of 0.45%.

In making calculations of atmospheric equilibrium solubilities from Bunsen solubilities measured at 1 atm of pure hydrogen, there is a question of whether Henry's law can be extrapolated accurately through six orders of magnitude (10, 11). Schmidt (12) considered this problem by making atmospheric solubility measurements of hydrogen at partial pressures of hydrogen of about 10^{-5} atm. He measured solubilities for pure water and sea water (24 values) at 31.6%. salinity over the temperature range 273.15 to 303.15°K by equilibrating sea water with air containing 21.5 ppmv hydrogen. The standard error of Schmidt's data (7%) is higher than that of the other data evaluated here (1, 2), but within the standard error of his data, Schmidt's data are consistent with the Bunsen coefficients measured at 1 atm.

References

- Crozier, T. E.; Yamamoto, S. *J. Chem. Eng. Data* <u>1974</u>, 19, 242. Gordon, L. I.; Cohen, Y.; Standley, D. R. *Deep-Sea Res.* <u>1977</u>, 24, 937.
- Wiesenburg, D. A.; Guinasso, N. L., Jr. J. Chem. Eng. Data 1979, 24, 3.
- 4.
- Weiss, R. F. Deep-Sea Res. 1970, 17, 721.

 Kester, D. in "Chemical Oceanography" v. 1 2nd Edition, J. P. Riley and G. Skirrow, eds. Academic Press, New York, 1975, pp. 497-556.

 Bridgeman, O. C.; Aldrich, E. W. J. Heat Transfer 1964, 86, 279.

 Robinson, R. A. J. Mar. Biol. Assoc. U.K. 1954, 33, 449.
- 7.
- 8.
- 9.
- Knudsen, M. Hydrographical Tables, G. E. Gad, Copenhagen, 1901. Schmidt, U. J. Geophys. Res. 1978, 83, 941. Bieri, R. H. in "The Sea', v. 5, E. D. Goldberg, ed., Wiley Interscience, New York, 1974, pp. 199-218. Meadows, R. W.; Spedding, D. J. Tellus 1974, 26, 143. 10.
- 12. Schmidt, U. Tellus 1979,31, 68.

Seawater 19

COMPONENTS:

- 1. Hydrogen; H₂;1333-74-0
- Sea Water

ORIGINAL MEASUREMENTS:

Crozier, T. E.; Yamamoto, S.

J. Chem. Eng Data 1974, 19, 242 - 244.

VARIABLES:

T/K:

274.60 - 303.49 101.325 (1 atm) H₂ P/kPa: Salinity/% o: 0 - 39.927

PREPARED BY:

Denis A. Wiesenburg

EXPERIMENTAL VALUES:

Salinity %。	Temp/K	Bunsen Coefficient	Salinity %。	Temp/K	Bunsen Coefficient
·		α			α
0.0	274.60	0.02150	0.0	287.85	0.01871
	274.63	0.02148		287.91	0.01882
	274.64	0.02152		287.92	0.01869
	277.54	0.02081		287.94	0.01871
	277.70	0.02074		287.94	0.01890
	277.70	0.02067		287.94	0.01885
	277.73	0.02072		287.95	0.01880
	277.74	0.02079		290.01	0.01806
	282.98	0.01954		290.01	0.01812
	282.99	0.01964		290.02	0.01811
	282.99	0.01949		290.03	0.01804
	283.00	0.01947		290.03	0.01805
	283.00	0.01949		297.85	0.01740
	283.00	0.01955		297.85	0.01754
	283.01	0.01960		297.88	0.01747
	283.01	0.01957		297.88	0.01741
	283.02	0.01957		297.92	0.01742
	283.03	0.01960		301.99	0.01696
	287.77	0.01882		302.17	0.01709
	287.80	0.01876		302.31	0.01706
	287.82	0.01873		302.47	0.01712

Continued on next page.

AUXILIARY INFORMATION

METHOD APPARATUS / PROCEDURE:

Solubility determinations were made using the Scholander microgasometric technique (1) as modified by Douglas (2). Pure hydrogen and degassed sea water were introduced into a reaction vessel in a constant temperature room. The vessel was shaken vigor-Ously to allow equilibration between the hydrogen and sea water. amount of gas absorbed and the Volume of sea water were measured volumetrically with a microburet. Bunsen solubility coefficients were calculated from the observed volumes.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Linde Specialty Gas, specified 99.9995% purity.
- Sea Water. Passed through $0.45\text{-}\mu\text{m}$ millipore filter and poisoned with 1 mg/l of MgCl2. Sea water was boiled or diluted with glass distilled water (used for 0 % o) to obtain desired salinities.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta S/\%_o = 0.003$

REFERENCES:

- 1. Braun, L.
 - Z. Phys. Chem. 1900,33, 721.
- 2. Douglas, E. J. Phys. Chem. 1964,68, 169. ibid. 1965,69, 2608.

20		Hydrogen Solub	oilities up to 200kPa	l		
COMPONENTS:			ORIGINAL MEASUR	EMENTS:		
1. Hydroge	n; H ₂ ; 1333	-74-0	Crozier, T.	E.; Yamam	oto, S.	
2. Sea Water		J. Chem. En 242 - 244.	J. Chem. Eng. Data <u>1974</u> , 19,			
VARIABLES: T/K H ₂ P/kPa Salinity/°/	: 101.325	- 303.49 (1 atm) 927	PREPARED BY:	nis A. Wie	senburg	
EXPERIMENTAL V	ALUES:					
Salinity %。	Temp/K	Bunsen Coefficient	Salinity %。	Temp/K	Bunsen Coefficient	
27.665	274.78 274.81 274.83 274.83 274.83 274.84 274.84 274.84 274.85 280.17 280.18 280.18 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19 280.19	0.01856 0.01859 0.01847 0.01850 0.01853 0.01851 0.01851 0.01860 0.01861 0.01754 0.01751 0.01755 0.01755 0.01755 0.01755 0.01752 0.01754 0.01754 0.01752 0.01754 0.01680 0.01682	27.665	285.23 285.23 285.24 285.24 285.25 285.25 292.23 292.23 292.23 292.24 292.24 292.24 292.24 292.24 292.24 292.24 292.25 298.35 298.35 298.35	0.01680 0.01681 0.01681 0.01684 0.01684 0.01688 0.01599 0.01598 0.01595 0.01596 0.01597 0.01598 0.01599 0.01601 0.01602 0.01541 0.01541 0.01547	
Continued	on next pag	ge.				
		AUXILIARY	INFORMATION			
METHOD 'APPARAT	US/PROCEDURE:	<u></u>	SOURCE AND PURI	TY OF MATERI	ALS:	
See prev	ious page.		See previ	ous page.		

AUXILIARY INFORMATION METHOD 'APPARATUS/PROCEDURE: See previous page. See previous page. ESTIMATED ERROR: See previous page. REFERENCES: See previous page.

Seawater 21 COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; 1333-74-0 Crozier, T. E.; Yamamoto, S. Sea Water J. Chem. Eng. Data 1974, 19, 242 - 244.VARIABLES: PREPARED BY: 274.60 - 303.49 101.325 (1 atm) T/K: H₂ P/kPa: Denis A. Wiesenburg Salinity/% .: 0 - 39.927EXPERIMENTAL VALUES: Salinity Salinity Temp/K Bunsen Temp/K Bunsen %。 Coefficient %。 Coefficient α α 27.665 298.37 0.01548 33.680 275.15 0.01783 298.37 0.01550 275.16 0.01783 298.38 0.01540 281.42 0.01679 298.40 0.01549 281.44 0.01682 303.41 0.01511

0.01684 281.44 303.41 0.01508 281.44 0.01678 303.42 0.01503 281.45 0.01686 303.43 0.01507 281.46 0.01684 303.43 0.01511 281.46 0.01690 303.44 0.01501 281.47 0.01682 303.47 0.01510 281.47 0.01682 303.47 0.01512 281.48 0.01679 303.47 0.01513 286.63 0.01618 303.48 0.01516 286.63 0.01616 286.63 0.01609 33.680 275.10 0.01778 286.63 0.01606 275.12 0.01789 286.63 0.01608 275.12 0.01782 286.63 0.01619 275.13 0.01783 0.01621 286.63 275.13 0.01784 286.63 0.01618 275.14 0.01787 286.63 0.01617 275.14 0.01795 286.64 0.01619 275.14 0.01778 292.33 0.01559

Continued on next page.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
See previous page.	See previous page.
	ESTIMATED ERROR:
	See previous page.
	REFERENCES:
	See previous page.

22 Hydrogen Solubilities up to 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; 1333-74-0 Crozier, T. E.; Yamamoto, S. 2. Sea Water J. Chem. Eng. Data 1977, 19, 242 - 244.VARIABLES: PREPARED BY: T/K: 274.60 - 303.49 H₂ P/kPa: 101.325 (1 atm) Denis A. Wiesenburg Salinity/% .: 0 - 39.927 EXPERIMENTAL VALUES: Salinity Temp/K Salinity Temp/K Bunsen Bunsen %。 Coefficient %。 Coefficient 33.680 292.36 0.01555 33.680 303.11 0.01472 303.11 0.01477 292.37 0.01554 292.38 303.11 0.01482 0.01557 292.38 0.01545 303.12 0.01486 0.01473 292.40 303.13 0.01550 292.41 0.01555 303.14 0.01491 292.43 0.01547 274.65 0.01730 292.44 0.01554 39.927 292.46 0.01555 274.65 0.01730 274.65 0.01734 298.10 0.01519 298.13 274.65 0.01729 0.01502 298.13 274.65 0.01744 0.01502 298.14 274.66 0.01728 0.01515 274.66 298.14 0.01739 0.01507 298.15 0.01506 274.66 0.01723 274.66 0.01734 298.16 0.01513 298.16 274.67 0.01723 0.01515 298.16 279.63 0.01658 0.01504 279.63 298.17 0.01655 0.01517 303.08 0.01480 279.65 0.01655 303.11 279.66 0.01658 0.01486 279.67 303.11 0.01656 0.01477 303.11 0.01469 279.68 0.01652 Continued on next page. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: See previous page. See previous page. ESTIMATED ERROR:

See previous page.

REFERENCES:

See previous page.

Seawater 23

ORIGINAL MEASUREMENTS:

1. Hydrogen; H₂; 1333-74-0

2. Sea Water

VARIABLES:

T/K: 274.60 - 303.49

H₂ P/kPa: 101.325 (1 atm)
Salinity/% : 0 - 39.927

ORIGINAL MEASUREMENTS:

Crozier, T. E.; Yamamoto, S.

J. Chem. Eng. Data 1974, 19,
242 - 244.

PREPARED BY:
Denis A. Wiesenburg

EXPERIMENTAL VALUES:

Salinity %。	Temp/K	Bunsen Coefficient	Salinity %	Temp/K	Bunsen Coefficient
		α			α
39.927	279.68	0.01649	39.927	291.79	0.01519
	279.68	0.01654		291.83	0.01517
	279.68	0.01658		297.52	0.01469
	279.69	0.01653		297.52	0.01466
	285.63	0.01573		297.53	0.01465
	285.63	0.01573		297.53	0.01467
	285.63	0.01573		297.53	0.01471
	285.63	0.01575		297.54	0.01466
	285.63	0.01574		297.54	0.01461
	285.63	0.01569		297.54	0.01466
	285.65	0.01577		297.55	0.01465
	285.65	0.01574		297.55	0.01470
	285.66	0.01573		303.40	0.01446
	285.68	0.01571		303.41	0.01431
	291.73	0.01515		303.41	0.01441
	291.75	0.01516		303.41	0.01449
	291.75	0.01516		303.41	0.01439
	291.76	0.01514		303.42	0.01432
	291.76	0.01526		303.43	0.01444
	291.79	0.01519		303.44	0.01434
	291.79	0.01517		303.44	0.01440
	291.79	0.01525		303.44	0.01431

AUXILIARY INFORMATION .

	AUXILIARI INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
See previous page.	See previous page.
	ESTIMATED ERROR:
	See previous page.
	REFERENCES:
	See previous page.

COMPONENTS:

- 1. Hydrogen; H₂; 1333-74-0
- 2. Sea Water

ORIGINAL MEASUREMENTS:

Gordon, L. I.; Cohen, Y.; Standley, D. R.

Deep-Sea Res. 1977, 24, 937 - 941.

VARIABLES:

T/K: 272.80 - 302.41

 H_2 P/kPa: 101.325 (1 atm) Salinity/% o: 0 - 39.096 PREPARED BY:

Denis A. Wiesenburg

EXPERIMENTAL VALUES:

Temp/K	Salinity %。	Bunsen Coefficient	Temp/K	Salinity %。	Bunsen Coefficient
		$\alpha \times 10^3$			$\alpha \times 10^3$
272.80	29.931	18.75	296.78	0.000	17.62
273.29 273.18 273.17 278.19 278.20 278.20 278.21 283.15 283.15 283.17 283.11 283.17 283.19 283.12 289.82 289.82	0.000 10.626 20.396 35.109 0.000 9.470 19.757 30.060 37.810 0.000 10.063 19.694 19.736 38.079 0.000 10.524	22.17 21.00 19.90 18.44 20.63 19.55 18.94 17.68 17.03 19.66 19.67 18.80 17.68 17.75 16.26 18.66 17.72	296.78 296.77 296.77 296.77 296.77 296.77 297.91 302.40 302.41 302.40 302.41 302.40 302.41 302.40 302.41	4.919 10.385 17.115 19.675 34.728 39.096 32.901 0.000 7.946 12.260 17.154 21.898 25.171 25.325 32.022 32.570 38.981	17.50 17.02 16.53 16.20 15.13 14.88 15.39 17.18 16.68 16.28 16.02 15.68 15.31 15.23 14.97 14.82 14.39
289.83 289.83	20.156 32.284	16.94 15.93			
289.79	37.317	15.50			

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

Solubility determinations were made using the method of Ben-Naim and Baer (1) as modified by Murray et al. (2), with slight further modifications. Pure hydrogen which had been saturated with sea water was placed in contact with a known volume of sea water in a thermostated dissolution flask. The sea water was mechanically stirred and the total gas pressure was maintained at 1 atm, using a gas manometer and a mercury leveling bulb. Solubility was calculated from the difference in buret readings, before and after solubility equilibrium had been maintained (about 7 hours duration), and the known volume of sea water.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Ultra-pure electrolytically generated hydrogen was used.
- 2. Sea Water. Aged surface sea water filtered and adjusted to pH < 3.2 with 4N HCl. Sea waters of various salinities were made by addition of distilled water or by evaporation.

ESTIMATED ERROR:

REFERENCES:

- Ben-Naim, A.; Baer, S. Trans. Faraday Soc. <u>1963</u>, 59, 2735.
- Murray, C.N.; Riley, J.P.;
 Wilson, T.R.S.
 Deep-Sea Res. 1969,16, 297.

COMPONENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Electrolyte

EVALUATOR:

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

1980, October

CRITICAL EVALUATION:

An Evaluation of the Solubility of Hydrogen in Aqueous Electrolyte Solutions at a Hydrogen Partial Pressure of 101.325 kPa.

Not enough workers have measured the solubility of hydrogen in any one aqueous electrolyte system over common ranges of concentration and temperature to recommend solubility values. Most of the available data are classed as tentative.

In order to have a common basis for comparison, the solubility data have been converted to Sechenow salt effect parameters in the form

$$k_{CSG}/dm^3 \text{ mol}^{-1} = (1/(c/mol dm^{-3}))\log(\alpha^{\circ}/\alpha)$$

where c is the electrolyte concentration in mol dm $^{-3}$ and α ° and α are the Bunsen coefficients in pure water and electrolyte solution, respectively. The Ostwald coefficient ratio, L°/L, will give the same value, but the salt effect parameter is symbolized, k_{SCL} . Both ratios are equivalent to a molar gas solubility ratio.

Other forms of the salt effect parameter will be found on the data sheets that follow this discussion. They include

$$k_{sms}/kg \text{ mol}^{-1} = (1/(m/mol kg^{-1}))log(s^{\circ}/s)$$

$$k_{SCx}/dm^3 \text{ mol}^{-1} = (1/(c/\text{mol dm}^{-3}))\log(x^\circ/x)$$

$$k_{smx}/kg \text{ mol}^{-1} = (1/(m/mol kg^{-1}))log(x^{\circ}/x)$$

where m is the electrolyte molality, s°/s is the Kuenen coefficient ratio, and x°/x is the mole fraction gas solubility ratio usually calculated with respect to all ions in the solution. The Kuenen coefficient, s, is referenced to 1 gof water whether it is for pure water or the electrolyte solution. Thus the s°/s ratio is proportional to a gas molality ratio m°/m. The density data required to convert the salt effect parameter from one form to another were taken from the International Critical Tables, McGraw-Hill, 1928, v. III.

The salt effect parameter is often assumed to be independent of electrolyte concentration. This is definitely not true of aqueous sulfuric acid solutions. It is probably true only as an approximation for many other solutions. There are indications through out the literature that the salt effect parameter values are larger in dilute solutions than at higher concentrations but there are no definitive studies on the point.

The effect of the electrolyte concentration on the salt effect parameter was checked by one of two ways. A graph was prepared either of $\log{(\alpha\,^{\circ}/\alpha)}$ vs. c or of $k_{SC\alpha}$ vs. c. A linear $\log{(\alpha\,^{\circ}/\alpha)}$ vs. c plot shows no concentration dependence to the salt effect parameter and the slope is $k_{SC\alpha}$.

A linear k vs. c plot of zero slope

shows no concentration dependence to the salt effect parameter. The second type of graph is more sensitive to small changes in $k_{\mbox{sc}\alpha}$ with concentration than the first type.

The solubility of hydrogen in water has usually been taken from the paper under evaluation for the calculation of the salt effect parameter. The reason for using the water solubility of the author, instead of the recommended solubility of hydrogen in water, is that systematic errors in a given authors work may cancel in the $\alpha^{\,\circ}/\alpha$ ratio.

The use of a salt effect parameter of the Sechenow type should not be taken to mean that it is necessarily the best way to represent salt effect results. It is used here as a convenient parameter for the comparison of data from several sources.

Studies of the solubility of hydrogen in aqueous electrolyte solutions appear in about fifteen papers. Some specific comments on several of the papers follow.

Geffcken (1) measured the solubility of hydrogen in five aqueous systems over an extended electrolyte range of concentration. His average value of the Ostwald coefficient of hydrogen in water of 0.01926 at 298.15 K is 0.78 per cent higher than the recommended value. His salt effect parameters usually show a small decrease in value as the electrolyte concentration increases.

Morrison and Billett (4) measured the solubility of hydrogen at four temperatures in four aqueous systems. Their values of the solubility of hydrogen in water agree well with the recommended values. A weakness of their work is that they report only the salt effect parameter, which is based on a solubility measurement at just one electrolyte concentration. They have reported what is equivalent to a molal gas solubility ratio.

Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in eight aqueous systems at temperatures up to 523 K in a high pressure apparatus. Their solubilities are given as Bunsen coefficients which are treated here as if they apply at a hydrogen partial pressure of 101.325 kPa. They did not measure the solubility of hydrogen in water, but they did their own evaluation of the solubility of hydrogen in water from literature data. Their data table includes both the solubility, α , and the corresponding ratio α/α° . From the α/α° values one can deduce the solubility values of hydrogen in water used by them are

T/K	298.15	323.15	348.15	373.15
$\alpha^{\circ}/\text{cm}^3 \text{ cm}^{-3} \text{ atm}^{-1}$	0.01744	0.01629	0.01637	0.01835
T/K	398.15	423.15	473.15	523.15
$\alpha^{\circ}/\text{cm}^3 \text{ cm}^{-3} \text{ atm}^{-1}$	0.02031	0.02328	0.03149	0.04456

The salt effect parameters, k_{SCQ} , at the electrolyte concentrations of 0.5, 1.0, and 1.5 mol dm $^{-3}$ were calculated directly from the inverse of the α/α° ratio tabulated in the paper. The values, which scatter widely, do not appear to show a correlation with either electrolyte concentration or temperature. The tabulated values of k_{SCQ} are average values of the three values measured at the three electrolyte concentrations. Although

three values measured at the three electrolyte concentrations. Although the data are classed as tentative they do not appear to be quite as reliable as the data from most of the other papers. In general the salt effect parameters calculated from the data in their paper are greater than the values obtained by other workers. This is probably due in part to the difficulties in making measurements at high pressure.

Deckwer (14) measured the solubility of hydrogen in aqueous manganese (II) sulfate solution at several temperatures between 293.15 and 353.15 K. He did not measure the solubility of hydrogen in water, but he took literature values from the Seidell Linke Handbook. A more consistent set of salt effect parameters was obtained when the recommended water solubility values from this volume were used. They are the salt effect parameters presented.

Shoor, Walker, and Gubbins (9) measured the solubility of hydrogen in aqueous KOH solutions. They calculated their salt effect parameters from the hydrogen mole fraction solubility ratio, x^0/x . Their salt effect parameters were not converted from the k_{SCX} to the k_{SCX} form because (1) reliable density data for aqueous KOH was not readily available, and (2) the authors did not define whether their mole fraction values were based on the KOH ion pairs or on the K+ and OH- ions.

Hydrogen solubility measurements have been reported in over 20 aqueous electrolyte systems. Each system is discussed briefly on the following pages. Unless otherwise stated, the salt effect parameters are for a one mole dm⁻³ solution at a hydrogen partial pressure of 101.325 kPa. Tentative values of the salt effect parameters are given as calculated from the various papers. The systems are given in the order of the standard arrangement for electrolytes used in U.S. National Bureau of Standards publications.

1. Hydrogen + water + Hydrochloric acid [7647-01-0]

Geffcken (1) measured the solubility of hydrogen in aqueous hydrochloric acid at nine concentrations up to 2.836 mol $\rm dm^{-3}$ at 298.15 K. The salt effect parameter decreases with increasing HCl concentration

$$k_{SCQ}/cm^3 \text{ mol}^{-1} = 0.0297 - 2.20 \times 10^{-4} (c_3/mol dm^{-3})$$

At 298.15 K and one mole dm^{-3} HC1 the tentative value of $k_{_{\mbox{SC}\alpha}}$ is 0.0295.

2. Hydrogen + water + Sulfuric acid [7664-93-9]

Although the solubility of hydrogen in aqueous sulfuric acid has been measured in four laboratories, no two laboratories report data at a common temperature. Christoff (2) measured the solubility at 293.15 K and three concentrations between 35.8 and 95.6 weight per cent sulfuric acid. There is not enough data to identify the acid concentration of minimum hydrogen solubility, but it is probably near 80 weight percent. Salt effect parameters of 0.0729 and 0.0490 were calculated from the Christoff data at 4.63 and 9.53 mol dm $^{-3}$ $\rm H_2SO_4$. Assuming a linear change of $\rm k_{SCO}$ with concentration gives

$$k_{sc\alpha}/dm^3 \text{ mol}^{-1} = 0.0955 - 4.88 \times 10^{-3} c_3/\text{mol} dm^{-3}$$

Geffcken (1) measured the solubility at 298.15 K at eleven sulfuric acid concentrations up to 2 mol $\rm dm^{-3}$. The salt effect parameter decreases with increasing acid concentration

$$k_{SCG}/dm^3 \text{ mol}^{-1} = 0.0718 - 7.16 \times 10^{-4} c_3/\text{mol dm}^{-3}$$

Ruetschi and Amlie (8) measured the solubility of hydrogen at ten concentrations up to $7.6~\text{mol}~\text{dm}^{-3}$ sulfuric acid. The salt effect parameter decreases with increasing acid concentration

$$k_{SCN}/dm^3 \text{ mol}^{-1} = 0.0932 - 6.68 \times 10^{-3} c_3/\text{mol} dm^{-3}$$

The data of Christoff and of Ruetschi and Amlie roughly parallel each other as a function of concentration, but the data of Christoff is too limited for the agreement to be meaningful.

Bruhn, Gerlach and Pawlek (7) measured the solubility of hydrogen at sulfuric acid concentrations of 0.5, 1.0, and 1.5 mol dm $^{-3}$ at five temperatures between 323.15 and 523.15 K. As discussed earlier in the section their salt effect parameter values show considerable scatter and poor correlation with both acid concentration and temperature. The average of their $k_{\mbox{\scriptsize SC}\alpha}$ values at each temperature show little change with temperature.

Tentative values of the salt effect parameters at a sulfuric acid concentration of one mole dm^{-3} from the four papers are:

T/K	293.15	298.15	303.15	323.15
$k_{sca}/dm^3 mol^{-1}$	0.0906	0.0711	0.0865	0.075
σ^1				0.014
T/K	373.15	423.15	473.15	523.15
$k_{sca}/dm^3 mol^{-1}$	0.074	0.080	0.074	0.074
σ^1	0.023	0.001	0.003	0.026

3. Hydrogen + water + Nitric acid [7697-37-2]

Geffcken (2) made ten measurements of the hydrogen solubility at 298.15 K up to a concentration of 4.23 mol $\rm dm^{-3}$ nitric acid. The salt effect parameters show some scatter but there is a tendency to a decrease in the parameters as the acid concentration increases.

$$k_{sca}/dm^3 \text{ mol}^{-1} = 0.0220 - 5.3 \times 10^{-4} c_3/\text{mol} dm^{-3}$$

The tentative value of the salt effect parameter at 298.15 K and one mol dm-3 nitric acid is 0.0215 dm 3 mol $^{-1}$.

4. Hydrogen + water + Ammonium hydroxide [1336-21-6]

Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in aqueous solutions of ammonium hydroxide at concentrations of 2.87, 3.63, and 8.28~mol dm $^{-3}$ at temperatures up to 423 K. Ammonium hydroxide shows only a small salt effect. There is no discernable trend with either concentration or temperature. The tentative values are the average of the three salt effect parameters at each temperature.

T/K	298.15	323.15	348.15	373.15	423.15
$k_{sc\alpha}/dm^3 mol^{-1}$	0.0043	0.0064	0.0025	0.0040	0.0042
σ^1	0.0016	0.0012	0.0015	0.0012	0.0014

5. Hydrogen + water + Ammonium chloride [12125-02-9]

Gerecke and Bittrich (12) measured the solubility of hydrogen in several ammonium chloride solutions at temperatures of 288.15 and 323.15 K. They cite a salt effect parameter value at 298.15 K from the thesis of Gerecke (10). The hydrogen solubility is reported as a Kuenen coefficient and the salt concentration is reported as molality (mol kg-l). Their salt effect parameter, $k_{\rm Sms}$, was converted to a $k_{\rm SCC}$ value. The tentative values for a one mol dm-3 solution are

T/K	288.15	298.15	323.15
$k_{sms}/kg mol^{-1}$	0.055	0.057	0.044
$k_{sca}/dm^3 mol^{-1}$	0.057	0.059	0.046

6. Hydrogen + water + Ammonium sulfate [7783-20-2]

Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in aqueous ammonium sulfate at 0.25, 0.75, 1.5 and 3.0 mol dm $^{-3}$ at temperatures up to 523 K. The individual $k_{\rm SC}\alpha$ values show considerable scatter, The four values at each temperature were averaged for the tentative salt effect parameter values. They are

¹ Standard deviation

T/K						
$k_{sc\alpha}/am^3 mol^{-1}$	0.148	0.145	0.152	0.140	0.156	0.151
σ	0.022	0.046	0.025	0.024		

7. Hydrogen + water + Ammonium nitrate [6684-52-2]

Knopp (15) made measurements on this system for six different concentrations at 293.15K. The results show some scatter. The tentative value of k is 0.033 dm 3 mol 1

8. Hydrogen + water + Zinc sulfate [7732-02-0]

Steiner (16) made measurements on this system for four different concentrations at temperatures near 288K and "adjusted" values to 288.2K. The tentative value of k is 0.237 dm mol $^{-1}$ at a salt concentration of 1 mol dm 3 . There appears to be a slight decrease of k with increasing concentration.

9. Hydrogen + water + Copper (II) sulfate [7758-98-7]

Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in aqueous copper sulfate of 0.5, 1.0, and 1.5 mol dm $^{-3}$ and temperatures up to 398.15 K. There is no definite trend in the salt effect parameter with either copper sulfate concentration or temperature. The three values of $k_{\mbox{\footnotesize SC}\alpha}$ at each temperature were averaged to give the tentative salt effect parameters below.

T/K			348.15		
$k_{sc\alpha}/dm^3 mol^{-1}$	0.169	0.170	0.156	0.158	0.176
σ	0.021	0.037	0.015	0.023	0.018

10. Hydrogen + water + Nickel sulfate [7786-81-4]

Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in aqueous nickel sulfate at 0.5, 1.0, and 1.5 mol dm $^{-3}$ and temperatures up to 398.15 K. There is no definite trend in the salt effect parameter with either nickel sulfate concentration or temperature. The three values of $k_{\text{SC}\alpha}$ at each temperature were averaged to obtain the tentative salt effect parameters below.

T/K		323.15			
$k_{sc\alpha}/dm^3 mol^{-1}$	0.174	0.184	0.164	0.177	0.173
σ	0.021	0.036	0.018	0.033	0.015

11. Hydrogen + water + Cobalt (II) sulfate [10124-43-3]

Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in aqueous cobalt sulfate at 0.5, 1.0, and 1.5 mol dm^{-3} and temperatures up to 398.15 K. There is no definite trend in the salt effect parameter with either cobalt sulfate concentration or temperature. The three values of $k_{\mbox{\footnotesize SCC}}$ at each temperature were averaged to obtain the tentative salt effect parameters below.

T/K			348.15		
$k_{sc\alpha}/dm^3 mol^{-1}$	0.157	0.156	0.157	0.159	0.155
σ	0.019	0.036	0.006	0.012	0.027

12. Hydrogen + water + Hydrate iron (III) oxide [12259-21-1]

The data of Shkol'nikova (6) are classed as tentative. She made no solubility measurements in pure water. No salt effect parameters were calculated for the colloidal solutions.

13. Hydrogen + water + Manganese (II) sulfate [7785-87-7]

Deckwer (14) measured the solubility of hydrogen in aqueous manganese (II) sulfate up to a concentration of 3.5 mol dm^{-3} at six temperatures between 293.15 and 353.15 K. He did not measure the solubility of hydrogen in water. The salt effect parameters were calculated using the recommended hydrogen in water values of this volume, rather than the literature values picked by Deckwer.

The salt effect parameters appear to be a function of the electrolyte concentration at each temperature. An equation for the salt effect parameter as a linear function of the Manganese (II) sulfate concentration and the $k_{\rm SCC}$ values at concentrations of one and three mol dm-3 are given below.

T/K	$k_{sc\alpha} = a + b C_3$	1 mol dm ⁻³ ksca	3 mol dm^{-3}
293.15	0.111 + 0.037 C ₃	0.148	0.222
303.15	0.133 + 0.025 C ₃	0.158	0.208
313.15	0.155 + 0.013 C ₃	0.168	0.194
323.15	$0.154 + 0.010 C_3$	0.164	0.184
333.15	$0.175 + 0.003 C_3$	0.178	0.184
353.15	0.160 + 0.007 C ₃	0.167	0.181

14. Hydrogen + water + Hydrated aluminum oxide [1333-84-6]

The data of Shkol'nikova (6) are classed as tentative. She made no pure water hydrogen solubility measurements. No salt effect parameters were calculated for the colloidal solutions.

15. Hydrogen + water + Aluminium Chloride [7446-70-0]

This system has been studied by Steiner (16) at four different salt concentrations at temperatures near 288K. Values "adjusted" to 288.2K were reported and give a tentative value of $k_{SC}\alpha$ of 0.197 dm³ mol-1 at a salt concentration of 1 mol dm-3. There appears to be a slight decrease of $k_{SC}\alpha$ with increasing concentration.

16. Hydrogen + water + Lanthanum chloride [10099-58-8]

Morrison and Billett (4) measured the solubility of hydrogen in 0.333 mol kg⁻¹ LaCl $_3$ at four temperatures. Their salt effect parameter, k was recalculated as a k sc α value at 1 mol dm⁻³. The values are classed as tentative.

T/K	285.75	303.15	322.55	344.85
k _{sms} /kg mol ⁻¹	0.237	0.234	0.228	0.225
$k_{sc\alpha}/dm^3 mol^{-1}$	0.240	0.247	0.252	0.265

17. Hydrogen + water + Uranyl sulfate [1314-64-3]

Stephan, Hatfield, Peoples and Pray (5) measured the solubility of hydrogen in aqueous uranyl sulfate of 40, 100, and 243 g dm $^{-3}$ uranium at temperatures of 373.15, 408.15, and 435.93 K. Salt effect parameters were not calculated. The data are classed as tentative.

18. Hydrogen + water + Magnesium sulfate [7487-88-9]

This system has also been studied by Steiner (16) at four different salt concentrations at temperatures near 288K. Values "adjusted" to 288.2K were reported and give a tentative value of $k_{\rm SCQ}$ of 0.233 dm³ mol $^{-1}$ at a salt concentration of 1 mol dm $^{-3}$. There appears to be a slight increase of $k_{\rm SCQ}$ with increasing concentration.

19. Hydrogen + water + Calcium chloride [10043-52-4]

This system has been studied by Steiner (16) at six different salt concentrations at temperatures near 288K. Values "adjusted" to 288.2K were reported and give a tentative value of $k_{\text{SC}\alpha}$ of 0.194 dm³ mol $^{-1}$ at a salt concentration of 1 mol dm $^{-3}$. The salt effect parameters show some scatter but there is a tendency to a decrease in $k_{\text{SC}\alpha}$ as the salt concentration increases:

$$k_{SCQ}/dm^3 \text{ mol}^{-1} = 0.1976 - 3.2 \times 10^{-3} \text{ c}_3/\text{mol dm}^{-3}$$

where c3 is the salt concentration.

20. Hydrogen + water + Barium chloride [10361-37-2]

This system has been investigated by Braun (17). The salt effect parameters are as below at a concentration of 70g/kg (solution). The values calculated from Braun's data decrease with an increase in concentration. The Bunsen coefficients at the lowest temperature are thought to be considerably in error but the salting out parameters are probably more reliable, however the data are classified as doubtful.

T/K	278.2	283.2	288.2	293.2	298.2
$k_{\text{scc}}/\text{dm}^3 \text{ mol}^{-1}$	0.245	0.229	0.224	0.223	0.225

21. Hydrogen + water + Lithium chloride [7447-41-8]

Morrison and Billett (4) measured the solubility of hydrogen in one mol kg⁻¹ lithium chloride at four temperatures. Gerecke and Bittrich (12) and Gerecke (10) reported salt effect parameters at 288.15 and 298.15 K respectively. All of the salt effect parameters were converted to $k_{\mbox{sc}\alpha}$ values which are classed as tentative. The values for one mol dm⁻³ solutions are:

T/K	285.75	288.15	298.15	303.15	322.55	344.85
$k_{sca}/dm^3 mol^{-1}$	0.074	0.070	0.073	0.076	0.076	0.075

Steiners data (16) for this system give a value of $k_{\rm sca}$ of 0.078 mol dm⁻³.

22. Hydrogen + water + Sodium hydroxide [1310-73-2]

Geffcken (1) and Bruhn, Gerlach, and Pawlek (7) measured the solubility of hydrogen in aqueous sodium hydroxide. Geffcken made measurements at ten NaOH concentrations up to 4.687 mol dm⁻³ at 298.15 K. Bruhn et al. made measurements at 0.5, 1.0, and 1.5 mol dm⁻³ NaOH up to a temperature of 523 K. The salt effect parameter calculated from Geffcken's data is about 30 per cent lower than the values of Bruhn et al. at the higher temperatures.

The tentative salt effect parameters for a NaOH concentration of one mol dm^{-3} are

	298.15					
k _{sca} /dm ³ mol ⁻¹	0.137	0.181	0.190	0.179	0.173	0.189
	0.006					

23. Hydrogen + water + Sodium chloride [7647-14-5]

The solubility of hydrogen in aqueous sodium chloride was measured by Morrison and Billett (4) at four temperatures, by Gerecke and Bittrich (12) at two temperatures, by Gerecke (10) at one temperature, and by Crozier and Yamamoto (13) at five temperatures.

All measurements were converted to salt effect parameters, $k_{_{\rm SCO}}$. Morrison and Billett's measured the hydrogen solubility at one mol kg-l NaCl, while Crozier and Yamamoto made measurements at 0.1895 and 0.4815 mol kg NaCl. Gerecke and Bittrich made measurements over a range of 0.50 to 4.30 mol kg-l NaCl. Both Morrison and Billett and Gerecke and Bittrich reported log (S°/S) values and not the original solubility data. In the Morrison and Billett paper the ratio, S°/S, was identified as the hydrogen solubility ratio per kg of water. Gerecke and Bittrich identified the S°/S ratio as a ratio of Kuenen coefficients, which was taken to mean the solubility of hydrogen per g of water in both pure water and solution. Conversions to $k_{_{\rm SCO}}$ values were made consistent with the authors definitions.

The salt effect parameters scatter, but there is a general trend of a decrease of salt effect parameter magnitude as the temperature increases. A linear regression, over the 273-345 K temperature interval gave

$$k_{SCG}/dm^3 \text{ mol}^{-1} = 0.2256 - 4.09 \times 10^{-4} \text{ T/K}$$

The salt effect parameters calculated from the papers and the smoothed values are given below. The smoothed values have an uncertainty of about 10 per cent.

T/K	Braun	Morrison, Billett	Gerecke	Gerecke, Bittrich	Crozier, Yamamoto	Steiner	Value from Equation
274.04					0.1271		0.113
278.2	0.103				•••		0.111
283.2	0.095						0.109
283.97					0.101^{2}		0.109
285.75		0.107					0.109
288.15	0.093			0.107	•	0.106	0.108
289.55					0.1151		0.107
293.2	0.090						0.105
295.34					0.106^{2}		0.105
298.15	0.096		0.106	,		2	0.103
301.50		. 102		C	0.088 ¹ , 0.091		0.102
303.15		0.103					0.102 0.094
322.55		0.099		0.100			0.094
323.15 344.85		0.088		0.100			0.095

measurements at ca. 0.2 mol dm⁻³

The Bunsen coefficient data of Braun at the lowest temperatures are thought to be considerably in error but the salting and parameters are probably more reliable. The values quoted in the table are for a concentration of 1 mol $\rm dm^{-3}$. Braun's data gives larger values for more dilute solution and are classified as doubtful.

24. Hydrogen + water + Sodium sulfate [7757-82-6]

This system has been studied by Steiner (16) at three different concentrations. The average value of $k_{SC\alpha}$ is 0.279 dm³ mol⁻¹ at 288.2 K.

measurements at ca. 0.5 mol dm⁻³

25. Hydrogen + water + Sulfuric acid [7664-93-9] + Sodium sulfate [7757-82-6]

Kobe and Kenton (3) made two measurements of the solubility of hydrogen in a mixture that was 1.76 mol kg^{-1} Na_2SO_4 and 0.90 mol kg^{-1} H_2SO_4 . Using the sum of the component molalities gives the salt effect parameter, $k_{sm\alpha} = 0.157$. The value indicates the Na_2SO_4 contributes more to the salting out effect than does the H_2SO_4 . The value appears reasonable and is classed as tentative.

26. Hydrogen + water + Sodium nitrite [7632-00-0]

Longo, Delivoria-Papadopoulas, Power, Hill, and Forster (11) measured the solubility of hydrogen in water and in 0.14 mol dm $^{-3}$ NaNO2. The salt effect parameter calculated from their data is $k_{\mbox{\scriptsize SC}\alpha}$ 0.154 at 298.15 K. The value is greater than for other 1-1 electrolytes. It is classed as tentative.

27. Hydrogen + water + Sodium nitrate [7631-99-4]

Gerecke (10) measured the solubility of hydrogen in aqueous NaNO $_3$. He reported one value of the salt effect parameter, k_{SMS} , of 0.081 at 298.15 K. This was converted to a salt effect parameter value, $k_{\text{SC}\alpha}$, of 0.098. The value is classed as tentative.

This system has also been studied by Steiner (16) at five concentrations at temperatures near 288 K. Values "adjusted" to 288.2 K were reported and give a tentative value of $k_{\mbox{\footnotesize SC}\alpha}$ of 0.0986 dm³ mol^1 at a salt concentration of 1 mol dm^3. The salt effect parameters show some scatter but there is a tendency to a decrease in $k_{\mbox{\footnotesize SC}\alpha}$ as the salt concentration increases

$$k_{sca}/dm^3 \text{ mol}^{-1} = 0.1007 - 2.1 \times 10^{-4} \text{ c}_3/\text{mol dm}^{-3}$$

where c_3 is the salt concentration.

The data of Knopp (15) give salt effect parameters, $k_{\text{SG}\alpha}$ which scatter considerably with an average value of 0.094 dm³ mol⁻¹ at 293.15 K.

28. Hydrogen + water + Sodium carbonate [497-19-8]

Steiner (16) studied this system at four concentrations at temperatures near 288 K. Values "adjusted" to 288.2 K were reported and give a tentative value of $k_{\rm SC\alpha}$ of 0.294 $\rm dm^3~mol^{-1}$.

29. Hydrogen + water + Potassium hydroxide [1310-58-3]

The solubility of hydrogen in aqueous potassium hydroxide was measured by Geffcken (1), Knaster and Apel'baum (15), Bruhn, Gerlach, and Pawlek (7), Ruetschi and Amlie (8), and Shoor, Walker, and Gubbins (9).

The authors' results were converted to a Sechenow salt effect parameter of the form $k_{SC\alpha}=(1/c_3)\log(\alpha^\circ/\alpha)$, except for the results of Shoor, Walker, and Gubbins which were left in the original form of $k_{SC\alpha}=(1/c)\log(x^\circ/x)$. The value of $k_{SC\alpha}$ was taken as the slope of a linear regression of $\log(\alpha^\circ/\alpha)$ vs. c_3 , except for the data of Bruhn et al. for which $k_{SC\alpha}$ values were averaged.

T/K	Geffcken	Kaster, Apel'baum	Bruhn, Gerlach, Pawlek	Reutschi, Amlie	Shoor, Walker, Gubbins
294.15		0.123			
298.15	0.1371	*****			0.127^{3}
303.15				0.133	
313.15					0.130^{3}
318.15		0.132			
323.15			0.169²		
333.15					0.129³
348.15		0.137			
353.15					0.128 ³
373.15			0.156²		0.127^{3}
423.15			0.164^{2}		
473.15			0.151^{2}		

- Average of four values at KOH concentrations between 0.715 and 1.480 mol dm⁻³. Standard deviation 0.002.
- Average of three values at KOH concentrations 0.5, 1.0, and 1.5 mol dm⁻³. The standard deviations are 0.025, 0.024, 0.024 and 0.015 from top to bottom.
- 3 The salt effect parameters are given as ${\bf k}_{\rm SCX}$ values. Conversion to ${\bf k}_{\rm SCX}$ values will make them smaller by about 0.01.

30. Hydrogen + water + Potassium chloride [7747-40-7]

Gerecke and Bittrich (12) measured the solubility of hydrogen at two concentrations of potassium chloride at 288.15 K. They quote a salt effect parameter of Gerecke (10) at 298.15. They worked with electrolyte molality and gas Kuenen coefficients. Their values are classed as tentative. Values of both $k_{\mbox{sms}}$ and $k_{\mbox{sc}\alpha}$ are given.

T/K 288.15 298.15
$$k_{sms}/kg \text{ mol}^{-1}$$
 0.085 0.078 $k_{sc\alpha}/dm^3 \text{ mol}^{-1}$ 0.100 0.094

Steiner (16) also studied this system and the salt effect parameter $\mathbf{k}_{\text{SC}\alpha}$ at 288.2K is given by

$$k_{SCG}/dm^3 mol^{-1} = 0.1016 - 0.00295 \times c_3/mol dm^3$$

where c3 is the concentration of the salt.

Knopp's data (15) yield salt effect parameters which show no concentration dependence. The average value of $k_{\mbox{sc}\alpha}$ is 0.096 \mbox{mol}^{-1} dm 3 .

31. Hydrogen + water + Potassium iodide [7681-11-0]

The solubility of hydrogen in aqueous potassium iodide was measured at four temperatures by Morrison and Billett (4) and at one temperature by Gerecke (10). Their values of $k_{\mbox{sms}}$ were converted to $k_{\mbox{sc}\alpha}$ values. The salt effect parameters in both forms are given below.

T/K		298.15			
k _{sms} /kg mol ⁻¹					
$k_{sc\alpha}/dm^3 mol^{-1}$	0.113	0.110	0.108	0.097	0.078

0.0835

2.430

Hydrogen + water + Potassium nitrate [7757-79-1]

This system has been studied by Steiner (16), Gerecke (10) and Knopp (15). Values of the salt effect parameter derived from Knopp's data at 293.15K show considerable variation but no clear correlation with concentration the average value is 0.07 mol⁻¹ dm³. Steiner's data give values of k_{sca} which decrease with increasing concentration but show considerable The value of $k_{sca}/mol^{-1} dm^3$ are given below

$$k_{\text{sca}}/\text{mol}^{-1} \text{ dm}^3$$
 0.1012 0.1121 0.0853 0.0864 Conc. of salt /mol dm⁻³ 0.482 0.879 1.541 1.820

0.482

Gerecke (10) reports a salt effect parameter for aqueous potassium nitrate at 298.15 K. The value is classed as tentative. It is 0.061 as $k_{\rm sms}$ and 0.083 as k_{SCQ} .

0.879

1.541

1.820

33. Hydrogen + water + Potassium carbonate [584-08-7]

This system has been studied by Steiner (16) at seven different salt concentrations at temperatures near 288K. Values "adjusted" to 288.2K were reported and give a tentative value of $k_{SC\alpha}$ of 0.290 mol⁻¹ dm³ at a salt concentration of 1 mol dm³. Their values decrease slightly with increasing concentration.

References:

- Geffcken, G. Z. Phys. Chem. 1904, 49; 257.
- 2. Christoff, A. Z. Physik. Chem. 1906, 55, 622.
- Kobe, K. A.; Kenton, F. H. Ind. Eng. Chem., Anal. Ed. 1938, 10, 76.
- Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819.
- Stephan, E. L.; Hatfield, N. S.; Peoples, R. S.; Pray, H. A. H. Battelle Memorial Institute Report BMI-1067, 1956.
- Uch. Zap. Leningr. Gos. Univ., Shkol'nikova, R. I. Ser. Khim. Nauk. 1959, Nr. 18, 64.
- Bruhn, G.; Gerlach, J.; Pawlek, F. Zeit. Anorg. Allg. Chem. 1965, 337, 68.
- 8. Ruetschi, P.; Amlie, R. F. J. Phys. Chem. 1966, 70, 718.
- Shoor, S. K.; Walker, R. D. Jr.; Gubbins, K. E. J. Phys. Chem. 1969, 73, 312.
- 10. Gerecke, J. Dissertation (Dr. rer. nat.) 1969 THS "Carl Schorlemmer" Leuna-Merseburg, DDR
- 11. Longo, L. D.; Delivoria-Papadopoulas, M.; Power, G. G.; Hill, E. P.; Forster, R. E., Am. J. Physiology, 1970, 219, 561.
- 12. Gerecke, J.; Bittrich, H. J. Wiss. Z. Tech. Hocsch. Chem. "Carl Schorlemmer" Leuna-Merseburg 1971, 115 and 313.
- 13. Crozier, T. E.; Yamamoto, S. J. Chem. Eng. Data 1974, 19, 242.
- 14. Deckwer, W.-D. J. Chem. Eng. Data 1980, 25, 75.
- 15. Knopp, W. Z. Phys. Chem. 1904, 48, 97.
- 16. Steiner, P. Ann. der Phys. Chem. 1894, 52, 275
- 17. Braun, L. A. Phys. Chem. <u>1900</u>, 33, 721
- 18. Knaster, M.B.; Apel'baum, L.A. Zh. Fiz. Khim. 1964, 38, 223.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Geffcken, G.Z. Phys. Chem.
2. Water; H ₂ O; [7732-18-5]	1904,49,257-302
3. Hydrochloric acid; HCl; [7647-01-0]	
VARIABLES:	PREPARED BY:
Concentration	C.L. Young

T/K	Conc of acid/mol dm3 (soln)	Ostwald coefficient, $\it L$
298.15	0.426	0.01875
	0.432	0.01868
	1.063	0.01789
	1.062	0.01732
	1.802	0.01699
	1.928	0.01688
	2.338	0.01652
	2.438	0.01627
	2.836	0.01606

AUXILIARY INFORMATION

AUXILIARY INFORMATION		
METHOD /APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Volumetric method using simple adsorption pipet and buret. Diagram and detailed description given in original paper.	1. Prepared by the action of dilute hydrochloric acid on aluminium in the presence of mercury chloride. Washed in potassium hydroxide solution and potassium permanganate solution. Dried.	
	2. Degassed.	
	ESTIMATED ERROR:	
	$\delta T/K = \pm 0.1; \delta L = \pm 1%.$	
	(estimated by compiler).	
	REFERENCES:	

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Geffcken, G. Z. Phys. Chem. 2. Water; H₂O; [7732-18-5] 1904,49,257-302 3. Sulfuric acid; H₂SO₄; [7664-93-9] VARIABLES: PREPARED BY: Concentration C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc of acid/mol dm3 (soln)	Ostwald coefficient, L
298.15	0.2635 0.2344 0.4925	0.01869 0.01838 0.01780
	0.5610 0.9330 0.9525	0.01768 0.01642 0.01632 0.01575
	1.3025 1.5225 1.5870 1.9810 1.9945	0.01373 0.01496 0.01456 0.01422 0.01402

AUXILIARY	INFORMATION
METHOD /APPARATUS/PROCEDURE: Volumetric method using simple adsorption pipet and buret. Diagram and detailed description given in original paper.	SOURCE AND PURITY OF MATERIALS: 1. Prepared by the action of dilute hydrochloric acid on aluminium in the presence of mercury chloride. Washed in potassium hydroxide solution and potassium permanganate solution. Dried. 2. Degassed.
	ESTIMATED ERROR: $ \delta T/K = \pm 0.1; \ \delta L = \pm 1 \% $ (estimated by compiler). $ \text{REFERENCES:} $

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Christoff, A. (2) Water; H₂O; [7732-18-5] Z. Physik. Chem. 1906, 55, 622-634. (3) Sulfuric acid; H₂SO₄; [7664-93-9] VARIABLES: PREPARED BY: T/K: 293.15 M. E. Derrick H. L. Clever P: Atmospheric H₂SO₄/wt %: 0 - 95.6

EXPERIMENTAL VALUES:

T/K	H ₂ SO ₄ /wt %	m _{H2} SO ₄ /mol kg ⁻¹	Ostwald Coefficient L x 10 ²
293.15	0.0	0.0	2.077
	35.82	5.690	0.9544
	61.62	16.37	0.7081
	95.6	222.	1.097

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was an Ostwald type (1) with a lead capillary tube through which the gas flows to the absorption flask, the gas buret, and the gasometer.

The solvent was degassed by boiling under reflux. The author estimates a one per cent change in the acid concentration due to the degassing procedure. The absorption flask was filled with solvent, the gas was introduced, and the system shaken until equilibrium was reached.

SOURCE AND PURITY OF MATERIALS;

- Hydrogen. Prepared from the reaction of zinc and dilute sulfuric acid.
- (2) Water. Distilled.
- (3) Sulfuric acid. Merck (Darmstadt) Specific gravity 1.271, 1.523, and 1.839 for 35.82, 61.62, and 95.6 wt per cent, respectively.

ESTIMATED ERROR:

 $\delta T/K = 0.02 \ \text{for acid} \\ = 0.5 \ \text{for gas} \\ \text{Barometric fluctuation stated to be} \\ \text{negligible.}$

REFERENCES:

1. Ostwald, W.

Lehrbuch der allgem. Chemie
(2 Aufl.), 1, 615.

COME	ONENTS:	ORIGINAL MEASUREMENTS:
1.	Hydrogen; H ₂ ; [1333-74-0]	Bruhn, G.; Gerlach, J.; Pawlek, F.
2.	Water; H ₂ O; [7732-18-5]	Zeit. Anorg. Allg. Chem.
3.	Sulfuric acid; H ₂ SO ₄ ;[7664-93-9]	<u>1965</u> , <i>337</i> , 68-79
VAR	TABLES:	PREPARED BY:
	Temperature, concentration	C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc of acid/mol 1-1	Bunsen coefficient,α
323.15	0.5 1.0 1.5	0.01521 0.01348 0.01220
373.15	0.5 1.0 1.5	0.01733 0.01475 0.01398
423.15	0.5 1.0 1.5	0.02125 0.01935 0.01770
473.15	0.5 1.0	0.02900 0.02645
523.15	0.5 1.0	0.04180 0.03600

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping solution of gas and estimating volumetrically. ESTIMATED ERROR: ô T/K = ±2; ôa = ±2%. (estimated by compiler) REFERENCES: 1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute Report BMI-840, 1953.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Ruetschi, P.; Amlie, R. F. (2) Water; H₂O; [7732-18-5] J. Phys. Chem. 1966, 70, 718 - 723. (3) Sulfuric acid; H₂SO₄; [7664-93-9] VARIABLES: PREPARED BY:

303.15 T/K:

H₂ P/kPa: H₂SO₄/eq dm⁻³: 101.325 (1 atm) 0 - 15.2 H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature	Normality	Molarity	Solubility		(1 () 1
t/°c	T/K	mol dm ⁻³	mol dm ⁻³	cm ³ (STP) dm ⁻³	log 50/S	(1/c)log S ^O /S ¹
30	303.15	0.0	0.0	17.03 16.90 17.10 16.93		
				16.99 ± 0.08 Av	7. -	-
,		0.0011 0.100 0.502 1.02 3.04 5.05 6.95 9.67 12.4 15.2	0.00055 0.050 0.251 0.51 1.52 2.525 3.475 4.835 6.2 7.6	17.09 16.66 16.15 15.17 12.76 10.83 10.01 8.87 8.11 7.68	0 0.0083 0.0221 0.0495 0.1243 0.195 0.230 0.283 0.322 0.345	0 0.166 0.088 0.097 0.082 0.077 0.066 0.059 0.052

¹ The c is the molar c, $c_{\rm H_2SO_4}/{\rm mol~dm^{-3}}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

They used the apparatus of Ben-Naim and Baer (1). A calibrated dissolution vessel contains degassed water. Gas is introduced wet from a calibrated gas buret system. Stirring the liquid forces it up sidearms attached to the top of the flask and the liquid returns via a central tube. The amount of gas dissolved is determined via the gas burets. The gas burets and dissolution vessel are thermostated in a water bath. The original paper contains a diagram ESTIMATED ERROR: and a description of operation.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Prepurified grade (99.5% min purity).
- (2) Water. No comment by author.
- (3) Sulfuric acid. Source not given. Reagent grade.

REFERENCES:

1. Ben-Naim, A.; Baer, S. Trans. Faraday Soc. 1963, 59, 2735.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Geffcken, G.Z. Phys. Chem.
2. Water; H ₂ O; [7732-18-5]	1904,49,257-302
3. Nitric acid; HNO ₃ ; [7697-37-2]	
VARIABLES:	PREPARED BY:
Concentration	C.L. Young
PVDEDTAGNMAI MATHEC.	

EXPERIMENTAL VALUES:

Conc of acid/mol dm ⁻³ (soln)	Ostwald Coefficient, L
0.741	0.01851
0.753	0.01868
1.22	0.01812
1.45	0.01782
	0.01739
	0.01690
	0.01667
	0.01633
	0.01611
4.23	0.01589
	0.741 0.753 1.22 1.45 2.09 2.96 3.18 3.22 4.13

AUXILIARY INFORMATION

AUXILIAK	INFORMATION	
METHOD /APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
Volumetric method using simple adsorption pipet and buret. Diagram and detailed description given in original paper.	1. Prepared by the action of dilute hydrochloric acid on aluminium in the presence of mercury chloride. Washed in potassium hydroxide solution and potassium permanganate solution. Dried.	
	2. Degassed.	
	ESTIMATED ERROR:	
	$\delta T/K = \pm 0.1; \ \delta L = \pm 1\%.$	
•	(estimated by compiler.)	
	REFERENCES:	

l. Hydrogen, H ₂ ; [1333-74-0]	Bruhn, G.; Gerlach, J.; Pawlek, F.
2. Water, H ₂ O; [7732-18-5]	Zeit. Anorg. Allg. Chem.
Ammonium hydroxide; NH,OH; [1336-21-6]	<u>1965</u> , <i>337</i> ,68-79.
VARIABLES:	PREPARED BY:
Temperature, concentration	C.L. Young

T/K	Conc of salt/mol 1-1	Bunsen coefficient, α
298.15	2.87 5.63 8.28	0.01745 0.01659 0.01603
323.15	2.87 5.63 8.28	0.01571 0.01473 0.01460
348.15	2.87 5.63 8.28	0.01629 0.01569 0.01530
373.15	2.87 5.63 8.28	0.01791 0.01762 0.01656
423.15	2.87 5.63 8.28	0.02285 0.02175 0.02140

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Static equilibrium cell. Similar to that described by Pray and Stephan (1) Composition of liquid determined by stripping solution of gas and estimating volumetrically.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 2$; $\delta \alpha = \pm 2$ %. (estimated by compiler).

REFERENCES:

1. Pray, H.A.; Stephan, E.J..
Battelle Memorial Institute
Report BMI-840, 1953.

COMPONENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Ammonium chloride; NH,Cl; [12125-02-9]

ORIGINAL MEASUREMENTS:

Gerecke, J.; Bittrich, H. J.

Wiss. Z. Tech. Hocsch. Chem. "Carl Schorlemmer" Leuna-Merseburg 1971, 115 - 122, 313 - 231.

Chem. Abstr. 1972, 76, 77239, 77, 66741.

VARTABLES:

T/K:

288, 323 101.325 (1 atm) P/kPa: m_{NH,Cl}/mol kg-1:

0.50 - 5.00

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K	m _{NH₄Cl/mol kg⁻¹}	log (S°/S)
288	0.50 1.00 2.00 5.00	0.029 0.058 0.112 0.262
323	0.50 1.00 2.00 5.00	0.021 0.045 0.093 0.213

Values were taken from a graph in the paper by the compiler.

The solubility ratio, S°/S, is a ratio of Kuenen coefficients.

The authors value of the solubility of hydrogen in water at 298.15 K and one atm partial pressure is a Bunsen coefficient of 0.0177.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen solubilities appear to have been determined by the method of Morrison and Billett (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen.
- (2) Water.
- (3) Ammonium chloride.

No information on the materials.

ESTIMATED ERROR:

 $\delta \log (S^{\circ}/S) = +0.003$ from graph.

REFERENCES:

1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Gerecke, J. Dissertation (Dr. rer. nat.) 1969 (2) Water; H₂O; [7732-18-5] THC "Carl Schorlemmer" Leuna-Merseburg, DDR (3) Electrolyte VARIABLES: PREPARED BY: T/K: 298.15 P/kPa: 101.325 (1 atm) H. L. Clever EXPERIMENTAL VALUES: $k_{s} = (1/m) \log (S^{0}/S)$ T/K Ammonium chloride; NH₄Cl; [12125-02-9] 298.15 0.055 Lithium chloride; LiCl; [7447-41-8] 298.15 0.062 Sodium chloride; NaCl; [7647-14-5] 298.15 0.095 Potassium chloride; KCl; [7447-40-7] 298.15 0.078 Potassium iodide; KI; [7681-11-0] 298.15 Sodium nitrate; NaNO3; [7631-99-4] 298.15 0.081 Potassium nitrate; KNO3; [7757-79-1] 298.15 0.061 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: The values above were quoted in a No information on the source and paper by Gerecke and Bittrich (1). purity of materials. The solubility ratio, S^0/S , is ratio of Kuenen coefficients. The salt concentration is m/mol kg⁻¹. ESTIMATED ERROR: REFERENCES: Gerecke, J.; Bittrich, H.-J. Wiss. Z. Tech. Hochsch. Chem. "Carl Schorlemmer" Leuna-

Merseburg 1971, 13, 313 - 321.

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COMPONENTS:		ORIGINAL MEASUREMENTS:
. Hydrogen; H ₂	; [1333-74-0]	Bruhn, G.; Gerlach, J.; Pawlek, F.
2. Water; H ₂ O;	[7732-18-5]	Zeit. Anorg. Allg. Chem.
3. Ammonium sul	fate; (NH ₄) ₂ SO ₄ ;	<u>1965</u> , <i>337</i> , 68-79.
[7783-20-2]		
VARIABLES:		PREPARED BY:
Temperature,	concentration	C.L. Young
EXPERIMENTAL VALUES	:	
T/K	Conc of salt/mol :	Bunsen coefficient, α
298.15	0.25	0.01638
	0.75 1.5	0.01358 0.00953
	3.0	0.00766
323.15	0.25	0.01540
	0.75 1.5	0.01191 0.00854
	3.0	0.00747
373.15	0.25	0.01657
	0.75 1.5	0.01449 0.01029
	3.0	0.00759
423.15	0.25	0.02175
	0.75 1.5	0.01798 0.01300
	3.0	0.01030
473.15	1.5 3.0	0.01703 0.01250
523.15	1.5	0.02305
	3.0	0.02055
	AUXILIARY	INFORMATION
ŒTHOD /APPARATUS	S/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Static equilibr	rium cell. Similar	
Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping		No details given.
solution of gas volumetrically	s and estimating	
		ESTIMATED ERROR:
		$\delta T/K = \pm 2$; $\delta \alpha = \pm 2$ %.
	,	(estimated by compiler)
	•	REFERENCES:
		1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Knopp, W. 2. Water; H₂O; [7732-18-5] 3. Ammonium nitrate; NH₄NO₃; Z. Phys. Chem. [6484-52-2] 1904, 48, 97-108. VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Wt. of salt in 100 g soln.	Conc. of salt /mol dm ⁻³ (soln.)	Density of soln. /g cm ⁻³	Bunsen absorption coefficient, a	10 mole fraction of hydrogen, 10 H ₂
293.15	0	0	0.99823	0.01883	0.1511
	1.037	0.1308	1.00267	0.01872	0.1508
	2.167	0.2765	1.00722	0.01845	0.1492
	3.378	0.4363	1.01216	0.01823	0.1481
	4.823	0.6333	1.01815	0.01773	0.1450
	6.773	0.9069	1.02620	0.01744	0.1436
	11.550	1.6308	1.04652	0.01647	0.1384

AUXILIARY INFORMATION

METHOD 'APPARATUS/PROCEDURE:

Manometric method with absorption pipet and gas buret being used.

Densities were determined using a Sprengel pyknometer.

- SOURCE AND PURITY OF MATERIALS:
 - Prepared from pure zinc and dil. sulfuric acid in a Kipp's apparatus, passed through silver nitrate, potassium hydroxide and permanganate solutions.
 - 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta\alpha/\alpha = \pm 3\%$ (estimated by compiler).

REFERENCES:

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 3. Zinc sulfate; ZnSO₄; 1894, 52, 275-299. [7733-02-0] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K Conc. of salt at 288.2 K coeffi / mol dm ⁻³ /g cm ⁻³	cient, coefficient at 288.2 K
288.2 0 0.999 0.01	883 0.01883
288.2 0 0.999 0.01 290.94 0.397 1.0620 0.01	
291.10 0.899 1.1394 0.01	
291.37 1.277 1.1961 0.00	940 0.00961
291.71 2.180 1.3265 0.00	0.00605

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD/APPARATUS/PROCEDURE: Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source. ESTIMATED ERROR: $\delta \alpha/\alpha = \pm 0.02.$ REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Bruhn, G.; Gerlach, J.; Pawlek, F.
2. Water; H ₂ O; [7732-18-5]	Zeit. Anorg. Allg. Chem.
3. Copper (2+) sulfate; CuSO ₄ ; [7758-98-7]	<u>1965</u> , <i>337</i> , 68-79
VARIABLES:	PREPARED BY:
Temperature, concentration	C.L. Young

EXPE	RIMENTAL	VALUES:

METHOD/APPARATUS/PROCEDURE:

T/K	Conc of salt/mol l ⁻¹	Bunsen coefficient,α
298.15	0.5 1.0 1.5	0.01422 0.01222 0.01050
323.15	0.5 1.0 1.5	0.01280 0.01189 0.00935
348.15	0.5 1.0 1.5	0.01372 0.01102 0.01001
373.15	0.5 1.0 1.5	0.01490 0.01275 0.01149
398.15	0.5 1.0 1.5	0.01619 0.01384 0.01153

AUXILIARY INFORMATION

Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping solution of gas and estimating volumetrically.

REFERENCES:

ESTIMATED ERROR:

1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute Report BMI-840, 1953.

 $\delta T/K = \pm 2$; $\delta \alpha = \pm 2$ %. (estimated by compiler).

SOURCE AND PURITY OF MATERIALS:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Bruhn, G.; Gerlach, J.; Pawlek, F.
2. Water; H ₂ O; [7732-18-5]	Zeit. Anorg. Allg. Chem.
3. Nickel (2+) sulfate; NiSO ₄ ; [7786-81-4]	<u>1965</u> , <i>337</i> , 68-79.
VARIABLES:	PREPARED BY:
Temperature, concentration	C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc of salt/mol 1-1	Bunsen coefficient, α
298.15	0.5 1.0 1.5	0.01412 0.01205 0.01031
323.15	0.5 1.0 1.5	0.01260 0.01143 0.00897
348.15	0.5 1.0 1.5	0.01356 0.01076 0.00985
373.15	0.5 1.0 1.5	0.01425 0.01233 0.01135
398.15	0.5 1.0 1.5	0.01630 0.01390 0.01155

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping solution of gas and estimating volumetrically.	No details given.
	ESTIMATED ERROR:
	$\delta T/K = \pm 2$; $\delta \alpha = \pm 2$ %.
	(estimated by compiler).
·	REFERENCES:
	1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute Report BMI-840. 1953.

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Bruhn, G.; Gerlach, J.; Pawlek, F. 2. Water; H₂O; [7732-18-5] Zeit. Anorg. Allg. Chem. 3. Cobalt (2+) sulfate; CoSO₄; 1965,337, 68-79 VARIABLES: PREPARED BY: Temperature, concentration C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc of salt/mol l-1	Bunsen coefficient, α
298.15	0.5 1.0 1.5	0.01446 0.01250 0.01085
323.15	0.5 1.0 1.5	0.01297 0.01183 0.01038
348.15	0.5 1.0 1.5	0.01364 0.01125 0.00971
373.15	0.5 1.0 1.5	0.01506 0.01270 0.01105
398.15	0.5 1.0 1.5	0.01641 0.01455 0.01275

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping solution of gas and estimating volumetrically.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 2$; $\delta \alpha = \pm 2$ %. (estimated by compiler).

REFERENCES:

1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute Report, BMI-840, 1953.

COMPONENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Hydrated iron oxide; Fe₂O₃·xH₂O; [12259-21-1]

ORIGINAL MEASUREMENTS:

Shkol'nikova, R. I.

Uch. Zap. Leningr. Gos. Univ., Ser. Khim. Nauk. <u>1959</u>, Nr. 18, 64 - 86.

Chem. Abstr. 1961, 55, 25443b.

VARTABLES.

T/K: 293.15 - 313.15 P/kPa: 101.325 (1 atm)

Fe₂O₃/Wt %: 0 - 0.8

PREPARED BY:

A. L. Cramer H. L. Clever

EXPERIMENTAL VALUES:

Hydrated Fe ₂ O ₃ /Wt %	Bunsen Coefficient $\alpha \times 10^3$
0.1	17.4
0.5	16.1
0.8	15.3
0.1	15.7
0.5	15.1
0.8	13.4
0.1	14.1
0.5	12.6
0.8	10.9
	Fe ₂ O ₃ /Wt % 0.1 0.5 0.8 0.1 0.5 0.8 0.1 0.5

The enthalpy of solution of hydrogen was calculated from the temperature coefficient of the Bunsen coefficient. It is 1590, 1980, 2240, and 3090 cal mol^{-1} in water, and 0.1, 0.5, and 0.8 wt % Fe₂O₃, respectively.

The values for the solubility of hydrogen in water were not given in the paper.

The hydrated iron oxide is described as a sol (colloidal).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure of Lannung were modified (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Stated to be 99.99 per cent.
- (2) Water. No information.
- (3) Iron oxide. No information.

ESTIMATED ERROR:

REFERENCES:

Lannung, A.
 J. Am. Chem. Soc. <u>1930</u>, 52, 68.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Water; H₂O; [7732-18-5] (3) Manganese (II) sulfate; MnSO₄; [7785-87-7] VARIABLES: T/K: 293.15 - 353.15 (20 - 80 °C) P/kPa: 101.325 (1 atm) CMnSO₄/mol dm⁻³: 0.5 - 3.5

EXPERIMENTAL VALUES:

c _{MnSO4} /mol dm ⁻³	Bunsen coefficient, $\alpha \times 10^2$					
	293.15K	303.15K	313.15K	323.15K	333.15K	353.15K
0 1	1.820	1.700	1.640	1.610	1.600	1,600
0.5	1.672	1.508	1.429	1.342	1.302	1.236
1.0	1.339	1.212	1.141	1.141	1.072	1.108
1.5	1.002	0.945	0.867	0.856	0.835	0.920
2.0	0.725	0.696	0.690	0.686	0.690	0.782
2.5	0.515	0.524	0.573	0.585	0.592	0.631
3.0	0.375	0.399	0.427	0.464	0.462	0.477
3.5	0.304	0.312	0.330	0.352	0.339	0.352

¹ Water values not measured by author, but taken from reference 1.

Bunsen coefficients are the average of five determinations. The reproducibility was usually better than 1 per cent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A gas chromatograph technique was

The gas was presaturated by passing through a $MnSO_4$ solution, then passed through the solution, equilibrium was established in one hour.

A known volume (about $10~\rm{cm}^3$) was transferred to an evacuated, heated column. Most of the \rm{H}_2 desorbed from the saturated solution under these conditions, but any remaining was stripped by passage of argon gas.

The gas flow was dried on silica gel, and introduced to the gas chromatograph (Perkin-Elmer Fl16E). Peaks without tailing were obtained on a 2-cm column at 50 C filled with 5A molecular sieve and a heat conductivity detector.

The instrument was calibrated with ${\rm H}_{2}$ and ${\rm H}_{2}/{\rm Ar}$ mixtures.

The paper also reports solution den- | sities, viscosities, & vapor pressure lowering.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Commercial sample of 99.9 per cent purity.
- (2) Water. No information.
- (3) Manganese (II) sulfate. No information

ESTIMATED ERROR: Mean relative error is about 2 per cent at MnSO₄ concentration of 1 mol dm⁻³, increases to about 4 per cent at 3.5 mol dm⁻³ (author).

REFERENCES:

 Seidell, A.; Linke, W. F. Solubilities of Inorganic and Metalorganic Compounds, Van Nostrand, Princeton, NJ, 1958, Vol. I.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Shkol'nikova, R. I. (2) Water; H₂O; [7732-18-5] Uch. Zap. Leningr. Gos. Univ., Ser. Khim. Nauk. 1959, Nr. 18, 64 - 86. (3) Hydrated aluminium oxide; Al₂O₃·xH₂O; [1333-84-2] Chem. Abstr. 1961, 55, 25443b. VARIABLES: T/K: 293.15 - 313.15 P/kPa: 101.325 (1 atm) PREPARED BY: A. L. Cramer H. L. Clever

EXPERIMENTAL VALUES:

 $Al_2O_3/Wt %: 0 - 0.35$

т/к	Hydrated Al ₂ O ₃ /Wt %	Bunsen Coefficient $\alpha \times 10^3$
293.15	0.1 0.35	17.7 15.0
303.15	0.1 0.35	16.7 11.1
313.15	0.1 0.35	15.6 9.2

The enthalpy of solution of hydrogen was calculated from the temperature coefficient of the Bunsen coefficient. It is 1590, 1150, and 3920 cal mol^{-1} in water, 0.1 and 0.35 wt % $\mathrm{Al}_2\mathrm{O}_3$, respectively.

The values for the solubility of hydrogen in water were not given in the paper.

The hydrated aluminium oxide is described as a sol (colloidal).

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The apparatus and procedure of Lannung (1) were modified. (1) Hydrogen. Source not given. Stated to be 99.99 per cent. (2) Water. No information. (3) Aluminium oxide. No information. ESTIMATED ERROR: REFERENCES: 1. Lannung, A. J. Am. Chem. Soc. 1930, 52, 68.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Hydrogen; H₂; [1333-74-0] Water; H₂O; [7732-18-5] Aluminium chloride; AlCl₃ [7446-70-0] 	Steiner, P. Ann. der Phys. Chem. 1894, 52, 275-299.
VARIABLES:	PREPARED BY:
Concentration of salt	C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient,	Bunsen coefficient [#] at 288.2 K	
288.2	0	0.999	0.01883	0.01883	
290.61	0.541	1.0488	0.01460	0.01486	
290.45	1.019	1.0914	0.01190	0.01210	
290.43	1.802	1.1589	0.00860	0.00874	
290.29	3.080	1.2647	0.00525	0.00533	

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.

ESTIMATED ERROR: $\delta \alpha/\alpha = \pm 0.02.$ REFERENCES:

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Morrison, T. J.; Billett, F. (2) Water; H₂O; [7732-18-5] J. Chem. Soc. 1952, 3819 - 3822. (3) Lanthanum chloride; LaCl₃; [10099-58-8] VARIABLES: T/K: 285.75 - 344.85 P/kPa: 101.325 (1 atm) PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

Temperature			Sa	alt Effect Parameters		
t/ºC	T/K	1/(T/K)	(1/c) log(S ⁰ /S) 1	(1/m)log(S ⁰ /S)	$(1/m) \log(x^0/x)$	
12.6	285.75	0.0035	0.079	0.237	0.267	
30.0	303.15	0.0033	0.078	0.234	0.264	
49.4	322.55	0.0031	0.076	0.228	0.258	
71.7	344.85	0.0029	0.075	0.225	0.255	

¹ In the authors notation c represented g eq LaCl2 per 1.000 kg water.

The salt effect parameters were calculated from two solubility measurements. The solubility in 1.000 kg water, $S^{\,0}$, and the solubility in a l equivalent of salt per 1.000 kg of water, S. Values of the solubility of hydrogen in water are given in the paper, but not the solubility in the salt solution.

The compiler calculated the salt effect parameter on a salt molal basis, and on a salt molal and gas mole fraction basis.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The degassed solvent flows in a thin film down an absorption helix containing the hydrogen gas plus solvent vapor at a total pressure of one atmosphere. The volume of gas absorbed is measured in an attached buret system (1).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared from pure zinc and dilute hydrochloric acid.
- (2) Water. No information given.
- (3) Lanthanum chloride. "AnalaR" material.

ESTIMATED ERROR:

 $\delta k = 0.010$

REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Stephan, E. L.; Hatfield, N. S.; Water; H₂O; [7732-18-5] Peoples, R. S.; Pray, H. A. H. 2. Battelle Memorial Institute Report BMI-1067, 1956. З. Uranyl sulfate; UO₆S; [1314-64-3] VARIABLES: PREPARED BY: Temperature, pressure, composition C. L. Young EXPERIMENTAL VALUES: g Uranium P^{\dagger} bar Solubility* g Uranium P[†]/bar Solubility* T/K T/K per liter per liter 373.15 40 26.4 0.375 373.15 100 30.5 0.35 0.396 34.1 27.6 0.395 29.1 54.8 0.392 0.63 30.2 0.41 55.8 0.645 57.3 46.4 0.62 0.662 47.6 0.64 58.4 0.648 0.675 70.3 0.83 48.7 50.1 0.69 72.2 0.867 73.4 0.84 68.2 0.97 69.3 0.98 76.5 0.84 70.7 97.8 1.20 0.91 71.6 99.8 1.08 1.24 100.3 72.1 1.01 1.25 1.27 98.7 1.44 101.7 101.1 1.48 104.8 1.27 104.9 1.27 102.4 1.50 243 23.6 0.20 106.2 1.49 24.8 100 0.207 26.3 0.305 0.23 27.4 0.31 26.8 27.6 0.325 43.5 0.372 44.6 0.40 29.3 0.34 (cont.) † partial pressure of hydrogen ml of hydrogen at S.T.P./g of solution AUXILIARY INFORMATION SOURCE AND PURITY OF MATERIALS: METHOD /APPARATUS/PROCEDURE: Gas and liquid equilibrated for 18 hours. Pressure measured with Bourdon gauge and temperature measu-

Gas and liquid equilibrated for 18 hours. Pressure measured with Bourdon gauge and temperature measured with thermocouple. Composition of liquid estimated by volumetric method. Details in source. Partial pressure estimated by subtracting vapor pressure from total pressure.

No details given.

ESTIMATED ERROR: $\delta T/K = \pm 0.6$; $\delta P/bar = \pm 0.3$; $\delta (Solubility) = \pm 3\%$ (estimated by compiler).

REFERENCES:

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Water; H₂O; [7732-18-5]

3. Uranyl sulfate; UO₆S;[1314-64-3]

ORIGINAL MEASUREMENTS:

Stephan, E. L.; Hatfield, N. S.; Peoples, R. S.; Pray, H. A. H. Battelle Memorial Institute Report BMI-1067, 1956.

EXPERIMENTAL VALUES:

T/K	g Uranium per liter	P [†] /bar	Solubility*	T/K	g Uranium per liter	P [†] /bar	Solubility*
373.15	243	46.2	0.392	408.15	243	93.5	0.895
		73.6	0.62			95.0	0.95
		77.3	0.668	435.93	40	14.2	0.324
		78.5	0.65			15.4	0.330
		101.8	0.92			16.5	0.294
		103.1	0.93			37.9	0.705
		105.8	0.91			40.0	0.753
		106.8	0.95			41.4	0.782
		108.6	0.96			43.1	0.805
408.15	40	27.4	0.40			56.9	1.20
		29.0	0.40			61.4	1.112
		30.1	0.44			66.0	1.22
		46.0	0.676			93.4	1.71
		47.4	0.71			94.1	1.715
		47.6	0.702			96.5	1.77
		48.4	0.718		100	18.1	0.321
		49.5	0.77			18.6	0.316
		67.6	0.99			18.8	0.333
		68.5	1.04			19.2	0.358
		70.1	1.07			35.9	0.585
		71.4	1.05			35.9	0.617
		98.9	1.47			39.3	0.595
		102.1	1.59			40.0	0.663
		104.8	1.56			41.0	0.683
	100	18.8	0.270			43.4	0.745
	200	19.8	0.251			43.5	0.73
		21.4	0.272			46.5	0.77
		44.3	0.55			58.6	0.97
		45.9	0.613			60.7	1.03
		47.3	0.63			64.2	1.05
		69.2	0.855			66.0	1.09
		70.1	0.887			71.7	1.14
		71.4	0.95			84.0	1.41
		99.2	1.27			88.0	1.43
		100.3	1.265		243	32.3	0.391
		101.3	1.325		213	33.4	0.384
		102.9	1.30			34.1	0.395
	243	22.4	0.219			34.5	0.42
	~ · · · ·	23.9	0.236			71.0	0.82
		56.4	0.561			74.2	0.83
		57.6	0.558			78.3	0.91
		58.7	0.588			102.4	1.24
		60.7	0.625			105.1	1.27
		92.3	0.875			T00.T	+•4/
		92.3	0.875				

^{*} ml of hydrogen at S.T.P./g of solution † partial pressure of hydrogen

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 3. Magnesium sulfate; MgSO₄; 1894, 52, 275-299. VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

т/к	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient, a	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
290.25	0.433	1.0503	0.01479	0.01501
290.45	0.936	1.1064	0.01140	0.01159
290.70	1.631	1.1805	0.00783	0.00797
291.41	2.501	1.2679	0.00487	0.00499

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha = \pm 0.02.$
	REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. Ann. der Phys. Chem. 2. Water; H₂O; [7732-18-5] Calcium chloride; CaCl₂; 1894, 52, 275-299. [10043-52-4] VARIABLES: PREPARED BY: C. L. Young Concentration of salt

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient, α	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
291.67	0.321	1.0285	0.01579	0.01619
291.19	0.578	1.0513	0.01419	0.01450
291.55	1.122	1.0981	0.01112	0.01138
291.24	1.827	1.1568	0.00821	0.00839
290.99	2.556	1.2150	0.00606	0.00619
290.83	2.962	1.2470	0.00510	0.00519

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwalt type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR: $\delta \alpha / \alpha = \pm 0.02$.
	REFERENCES:

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Braun, L. 2. Water; H₂O; [7732-18-5] Z. phys. Chem. 3. Barium chloride; BaCl₂; 1900, 33, 721-741. [10361-37-2] VARIABLES: PREPARED BY: Temperature, concentration of salt C. L. Young

EXPERIMENTAL VALUES:

METHOD 'APPARATUS / PROCEDURE:

T/K	Wt. of salt per 100 g soln. /g	Bunsen coefficient, α	T/K	Wt. of salt per 100 g soln. /g	Bunsen coefficient,
278.2	0 3.291	0.02366 0.02110	288.2	6.453 7.002	0.01734 0.01715
	3.600 6.453	0.02089 0.01957	293.2	0 3.291	0.01905 0.01719
283.2	7.002 0	0.01937 0.02213		3.600 6.453	0.01700 0.01605
	3.291 3.600	0.01983 0.01971	298.2	7.002 0	0.01591 0.01750
	6.453 7.002	0.01857 0.01833		3.291 3.600	0.01570 0.01562
288.2	0 3.291 3.600	0.02059 0.01847 0.01839		6.453 7.002	0.01474 0.01455

N.B. The Bunsen coefficients at the lowest temperature are thought to be considerably in error but the salting out parameters at the lowest temperatures are probably more reliable (see water evaluation).

AUXILIARY INFORMATION

SOURCE AND PURITY OF MATERIALS:

Ostwald method, using gas buret and pipet. Measurement of volume of gas before and after absorption. Vapor pressure of water was allowed for by assuming Raoult's law. Solution was degassed. Concentration of salt solution estimated by titration with silver nitrate solution. $\delta \alpha/\alpha = \pm 0.03$ REFERENCES:

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 3. Lithium chloride; LiCl; 1894, 52, 275-299. [7447-41-8] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient, a	Bunsen coefficient [#] at 288.2 K
288.2	1.800	0.999	0.01883	0.01883
283.62		1.0192	0.01676	0.01619
285.55		1.0416	0.01396	0.01370
285.92		1.0843	0.01006	0.00990

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha = \pm 0.02$.
	REFERENCES:

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Morrison, T. J.; Billett, F. (2) Water; H₂O; [7732-18-5] J. Chem. Soc. 1952, 3819 - 3822.

(3) Lithium Chloride; LiCl; [7447-41-8]

VARIABLES: PREPARED BY:

T/K: 285.75 - 344.85 P/kPa: 101.325 (1 atm)

EXPERIMENTAL VALUES:

Temperature			Salt Effect	
t/C	T/K	1/(T/K)	$(1/m)\log(s^{o}/s)^{1}$	$(1/m)\log(x^{O}/x)$
12.6	285.75	0.0035	0.064	0.079
30.0	303.15	0.0033	0.065	0.080
49.4	322.55	0.0031	0.061	0.076
71.7	344.85	0.0029	0.054	0.069

¹The authors used $(1/c)\log(S^O/S)$ with c defined as g eq salt per kg of water. For the 1-1 electrolyte the compiler changed the c to an m for $m_{NaCl}/mol\ kg^{-1}$. The hydrogen solubility S is cm³(STP) kg⁻¹.

The salt effect parameters were calculated from two measurements. The solubility of hydrogen in water, SO, and in the one molal salt solution, S. Only the solubility of the hydrogen in water, and the value of the salt effect parameter are given in the paper. The solubility values in the salt solution are not given.

The compiler calculated the values of the salt effect parameter using the mole fraction gas solubility ratio.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The degassed solvent flows in a thin film down an absorption helix containing the hydrogen gas plus solvent vapor at a total pressure of one atmosphere. The volume of gas absorbed is measured in an attached buret system (1).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared from pure zinc and dilute hydrochloric acid.
- (2) Water. No information given.
- (3) Lithium Chloride. "AnalaR" material.

ESTIMATED ERROR:

 $\delta k = 0.010$

REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Lithium chloride; LiCl; [7447-41-8]

ORIGINAL MEASUREMENTS:

Gerecke, J.; Bittrich, H. J.

Wiss. Z. Tech. Hocsch. Chem. "Carl Schorlemmer" Leuna-Merseburg 1971, 115 - 122, 313 - 321.

Chem. Abstr. 1972, 76, 77239, 77, 66741.

VARIABLES: T/K: 288

P/kPa: 101.325 (1 atm)

 $m_{LiC1}/mol \ kg^{-1}: 0.43 - 3.75$

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K	m _{LiCl} /mol kg ⁻¹	log (S°/S)
288	0.43	0.026
	0.75	0.046
	1.43	0.089
	3.75	0.225

Values were taken from a graph in the paper by the compiler.

The solubility ratio, S°/S, is a ratio of Kuenen coefficients.

The authors value of the solubility of hydrogen in water at 298.15 K and one atm partial pressure is a Bunsen coefficient of 0.0177.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The hydrogen solubilities appear to have been determined by the method of Morrison and Billett (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen.
- (2) Water.
- (3) Lithium chloride.

No information on the materials.

ESTIMATED ERROR:

 $\delta \log (S^{\circ}/S) = \pm 0.003$ from graph.

REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]	Geffcken, G.Z. Phys. Chem.		
2. Water; H ₂ O; [7732-18-5]	1904,49,257-302		
3. Sodium hydroxide; NaOH; [1310-73-2]			
VARIABLES:	PREPARED BY:		
Concentration	C.L. Young		
PUDENTAGAMAY MATING.			

EXPERIMENTAL VALUES:

T/K	Conc. of Hydroxide/mol dm3 (soln)	Ostwald coefficient, $\it L$
298.15	0.543 0.571 0.962 0.974	0.01632 0.01608 0.01442 0.01409
	1.059 1.137 1.850 3.400 3.430	0.01372 0.01348 0.01018 0.00648 0.00639
	4.687	0.00483

METHOD /APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using simple adsorption pipet and buret. Diagram and detailed description given in original paper.	 Prepared by the action of dilute hydrochloric acid on aluminium in the presence of mercury chloride. Washed in potassium hydroxide solution and potassium permangan- ate. Degassed.
	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta L = \pm 1 \%.$
	(estimated by compiler) REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:	
l. Hydrogen; H ₂ ; [1333-74-0]	Bruhn, G.; Gerlach, J.; Pawlek, F.	
2. Water; H ₂ O; [7732-18-5]	Zeit. Anorg. Allg. Chem.	
3. Sodium hydroxide; NaOH;	<u>1965</u> <i>337</i> , 68-79	
[1310-73-2]		
VARIABLES:	PREPARED BY:	
Temperature, concentration	C.L. Young	

EXPERIMENTAL VALUES:

T/K	Conc of salt/mol l-1	Bunsen coefficient, α
323.15	0.5 1.0 1.5	0.01306 0.01108 0.00868
373.15	0.5 1.0 1.5	0.01433 0.01270 0.00933
423.15	0.5 1.0 1.5	0.01790 0.01682 0.01308
473.15	0.5 1.0 1.5	0.02597 0.02115 0.01710
523.15	0.5 1.0 1.5	0.03535 0.02930 0.02350

	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping solution of gas and estimating volumetrically.	No details given.
·	ESTIMATED ERROR: $\delta T/K = \pm 2; \ \delta \alpha = \pm 2 \%.$ (estimated by compiler).
	REFERENCES: 1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute Report BMI-840, 1953.

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Water; H₂O; [7732-18-5] 3. Sodium chloride; NaCl; [7647-14-5] VARIABLES: Concentration of salt ORIGINAL MEASUREMENTS: Steiner, P. Ann. der Phys. Chem. 1894, 52, 275-299. PREPARED BY: C. L. YOung

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient,	Bunsen coefficient [#] at 288.2 K
		0.000	0.01883	0.01883
288.2	0	0.999_		
286.71	0.825	1.0315	0.01565	0.01548
286.95	2.049	1.0807	0.01140	0.01130
286.32	2.801	1.1088	0.00938	0.00925
286.63	4.815	1.1817	0.00602	0.00595

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha = \pm 0.02$.
	REFERENCES:

Salt Solution			ons (Aqueo	us)	67
COMPONENTS: 1. Hydrogen; H ₂ ; [1333-74-0] 2. Water; H ₂ O; [7732-18-5]		Braun, Z. phy	ys. Chem.		
3. Sodium chloride; NaCl; [7647-14-5]			33, 721-741		
VARIABLES: Temperature, concentration of salt EXPERIMENTAL VALUES:		PREPARED	C. L. Youn	a	
T/K	Wt. of salt per 100 g soln. /g	Bunsen coefficient,	T/K	Wt. of salt per 100 g soln. /g	Bunsen coefficient, a
278.2	0 1.250 1.523 3.798 4.496 5.506 5.999	0.02366 0.02180 0.02155 0.01977 0.01920 0.01861 0.01839	288.2	4.496 5.506 5.999 0 1.250 1.523 3.798	0.01714 0.01665 0.01640 0.01905 0.01771 0.01754 0.01623
283.2	0 1.250 1.523 3.798 4.496 5.506 5.999	0.02213 0.02052 0.02030 0.01876 0.01817 0.01769 0.01749	298.2	4.496 5.506 5.999 0 1.250 1.523 3.798	0.01587 0.01532 0.01528 0.01750 0.01621 0.01603 0.01476
288.2	0 1.250 1.523 3.798	0.02059 0.01914 0.01896 0.01760		4.496 5.506 5.999	0.01429 0.01395 0.01383

The Bunsen coefficients at the lowest temperatures are thought to be considerably in error but the salting out parameters are probably more reliable (see water evaluation). N.B.

METHOD APPARATUS / PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Ostwald method, using gas buret and pipet. Measurement of volume of gas before and after absorption. Vapor pressure of water was allowed for by assuming Raoult's law. Solution was degassed. Concentration of salt solution estimated	No details given.
by titration with silver nitrate solution.	ESTIMATED ERROR: $\delta\alpha/\alpha = \pm 0.03.$
	REFERENCES:

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Water; H₂O; [7732-18-5] (3) Sodium Chloride; NaCl; [7647-14-5] VARIABLES: T/K: 285.75 - 344.85 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819 - 3822.

EXPERIMENTAL VALUES:

WIND AUDI	123.			
Temper	rature		Salt Effect	Parameters
t/°C	<u>T/K</u>	1/(T/K)	$(1/m)\log(S^{O}/S)^{1}$	$(1/m)\log(x^{O}/x)$
12.6 30.0 49.4 71.7	285.75 303.15 322.55 344.85	0.0035 0.0033 0.0031 0.0029	0.097 0.092 0.082 0.066	0.112 0.107 0.097 0.081

¹The authors used $(1/c)\log(S^{\circ}/S)$ with c defined as g eq salt per kg of water. For the 1-1 electrolyte the compiler changed the c to an m for $m_{\text{NaCl}}/\text{mol kg}^{-1}$. The hydrogen solubility S is cm³(STP) kg⁻¹.

The salt effect parameters were calculated from two measurements. The solubility of hydrogen in water, S^{O} , and in the one molal salt solution, S. Only the solubility of the hydrogen in water, and the value of the salt effect parameter are given in the paper. The solubility values in the salt solution are not given.

The compiler calculated the values of the salt effect parameter using the mole fraction gas solubility ratio.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The degassed solvent flows in a thin film down an absorption helix containing the hydrogen gas plus solvent vapor at a total pressure of one atmosphere. The volume of gas absorbed is measured in an attached buret system (1).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared from pure zinc and dilute hydrochloric acid.
- (2) Water. No information given.
- (3) Sodium Chloride. "AnalaR" material.

ESTIMATED ERROR:

 $\delta k = 0.010$

REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Sodium chloride; NaCl; [7647-14-5]

ORIGINAL MEASUREMENTS:

Gerecke, J.; Bittrich, H. J.

Wiss. Z. Tech. Hocsch. Chem. "Carl Schorlemmer" Leuna-Merseburg 1971, 115 - 122, 313 - 321.

Chem. Abstr. 1972, 76, 77239, 77, 66741.

VARIABLES:

T/K:

288, 323 101.325 (1 atm) P/kPa:

m_{NaCl}/mol kg⁻¹: 0.50 - 4.30 PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K	m _{NaCl} /mol kg ⁻¹	log (S°/S)
288	0.50 1.00 2.00 4.30	0.051 0.097 0.164 0.388
323	0.50 1.00 2.00 4.30	0.042 0.083 0.190 0.325

Values were taken from a graph in the paper by the compiler.

The solubility ratio, S°/S, is a ratio of Kuenen coefficients.

The authors value of the solubility of hydrogen in water at 298.15 K and one atm partial pressure is a Bunsen coefficient of 0.0177.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The hydrogen solubilities appear to have been determined by the method of Morrison and Billett (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen.
- (2) Water.
- (3) Sodium chloride.

No information on the materials.

ESTIMATED ERROR:

 $\delta \log (S^{\circ}/S) = +0.003$ from graph.

REFERENCES:

Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Crozier, T. E.; Yamamoto, S. (2) Water; H₂O; [7732-18-5] J. Chem. Eng. Data 1974, 19, 242-244. (3) Sodium chloride; NaCl; [7647-14-5] VARIABLES: PREPARED BY: T/K: 274.03 - 301.51 P/kPa: 101.325 (1 atm) P. L. Long H. L. Clever w_{NaCl}/⁶/₀₀: 10.950, 27.376

EXPERIMENTAL VALUES:

 T/K	Bunsen Coefficient a	Ostwald Coefficient L
10.950	parts NaCl per	1000
283.97 289.55 301.48 301.51	0.01852 0.01770 0.01770 0.01650 0.01651	0.01925 0.01876 0.01876 0.01821 0.01822
27.376	parts NaCl per	1000
274.03 274.04 295.34 295.37 301.47	0.01877 0.01881 0.01586 0.01585 0.01552	0.01883 0.01887 0.01715 0.01714 0.01713

The authors report 42 values of the solubility of hydrogen in pure water at temperatures between 274.60 and 302.47 K. See page 18.

The sodium chloride concentrations of 10.950 and 27.376 parts per 1000 are equivalent to molalities , $m_{\rm NaCl}/mol~kg^{-1}$, of 0.1895 and 0.4815, respectively.

The compiler calculated the Ostwald coefficients from the authors Bunsen coeffcients.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

The solubility measurements were made by the Scholander (1) microgasometric technique as modified by Douglas (2). Equilibration is with 6 cm³ of gas-free water. All volumes are read on a micrometer which adjusts (3) Sodium chloride. No information.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Linde Specialty Gas. Research grade, 99.9995 per cent pure.
- (2) Water. Distilled from glass apparatus.

ESTIMATED ERROR:

 $\delta T/K = 0.01$ $\delta(\text{Parts per }1000/\%_{00}) = 0.003$

REFERENCES:

- 1. Scholander, P. F. J. Biol. Chem. 1947, 167, 235.
- 2. Douglas, E. J. Phys. Chem. 1964, 68, 169.

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Hydrogen; H₂; [1333-74-0] Water; H₂O; [7732-18-5] Sodium sulfate; Na₂SO₄; [7757-82-6] 	Steiner, P. Ann. der Phys. Chem. 1894, 52, 275-299.
VARIABLES:	PREPARED BY:
Concentration of salt	C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient,	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
291.66	0.335	1.0412	0.01482	0.01519
291.72	0.638	1.0768	0.01223	0.01254
291.56	1.364	1.1608*	0.00757	0.00775

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR: $\delta \alpha / \alpha = \pm 0.02.$
	REFERENCES:

^{*} at 291.15 K.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Sodium sulfate; Na₂SO₄; [7757-82-6]
- (4) Sulfuric acid; H₂SO₄; [7664-93-9]

VARIABLES:

T/K: 298.15

H₂ P/kPa: 101.325 (760 mmHg)

ORIGINAL MEASUREMENTS:

Kobe, K. A.; Kenton, F. H.

Ind. Eng. Chem., Anal. Ed. 1938, 10. 76 - 77.

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature T/K	Solvent Volume cm ³	Hydrogen Volume Absorbed cm ³	Bunsen Coefficient a	Ostwald Coefficient L
25	298.15	49.54 99.54	0.37 0.72	0.0067	0.0073

The solvent was a mixture of 800 g $\rm H_2O$, 200 g $\rm Na_2SO_4$ (anhydrous), 40 ml $\rm H_2SO_4$ (conc., 36 N).

Thus the molality of the solution was

 $m_{\text{Na}_2\text{SO}_4}/\text{mol kg}^{-1} = 1.76$

 $m_{H_2SO_4}/mol \ kg^{-1} = 0.90$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was described in detail in an earlier paper (1). The apparatus consists of a gas buret, a pressure compensator, and a 200 \mbox{cm}^3 absorption bulb and mercury leveling bulb. The absorption bulb is attached to a shaking mechanism.

The solvent and the gas are placed in the adsorption bulb. The bulb was shaken until equilibrium was reached. The remaining gas was returned to the buret. The difference in final and initial volumes was taken as the gas absorbed.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Purity stated to be 99⁺ percent.
- (2) Water. Distilled.
- (3, 4) Sodium sulfate and sulfuric acid. Sources not given. Analytical grades.

ESTIMATED ERROR:

 $\delta\alpha/cm^3 = 0.001$ (authors)

REFERENCES:

1. Kobe, K. A.; Williams, J. S. Ind. Eng. Chem., Anal. Ed. 1935, 7, 37.

COMPONENTS: ORIGINAL MEASUREMENTS: Longo, L. D.; Delivoria-1. Hydrogen; H₂; [1333-74-0] 2. Water; H₂O; [7732-18-5] Papadopoulas, M.; Power, G. G.; Hill, E. P.; Forster, R. E., Sodium nitrite; NaNO₂; Am. J. Physiology, 1970, 219, [7632-00-0] 561-569. VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: Conc. of salt /mol dm $^{-3}$ Bunsen coefficient, α s.D.* T/K 310.15 0.0155 0.0003 0.14 standard deviation AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Liquid samples were equilibrated No details given. with gas and then the dissolved gas was stripped out under vacuum and measured in a manometric Van Slyke apparatus. Some details in ref. 1. ESTIMATED ERROR: $\delta T/K = \pm 0.03$.

REFERENCES:

1. Power, G. G.,

468.

J. Appl. Physiology, 1968, 24,

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Hydrogen; H₂; [1333-74-0] Water; H₂O; [7732-18-5] Sodium nitrate; NaNO₃; [7631-99-4] 	Steiner, P. Ann. der Phys. Chem. 1894, 52, 275-299.
VARIABLES:	PREPARED BY:
Concentration of salt	C. L. Young

EXPERIMENTAL VALUES:

т/к	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient,	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
290.95	0.679	1.0367	0.01572	0.01603
290.80	1.413	1.0765	0.01345	0.01370
290.55	2.656	1.1417	0.01034	0.01052
290.51	3.980	1.2099	0.00797	0.00810
290.42	5.711	1.2963	0.00568	0.00578

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source. ESTIMATED ERROR: $\delta \alpha/\alpha = \pm 0.02$. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Hydrogen; H₂; [1333-74-0] Water; H₂O; [7732-18-5] Sodium nitrate; NaNO₃; [7631-99-4] 	Knopp, W. Z. Phys. Chem. 1904, 48, 97-108.
VARIABLES: Concentration of salt	PREPARED BY: C. L. Young
EXPERIMENTAL VALUES:	

T/K	Wt. of salt in 100 g soln.	Conc. of salt /mol dm (soln.)	Density of soln. /g cm ⁻³	Bunsen absorption coefficient, α	10 mole fraction of hydrogen, $10^4 x_{\rm H_2}$
293.15	0	0	0.99823	0.01883	0.1511
	1.041	0.1236	1.00524	0.01839	0.1476
	2.192	0.2634	1.01303	0.01774	0.1428
	4.405	0.5416	1.02820	0.01694	0.1367
	6.702	0.8442	1.04411	0.01518	0.1229
	12.637	1.7394	1.08667	0.01300	0.1064

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Manometric method with absorption pipet and gas buret were used. Densities were determined using a Sprengel pyknometer.	 Prepared from pure zinc and dil. sulfuric acid in a Kipp's apparatus, passed through silver nitrate, potassium hydroxide and permanganate solutions. and 3. No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha$ = ±3% (estimated by compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
 Hydrogen; H₂; [1333-74-0] Water; H₂O; [7732-18-5] Sodium carbonate; Na₂CO₃; [497-19-8] 	Steiner, P. Ann. der Phys. Chem. 1894, 52, 275-299.
VARIABLES: Concentration of salt	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient,	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
285.09	0.207	1.0217	0.01677	0.01639
284.76	0.438	1.0457	0.01420	0.01385
285.23	0.819	1.0835	0.01106	0.01082
286.22	1.218	1.1213	0.00851	0.00839

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha = \pm 0.02$.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Geffcken, G.Z.Phys.Chem.
2. Water; H ₂ O; [7732-18-5]	1904,49,257-302
Potassium hydroxide; KOH; [1310-58-3]	
VARIABLES:	PREPARED BY:
Concentration	C.L. Young
EXPERIMENTAL VALUES.	

EXPERIMENTAL VALUES:

T/K	Conc of hydroxide/mol dm³ (soln)	Ostwald coefficient, ${\it L}$
298.15	0.536	0.01658
	0.715	0.01539
	1.059	0.01378
	1.056	0.01389
	1.480	0.01195

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Prepared by the action of dilute hydrochloric acid on aluminium Volumetric method using simple in the presence of mercury chloride. Washed in potassium adsorption pipet and buret. Diagram and detailed description hydroxide solution and potassium permanganate solution. Dried. given in original paper. 2. Degassed. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \delta L = \pm 1$ %. (estimated by compiler). REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Potassium hydroxide; KOH [1310-58-3]

ORIGINAL MEASUREMENTS:

Knaster, M. B.; Apel'baum, L. A.

Zh. Fiz. Khim. 1964, 38, 223 - 225.

Russ. J. Phys. Chem. <u>1964</u>, 38, 120 - 122.

VARIABLES: P/kPa: 101.325 (760 mmHg) c₃/mol dm⁻³: 0 - 10

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tem	perature	Potassium	Bunsen	Salt Effect
t/°C	T/K	Hydroxide c ₃ /mol dm ⁻³	Coefficient	Parameter k _{sc} /dm ³ mol ⁻¹
21	294.15	0 1 4 7 10	18.10 14.15 6.11 2.51 1.11	0.107 0.118 0.123 0.121
45	318.15	0 1 4 7 10	16.30 12.75 5.35 2.13 0.809	0.107 0.121 0.126 0.130
75	348.15	0 1 4 7 10	16.10 12.14 5.21 1.98 0.736	0.123 0.122 0.130 0.134

¹ Salt effect parameter, $k_{sca}/dm^3 \text{ mol}^{-1} =$ $(1/(c_3/\text{mol dm}^3)) \log (\alpha^0/\alpha)$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The KOH solution was introduced into the saturating vessel. The solution was saturated with gas, which was bubbled through the solution at a rate of 15 $dm^{3} h^{-1}$ for 5 h. The gas stream was turned off and the solution was allowed to stand for one h to allow suspended gas bubbles to escape. A known amount of the gassaturated solution was transferred to an evacuated flask. The gas evolved from the solution was withdrawn, together with water vapor, into an evacuated and calibrated portion of the apparatus. The water vapor was frozen out in a liquid oxygen trap. The pressure (ca. 1 mmHg) of the residual gas at a known temperature and volume was measured on a McLeod gage.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. The gas was produced by electrolysis and subjected to a standard purification process.
- (2) Water. No information.
- (3) Potassium hydroxide. No information.

ESTIMATED ERROR:

 $\delta T/K = 0.1$ $\delta\alpha/\alpha = 0.007$ (authors)

REFERENCES:

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Water; H₂O; [7732-18-5] 3. Potassium hydroxide, KOH; [1310-58-3] VARIABLES: Temperature, concentration C.L. Young EXPERIMENTAL VALUES:

т/к	Conc of salt/mol 1-1	Bunsen coefficient, α
323.15	0.5 1.0 1.5	0.01299 0.01146 0.00947
373.15	0.5 1.0 1.5	0.01528 0.01360 0.00992
423.15	0.5 1.0 1.5	0.01880 0.01620 0.01404
473.15	0.5 1.0 1.5	0.02650 0.02298 0.01313

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Static equilibrium cell. Similar to that described by Pray and Stephan (1). Composition of liquid determined by stripping solution of gas and estimating volumetrically.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 2$; $\delta \alpha = \pm 2$ %. (estimated by compiler).

REFERENCES:

1. Pray, H.A.; Stephan, E.L. Battelle Memorial Institute Report, BMI-840, 1953.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Ruetschi, P.; Amlie, R. F. (2) Water; H₂O; [7732-18-5] J. Phys. Chem. 1966, 70, 718 - 723. (3) Potassium hydroxide; KOH; [1310-58-3] **VARIABLES:** PREPARED BY: T/K: 303.15 101.325 (1 atm) H. L. Clever H₂ P/kPa: CKOH/mol dm-3:

EXPERIMENTAL.	17 AT 11DC .
LEVLEKTLIENTAL	AWTHES

0 - 10.23

Tempe t/ ^O c	rature T/K	Molarity ¹ C _{KOH} /mol dm ⁻³	Solubility cm ³ (STP)dm ⁻³	log(S ^O /S)	(1/c) log(s ⁰ /S)
30	303.15	0.0	17.03 16.90 17.10		
			$\frac{16.93}{16.99 \pm 0.08 \text{ A}}$	v. -	-
		0.0091 0.102 0.510	16.68 16.29 14.13	0.003 0.018 0.080	0.33 0.18 0.16
		1.03 1.98 3.04	12.13 9.27 6.71	0.146 0.264 0.404	0.141 0.133 0.133
		5.00 7.61 10.23	3.65 1.59 0.77	0.666 1.029 1.344	0.133 0.135 0.131

¹ The authors labeled the concentration as equivalents per liter.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

They used the apparatus of Ben-Naim and Baer (1). A calibrated dissolution vessel contains degassed water. Gas is introduced wet from a calibrated gas buret system. Stirring the liquid forces it up sidearms attached to the top of the flask and the liquid returns via a central tube. The amount of gas dissolved is determined via the gas burets. The gas burets and dissolution vessel are thermostated in a water bath. The original paper contains a diagram ESTIMATED ERROR: and a description of operation.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Prepurified grade (99.5% min purity).
- (2) Water. No comment by author.
- (3) Potassium hydroxide. Source not given. Reagent grade.

REFERENCES:

 Ben-Naim, A.; Baer, S. Trans. Faraday Soc. 1963, 59, 2735.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Potassium hydroxide; KOH; [1310-58-3]

ORIGINAL MEASUREMENTS:

Shoor, S. K.; Walker, R. D. Jr.; Gubbins, K. E.

J. Phys. Chem. 1969, 73, 312 - 317.

EXPERIMENTAL VALUES:

T/K	Potass:	ium Hydroxide	Mol Fraction	Solubility Ratio	
	KOH/wt %	c _{KOH} /mol dm ⁻³	$H_2/x_1 \times 10^5$	$\gamma = x^0/x$	Parameter $k_s = \log(x^0/x)/c$
298.15	0.0 5.00 9.00 19.50 41.40 52.40	0.0 0.92 1.70 4.12 10.37 14.35	1.43	1.00 1.36 1.71 3.50 20.1 72.0	0.145 0.137 0.132 0.127 0.129
313.15	0.0 5.00 9.00 19.50 32.40 41.40 52.40	0.0 0.92 1.70 4.12 7.60 10.37 14.35	1.29	1.00 1.28 1.64 3.29 8.70 20.4 73.7	0.129 (authors) 0.117 0.126 0.125 0.124 0.126 0.130 0.129 (authors)
333.15	0.0 5.00 9.00 19.50 32.40 41.40 52.40	0.0 0.92 1.70 4.12 7.60 10.37 14.35	1.30	1.00 1.32 1.74 3.58 9.16 21.4 76.7	0.131 0.141 0.134 0.127 0.128 0.131 0.129 (authors)
353.15	0.0 5.00 9.00 19.50 32.40 41.40 52.40	0.0 0.92 1.70 4.12 7.60 10.37 14.35	1.322	1.00 1.33 1.81 3.65 9.04 21.8 75.4	0.135 0.152 0.136 0.126 0.129 0.131 0.129 (authors)
373.15	0.0 38.00 41.40 52.40 56.50	0.0 9.27 10.37 14.35 16.20	1.342	1.00 15.3 21.9 82.6 108.	0.128 0.129 0.134 0.126

The compiler calculated the salt effect parameters, $k_{\rm S}=(1/{\rm c})\log{(x^0/x)}$, at the individual KOH concentrations. The authors values are noted.

Continued on next page.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Potassium hydroxide; KOH; [1310-58-3]

ORIGINAL MEASUREMENTS:

Shoor, S. K.; Walker, R. D., Jr.; Gubbins, K. E.

J. Phys. Chem. 1969, 73, 312 - 317.

VARIABLES:

T/K: 298.15 - 373.15 P/kPa: 101.325 (1 atm)

KOH/wt %: 0 - 56.50

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

See preceding page.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: A gas chromatographic method was used (1). The hydrogen saturated solutions were prepared by bubbling the gas through presaturators and then through the KOH solution. Samples were drawn from the solution over a 48 hour period to determine whether or not equilibrium was established. Samples were transferred from the saturator to the gas chromatograph in gas tight Hamilton syringes. All analyses were made with a thermal conductivity detector, and with nitrogen as the carrier gas.

The results are reported as activity coefficients, which are the mole fraction solubility ratio, x^0/x , where $x^{\,0}$ is the gas mol fraction solubility in water, and x is the gas mol fraction solubility in the aqueous KOH solution, both at a gas partial pressure of one atm. Solubility values were corrected to one atm assuming Henry's law is obeyed. The activity coefficients are the average of at least four measurements.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Minimum purity stated to be 99.9 per cent.
- (2) Water. Specially distilled and degassed from an all glass-Teflon still.
- (3) Potassium hydroxide. Baker Analyzed Reagent Grade. Contained a maximum of 1 per cent K2CO3. The KOH solutions were protected from atmospheric CO2 with Ascarite.

ESTIMATED ERROR:

 $\delta T/K = 0.05$ $\delta \gamma / \gamma = 0.01$

REFERENCES:

1. Gubbins, K. E.; Carden, S. N.;
 Walker, R. D. Jr. J. Gas Chromatog. 1965, 3, 98.

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 3. Potassium chloride; KC1; 1894, 52, 275-299. [7747-40-7] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient, a	Bunsen coefficient [#] at 288.2 K
288.2		0.999	0.01883	0.01883
292.38	0 0.526	1.0240	0.01618	0.01667
292.15	1.051	1.0480	0.01447	0.01489
291.86	1.755	1.0794	0.01246	0.01279
291.97	2,909	1.1294	0.00985	0.01012
291.77	3.554	1.1565	0.00869	0.00892

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

	_
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha = \pm 0.02$.
	REFERENCES:

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Knopp, W. 2. Water; H₂O; [7732-18-5] Z. Phys. Chem. 3. Potassium chloride; KCl; 1904, 48, 97-108. [7447-40-7] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Wt. of salt in 100 g soln.	Conc. of salt /mol dm ⁻³ (soln.)	Density of soln. /g cm ⁻³	Bunsen absorption coefficient, a	10 mole fraction of hydrogen, 10 x H ₂
293.15	0	0	0.99823	0.01883	0.1511
	1.089	0.1475	1.00520	0.01823	0.1464
	2.123	0.2907	1.01182	0.01757	0.1413
	4.070	0.5687	1.02431	0.01661	0.1339
	6.375	0.9127	1.03936	0.01531	0.1239
	7.380	1.0682	1.04600	0.01472	0.1194
	13,612	2.1222	1.08754	0.01255	0.1030

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Manometric method with absorption pipet and gas buret were used. Densities were determined using a Sprengel pyknometer.

SOURCE AND PURITY OF MATERIALS:

- 1. Prepared from pure zinc and dil. sulfuric acid in a Kipp's apparatus, passed through silver nitrate, potassium hydroxide and permanganate solutions.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta\alpha/\alpha$ = ±3% (estimated by compiler).

REFERENCES:

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Water; H₂O; [7732-18-5] (3) Potassium chloride; KC1; [7747-40-7] VARIABLES: T/K: 288 P/kPa: 101.325 (1 atm) m_{KC1}/mol kg-1: 0.50, 1.0 PREPARED BY: ORIGINAL MEASUREMENTS: Gerecke, J.; Bittrich, H.-J. Wiss. Z. Tech. Hocsch. Chem. "Carl Schorlemmer" Leuna-Merseburg 1971, 115 - 122, 313 - 321. Chem. Abstr. 1972, 76,77239,77,66741 PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

T/K	m _{KCl} /mol kg ⁻¹	log (S°/S)
288	0.50	0.043

Values were taken from a graph in the paper by the compiler.

The solubility ratio, S^0/S , is a ratio of Kuenen coefficients.

The authors value of the solubility of hydrogen in water at 298.15 K and one atm partial pressure is a Bunsen coefficient of 0.0177.

AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: The hydrogen solubilities appear to have been determined by the method of Morrison and Billett (1). (1) Hydrogen. (2) Water. (3) Potassium chloride. No information on the materials. ESTIMATED ERROR: &log (S°/S) = ±0.003 from graph. REFERENCES: 1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Potassium Iodide; KI; [7681-11-0]

ORIGINAL MEASUREMENTS:

Morrison, T. J.; Billett, F.

- J. Chem. Soc. 1952, 3819 3822.

VARIABLES:

T/K: 285.75 - 344.85 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

			Salt Effect	Daramotora
Temperature				
t/°C	<u> T/K</u>	1/(T/K)	$(1/m)\log(s^{O}/s)^{1}$	$(1/m)\log(x^{O}/x)$
12.6	285.75	0.0035	0.088	0.103
30.0	303.15	0.0033	0.081	0.096
49.4	322.55	0.0031	0.066	0.081
71.7	344.85	0.0029	0.043	0.058

¹The authors used $(1/c)\log(S^{O}/S)$ with c defined as g eq salt per kg of water. For the 1-1 electrolyte the compiler changed the c to an m for m_{NaCl}/mol kg⁻¹. The hydrogen solubility S is cm³(STP) kg⁻¹.

The salt effect parameters were calculated from two measurements. solubility of hydrogen in water, So, and in the one molal salt solution, S. Only the solubility of the hydrogen in water, and the value of the salt effect parameter are given in the paper. The solubility values in the salt solution are not given.

The compiler calculated the values of the salt effect parameter using the mole fraction gas solubility ratio.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The degassed solvent flows in a thin film down an absorption helix containing the hydrogen gas plus solvent vapor at a total pressure of one atmosphere. The volume of gas absorbed is measured in an attached buret system (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared from pure zinc and dilute hydrochloric acid.
- (2) Water. No information given.
- (3) Potassium Iodide. "AnalaR" material.

ESTIMATED ERROR:

 $\delta k = 0.010$

REFERENCES:

 Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033.

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 3. Potassium nitrate; KNO₃; 1894, 52, 275-299. [7757-79-1] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient,	Bunsen coefficient [†] at 288.2 K
288.2 290.97 290.73 289.96 290.42 290.96	0 0.482 0.879 1.541 1.820 2.430	0.999 1.0295 1.0539 1.0936 1.1101	0.01883 0.01650 0.01530 0.01373 0.01290 0.01157	0.01883 0.01683 0.01501 0.01391 0.01311

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR:
	$\delta\alpha/\alpha = \pm 0.02.$
	REFERENCES:

EXPERIMENTAL VALUES:

T/K	Wt. of salt in 100 g soln.	Conc. of salt /mol dm ⁻³ (soln.)	Density of soln. /g cm-3	Bunsen absorption coefficient, α	10 4 mole fraction of hydrogen, $10^4 x_{ m H_2}$
293.15	0	0 0.1245	0.99823 1.00593	0.01883 0.01835	0.1511 0.1475
	2.094	0.2114	1.01133	0.01818	0.1464
	4.010	0.4127	1.02362	0.01785	0.1443
	5.925	0.6225	1.03592	0.01743	0.1415
	7.742	0.8293	1.04768	0.01667	0.1358
	13.510	1.5436	1.08646	0.01436	0.1198

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Manometric method with absorption pipet and gas buret being used. Densities were determined using a Sprengel pyknometer.

SOURCE AND PURITY OF MATERIALS;

- Prepared from pure zinc and dil. sulfuric acid in a Kipp's apparatus, passed through silver nitrate, potassium hydroxide and permanganate solutions.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta\alpha/\alpha$ = ±3% (estimated by compiler).

REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H_2 ; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 1894, 52, 275-299. Potassium carbonate; K₂CO₃; [584-08-7] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient, a	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
284.38	0.209	1.0248	0.01675	0.01628
285.44	0.341	1.0405	0.01532	0.01501
284.47	0.690	1.0807	0.01216	0.01183
285.66	1.376	1.1555	0.00775	0.00761
285.77	2.156	1.2353	0.00470	0.00462
285.92	2.939	1.3112	0.00290	0.00285
286.32	4.352	1.4395	0.00162	0.00160

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source.	No details given.
	ESTIMATED ERROR: $\delta\alpha/\alpha = \pm 0.02.$
	REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Urea; CH_4N_2O or $(NH_2)_2CO$; [57-13-6]

ORIGINAL MEASUREMENTS:

Hüfner, G.

Z. Physik. Chem. 1907, 57, 611-624.

VARIABLES:

T/K: 293.29, 293.36 H₂ P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempe t/°C	rature T/K	C _{urea} / mol cm ⁻³	Gas Pressure/ mmHg	Absorbed Gas Volume ¹	Bunsen Coefficient $\alpha \times 10^2$
20.11	293.26	0.0			1.8102
20.21 20.14	293.36 293.29	1.0 1.0	668.4 699.3	6.13 6.39	1.700 1.706

 $^{^1\}mathrm{Volume}$ of gas reduced to 273.15 K and 760 mmHg absorbed in 490.94 cm^3 solution at stated pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, described in reference (1), was the Bunsen absorption type. It consisted of an absorption flask, which holds 409.94 cm³ of solvent, and gas burets.

The final partial pressure of the gas ranged between 662.5 and 694.3 mmHg. The author reported both the volume of gas absorbed at the final pressure in $409.94~{\rm cm}^3$ of solvent reduced to 273.15 K and 760 mmHg, and the Bunsen coefficient, which was calculated assuming Henry's law.

Urea name Harnstoff in paper.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Formed by the reaction of dilute sulfuric acid on zinc.

 The gas was washed with permanganate and caustic solutions and stored over mercury.
- (2) Water. Pure.
- (3) Urea. Source not given.

ESTIMATED ERROR:

 $\delta T/K = 0.01$

REFERENCES:

1. Hüfner, G.
Archiv. F. Anatomie und
Physiologie, Physiolog. Abtly.
1894, 5, 191.

²Average of three runs, see Hüfner's H₂ + H₂O data sheet.

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]	Geffcken, G.Z.Phys.Chem.		
2. Water; H ₂ O; [7732-18-5]	1904, 49, 257-302		
3. Chloroacetic acid; C ₂ H ₃ ClO ₂ [79-11-8]			
VARIABLES:	PREPARED BY:		
Temperature	C.L. Young		
EXPERIMENTAL VALUES:			
T/K Conc of acid/mol dm ³ (se	oln) Ostwald coefficient, L		
288.15 0.527 0.990 1.773	0.01905 0.01852 0.01783		
AUXILIAR	Y INFORMATION		
METHOD /APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Volumetric method using simple adsorption pipet and buret. Diagram and detailed description given in original paper.	 Prepared by the action of dilute hydrochloric acid on aluminium in the presence of mercury chloride. Washed in potassium hydroxide solution and potassium permanganate solution. Dried. Degassed. 		
	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta L = \pm 1 \%.$ (estimated by compiler).		

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Knopp, W. 2. Water; H₂O; [7732-18-5] Z. Phys. Chem. 3. 2,2,2-Trichloro-1,1 -Ethanediol (Chloralhydrate); C₂H₃Cl₃O₂; [302-17-0] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Wt. of salt in 100 g soln. /g	Conc. of salt /mol dm ⁻³ (soln.)	Density of soln. /g cm ⁻³	Bunsen absorption coefficient α	10^4 × Mole fraction of hydrogen $10^4 x_{ m H_2}$
293.15	0	0	0.99823	0.01883	0.1511
	4.911	0.310	1.02017	0.01839	0.1509
	7.69	0.504	1.03199	0.01802	0.1501
ì	14.56	1.030	1.06687	0.01712	0.1476
	18.77	1.397	1.08844	0.01653	0.1460
	29.50	2.530	1.14659	0.01542	0.1461
	32.00	2.845	1.16175	0.01518	0.1463
Į.	38.42	3.770	1.19817	0.01440	0.1463
[49.79	6.000	1.27242	0.01353	0.1530
	60.12	9.120	1.34522	0.01324	0.1697
	63.90	10.700	1.37426	0.01307	0.1768

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Manometric method with absorption pipet and gas buret were used. Densities were determined using a Sprengel pyknometer.

SOURCE AND PURITY OF MATERIALS:

- 1. Prepared from pure zinc and dil. sulfuric acid in a Kipp's apparatus, passed through silver nitrate, potassium hydroxide and permanganate solutions.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta\alpha/\alpha$ = ±3% (estimated by compiler).

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0]

- 2. Water; H₂O; [7732-18-5]
- 2,2,2-Trichloro-1,1,-Ethanediol (Chloralhydrate); C₂H₃Cl₃O₂; [302-17-0]

ORIGINAL MEASUREMENTS:

Muller, C.

Z. Phys. Chem. 1912-13, 81,

483-503.

VARIABLES:

Concentration of component 3

PREPARED BY:

C. L. Young

	Conc. of		Bunsen [#]	Density	
	comp. (3)	Bunsen	coefficient	of soln.	
T/K	(wt-%)	coefficient	at 288.2 K	at t/°C	t/°C
	Fi	st set of experi	mental data		
288.15	10	0.01740	0.01740	1.045	4
289.55	16.1	0.01719	0.01737	1.0772	16
288.95	33.35	0.01475	0.01484	1.1734	15
288.15	39.4	0.01470	0.01470	1.2144	15
288.75	51	0.01300	0.01306	1.2848	16
289.35	60.8	0.01281	0.01230	1.3585	16
288.65	70.7	0.01282	0.01287	1.44	16
288.15	79	0.01320	0.01320	1.5105	15
	Sec	cond set of expen	imental data		
292,55	15.5	0.01732	0.01724	1.0728	19
290.55	28.3	0.01569	0.01540	1.1444	17.4
291.85	46.56	0.01388	0.01375	1.2527	18.7
289.65	52	0.01314	0.01280	1.2899	17
290.15	63	0.01270	0.01243	1.3735	17
290.35	66	0.01285	0.01260	1.398	17.5
291.05	68	0.01286	0.01270	1.4121	18
291.45	78.4	0.01398	0.01380	1.4997	18

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric method in which pressure was determined using a mercury manometer. Solution was degassed by boiling under reduced pressure. A considerable amount of water was removed by this process. Gas was saturated with water vapor before being admitted to absorption buret.

SOURCE AND PURITY OF MATERIALS:

- Prepared by reaction of acid on zinc, washed with caustic potash solution.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$ $\delta P/P = \pm 0.001;$ $\delta \alpha/\alpha = \pm 3\%$ (estimated by compiler).

94	Hydrogen Solubil	ities up to 200kPa
COMPONENTS:	· · · · · · · · · · · · · · · · · · ·	ORIGINAL MEASUREMENTS:
1. Hydrogen; H	2; [1333-74-0]	Geffcken, G.Z. Phys. Chem.
2. Water; H ₂ O;	[7732-18-5]	1904,49,257-302
3. Acetic acid	; C ₂ H ₄ O ₂ ; [64-19-7]	
VARIABLES:		PREPARED BY:
Concentrati	on	C.L. Young
EXPERIMENTAL VALUES	3:	· · · · · · · · · · · · · · · · · · ·
т/к	Conc of acid/mol	${ m dm^3}$ (soln) Ostwald coefficient,
298.15	0.517 0.528 1.160 1.20 1.963 1.980 3.178 3.220	0.01925 0.01923 0.01903 0.01895 0.01885 0.01882 0.01862 0.01858

3.220 4.157

AUXILIARY INFORMATION

METHOD	/APPARATUS	/PROCEDURE:

Volumetric method using simple adsorption pipet and buret. Diagram and detailed description given in original paper.

SOURCE AND PURITY OF MATERIALS:

1. Prepared by the action of dilute hydrochloric acid on aluminium in the presence of mercury chloride. Washed in potassium hydroxide solution and potassium permanganate solution. Dried.

0.01849

2. Degassed.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta L = \pm 1$ %. (estimated by compiler).

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Acetamide; C_2H_5NO or CH_3CONH_2 ; [60-35-5]

ORIGINAL MEASUREMENTS:

Hüfner, G.

Z. Physik. Chem. 1907, 57, 611-624

VARIABLES:

T/K: 293.10, 293.43 H₂ P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature		CC2H5NO/mol dm-3	Gas Pressure/ mmHg	Absorbed Gas Volume ¹	Bunsen Coefficient $\alpha \times 10^2$	
20.11	293.26	0.0			1.8102	
20.28 19.95	293.43 293.10	1.0 1.0	662.5 682.0	6.42 6.60	1.796 1.794	

 $^{^1\}mathrm{Volume}$ of gas reduced to 273.15 K and 760 mmHg absorbed in 490.94 cm 3 solution at the stated pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, described in reference (1), was the Bunsen absorption type. It consisted of an absorption flask, which holds 409.94 cm³ of solvent, and gas burets.

The final partial pressure of the gas ranged between 662.5 and 694.3 mmHg. The author reported both the volume of gas absorbed at the final pressure in 409.94 cm³ of solvent reduced to 273.15 K and 760 mmHg, and the Bunsen coefficient, which was calculated assuming Henry's law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Formed by the reaction of dilute sulfuric acid on zinc. The gas was washed with permanganate and caustic solutions and stored over mercury.
- (2) Water. Pure.
- (3) Acetamide. Source not given.

ESTIMATED ERROR:

 $\delta T/K = 0.01$

REFERENCES:

1. Hüfner, G.
Archiv. F. Anatomie und
Physiologie, Physiolog. Abtly.
1894, 5, 191.

²Average of three runs, see Hüfner's H₂ + H₂O data sheet.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Glycine; C₂H₅NO₂ or CH₂(NH₂)COOH; [56-40-6]

ORIGINAL MEASUREMENTS:

Hüfner, G.

Z. Physik. Chem. 1907, 57, 611-624.

VARIABLES:

T/K: 293.26, 293.31 H₂ P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempera t/°C	ture T/K	C ₂ H ₅ NO ₂ /mol dm ⁻³	Gas Pressure mmHg	Absorbed Gas Volume ¹	Bunsen Coefficient $\alpha \times 10^2$
20.11	293.26	0.0			1.810 ²
20.16	293.31	1.0	666.7	5.67	1.577

¹ Volume of gas reduced to 273.15 K and 760 mmHg absorbed in 490.94 cm³ solution of the stated pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, described in reference (1) Hydrogen. Formed by the reaction (1), was the Bunsen absorption type. It consisted of an absorption flask, which holds 409.94 cm³ of solvent, and gas burets.

The final partial pressure of the gas ranged between 662.5 and 688.1 mmHg. The author reported both the volume of gas absorbed at the final pressure in 409.94 cm³ of solvent reduced to 273.15 K and 760 mmHg, and the Bunsen coefficient, which was calculated assuming Henry's law.

Glycine name glykoholl (aminoessigsaure) in the paper.

SOURCE AND PURITY OF MATERIALS:

- of dilute sulfuric acid on zinc. The gas was washed with permanganate and caustic solutions and stored over mercury.
- (2) Water. Pure.
- (3) Glycine. Merck.

ESTIMATED ERROR:

 $\delta T/K = 0.01$

REFERENCES:

1. Hüfner, G.
Archiv. F. Anatomie und Physiologie, Physiolog. Abtly. 1894, 5, 191.

²Average of three runs, see Hüfner's H₂ + H₂O data sheet.

- Hydrogen; H₂; 1333-74-0
- 2. Ethanol or Ethyl Alcohol; C2H5OH; 64-17-5
- 3. Water; H₂O; 7732-18-5

ORIGINAL MEASUREMENTS:

Cargill, R.W.

J Chem. Soc., Faraday Trans. I 1978, 74, 1444-1456

VARIABLES:

T/K : 277.4 - 335.2 P/kPa : 101.325 (1 atm) C₂H₅OH/X₂: 0.0 - 1.0 PREPARED BY:

R.W. Cargill

EXPERIMENTAL VALUES:

Mol Fraction Ethanol/X2	T/K	104 T-1	log(S _O /cm ³ kg ⁻¹)	S _O /cm ³ kg ⁻¹
0.98	278.9	35.87	1.962	91.6
0.98	289.2	34.59	1,984	96.4
0.98	299.2	33.43	2,000	100
0.98	309.2	32.35	2.025	106
0.98	320.2	31.24	2.045	111
0.98	333.2	30.02	2.061	115

aValues from reference 3.

The Solubility, S $_{\rm O}$, calculated as cm 3 gas at 273.15 K and Ar partial pressure of 101.325 kPa (1 atm) per kg of solvent.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

METHOD: Absorption of gas by a thin film of liquid. The Morrison and Billett (1) method was modified by replacing valve A with a constant flow pump and by measuring the mass of the solvent leaving the absorption tube (instead of the volume) on a top-pan balance.

APPARATUS/PROCEDURE: The solvent is degassed using the vapor pump principle (1). Fach determination absorbs about 20 cm³ of gas in up to 500 cm³ of solvent, which was recycled. The density of the solvent was checked after each run, so that the exact composition of the solution could be determined (2).

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. British Oxygen Co. Gas 99.9 percent pure, stored over saturated brine.
- 2. Ethanol. Absolute alcohol.
- 3. Water. Distilled then deionized.

ESTIMATED ERROR:

 $\delta T/K = 0.1$

 $\delta P/mmHg = 0.5$

Solubilities reproducible within 0.5 percent.

- Morrison, T. J.,; Billett, F. J. Chem. Soc. <u>1948</u>, 2033; <u>1952</u>, 3819
- International Critical Tables, Volume III, pp 112-118.
- Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819.

- 1. Hydrogen; H₂; 1333-74-0
- 2. Ethanol or Ethyl Alcohol; C₂H₅OH; 64-17-5
- 3. Water; H₂O; 7732-18-5

ORIGINAL MEASUREMENTS:

Cargill, R.W.

J. Chem. Soc., Faraday Trans I 1978, 74, 1444-1456.

EXPERIMENTAL VALUES:

ol Fraction Ethanol/X2	T/K	104 T-1	log(S _o /cm ³ kg ⁻¹)	S _o /cm ³ kg ⁻¹
0.18	279.1	35.84	1.296	19.8
0.18	289.3	34.58	1.325	21,1
0.18	298.9	33.47	1.330	21.4
0.18	309.8	32.29	1.354	22.6
0.18	321.2	31.24	1.403	25.3
0.18	332.9	30.05	1.433	27.1
0.22	278.4	35.93	1.327	21.2
0.22	286.6	34.91	1.348	22.3
0.22	295.9	33.81	1.365	23.2
0.22	304.7	32.83	1.400	25.1
0.22	315.4	31.72	1.422	26.4
0.22	324.7	30.80	1.457	28.6
0.22	333.5	29.99	1.487	30.7
0.22	335.1	29.85	1.506	32.1
0.31	279.1	35.84	1.433	27.1
0.31	289.5	34.55	1.475	29.9
0.31	298.8	33.48	1.496	31.3
0.31	309.8	32.29	1.536	34.4
0.31	321.9	31.07	1.573	37.4
0.31	333.4	30.00	1.600	39.8
0.41	278.4	35.95	1.542	34.8
0.41	286.7	34.90	1.561	36.3
0.41	305.2	32.78	1.649	44.6
0.41	315.0	31.76	1.679	47.8
0.41	324.7	30.80	1.709	51.2
0.41	335.2	29.84	1.735	54.3
0.59	278.6	35.90	1.699	50.0
0.59	288.8	34.64	1.729	53.6
0.59	297.7	33.60	1.753	56.6
0.59	310.9	32.18	1.795	62.4
0.59 0.59	321.3	31.13	1.827	67.1
0.59	332.9	30.05	1.865	73.3
0.68	279.7	35.76	1.786	61.1
0.68	288.8	34.80	1.802	63.4
0.68	309.7	32.30	1.865	73.3
0.68	320.6	31.20	1.889	77.5
0.68	332.7	30.07	1.919	83.0
0.89	278.6	35.90	1.904	80.2
0.89	294.9	33.92	1.944	87.9
0.89	314.3	31.83	1.996	99.1
0.89	328.8	30.42	2.046	111
0.89	332.2	30.11	2.036	108

- 1. Hydrogen; H₂; 1333-74-0
- 2. Ethanol or Ethyl Alcohol; C₂H₅OH; 64-17-5
- 3. Water; H₂O; 7732-18-5

ORIGINAL MEASUREMENTS:

Cargill, R.W. J. Chem. Soc., Faraday Trans.I 1978, 74, 1444-1456

EXPERIMENTAL VALUES:

l Fraction thanol/X2	T/K	104 T-1	log(S _O /cm ³ kg ⁻¹)	So/cm3kg-1
0.00	277.8	36.01	1.319	20.8
0.00	278.4	35.93	1,320	20.9
0.00	284.1	35.21	1.289	19.5
			1.284	19.2a
0.00	285.5	35.04		
0.00	289.3	34.58	1.272	18.7ª
0.00	290.5	34.42	1.268	18.5 ^a
0.00	294.5	33.97	1.257	18.1
0.00	296.2	33.77	1.252	17.9 ^a
0.00	297.0	33.68	1.251	17.8
0.00	298.2	33.55	1.248	17.7 ^a
0.00		32.77	1.233	17.1
	305.3			17.0a
0.00	306.4	32.63	1.230	
0.00	318.2	31.44	1.214	16.4ª
0.00	320.5	31.20	1.212	16.3ª
0.00	327.6	30.53	1.206	16.2 ^a
0.00	332.4	30.09	1.212	16.3
0.00	333.5	29.99	1.206	16.1 ^a
0.00		29.54	1.208	16.1ª
	338.7			16.1a
0.00	344.9	29.00	1.208	10.10
0.008	277.4	36.06	1.330	21.4
0.008	278.8	35.88	1.326	21.2
0.008	285.5	35.04	1.295	19.7
0.008	294.2	34.00	1.267	18.5
0.008	304.0	32.90	1.244	17.5
0.008	314.3	31.83	1.222	16.7
0.008	324.6	30.81	1.222	16.7
0.008	332.8	30.06	1.218	16.5
0.021			3 227	21.2
	277.9	36.00	1.327	
0.021	285.3	35.07	1.312	20.5
0.021	294.3	33.99	1.269	18.6
0.021	303.5	32.96	1.253	17.9
0.021	313.2	31.94	1.232	17.1
0.021	323.0	30.95	1.231	17.0
0.021	332.7	30.07	1.228	16.9
0.048	277.4	36.06	1,338	21.8
0.048	285.8	35.01	1.307	20.3
0.048			1.272	18.7
	295.4	33.87		
0.048	303.8	32.93	1.257	18.0
0.048	314.3	31.83	1.245	17.6
0.048	323.9	30.88	1.238	17.3
0.048	334.5	29.90	1.251	17.8
0.075	281.6	35.53	1.296	19.8
0.075	285.5	35.04	1,286	19.3
0.075	298.8	33.48	1.262	18.3
0.075		31.89	1.264	18.4
	313.7	31.09		
0.10	277.9	36.00	1.290	19.5
0.10	285.4	35.05	1.278	19.0
0.10	293.2	34.00	1.278	19.0
0.10	304.1	32.89	1.259	18.2
0.10	312.6	32.00	1.264	18.4
0.10	323.6	30.94	1.296	19.8
0.10	333.5	29.99	1.325	21.1
	JJJ - J		- · · · ·	

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Sulfinylbismethane or dimethyl sulfoxide; C₂H₆OS; [67-68-5]
- (4) N,N,N-Trimethylmethanaminium hydroxide; C₄H₁2N.HO; [75-59-2]

VARIABLES:

T/K: 298.15 - 353.15

P/kPa: 101.325 (1 atm) C₂H₆SO/mo1 %: 0 - 100 C_{Salt}/mo1 dm⁻³: 0.0 - 0.42

EXPERIMENTAL VALUES:

ORIGINAL MEASUREMENTS:

Symons, E. A.

Can. J. Chem. 1971, 49, 3940 - 3947.

PREPARED BY:

H. L. Clever

See preceding page.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Matheson Co., Inc. Lecture bottle, extra dry, used as received.
- (2) Water. Deionized distilled water.
- (3) Dimethylsulfoxide. Fisher Co. Certified Reagent grade. Dried at least 48 h over Linde type 4A molecular sieves, then vacuum distilled with nitrogen bled through a 16 in Vegreux column. The central fraction, 38-40°C (ca. 1 mmHg), was retained for use under a nitrogen atmosphere at ambient temperature.
- (4) N,N,N-Trimethylmethanaminium hydroxide or tetramethyl ammonium hydroxide. Matheson, Coleman and Bell Co., Inc., A 25 per cent aqueous solution in a polyethylene bottle, titrated against standard sulfuric acid solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas chromatographic method (1).

The gas-liquid equilibrium cell was a modified 100 cm³ round bottom flask equipped with magnetic stirrer, syringe sampling portal, and vacuum/gas line. The solvent was added, the flask evacuated several minutes to remove dissolved gases. Then the gas was introduced to a partial pressure of one atm. The solution was stirred for five minutes, then sampled. Three to four successive samples were taken.

The 5.0 cm³ samples were taken by gas tight syringe. The sample was introduced to a stripping cell, stripped out over a period of 1-2 minutes by the nitrogen carrier gas and then passed into a Varian Aerograph (No. 1420) equipped with an injection portal, column (10' ½" stainless steel, packed with 40-60 mesh 13X molecular sieve) at ambient temperature, and a thermal conductivity cell at 65°C.

SOURCE AND PURITY OF MATERIALS:

See above.

ESTIMATED ERROR:

 $\delta T/K = 0.05$ $\delta c/c = 0.02$ (author's estimate)

- Gubbins, K. E.; Carden, S. N.; Walker, R. D. Jr. J. Gas Chromatogr. 1965, 98.
- 2. Symons, E. A.; Buncel, E. Can. J. Chem. 1973, 51, 1673.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Sulfinylbismethane or dimethyl sulfoxide; C_2H_6OS ; [67-68-5]
- (4) N,N,N-Trimethylmethanaminium hydroxide; C₄H₁₂N.HO; [75-59-2]

ORIGINAL MEASUREMENTS:

Symons, E. A.

Can. J. Chem. 1971, 49, 3940 - 3947.

EXPERIMENTAL VALUES:

m values.							
	_	rature	Dimethylsulfoxide	c _{base} 1	Solubility -3		
	t/°C	T/K	mol %		C _{H2} /mol dm ⁻³		
					c x 10 ³		
	25.0 35.0 50.0 65.0	298.15 308.15 323.15 338.15	100	0	1.05,1.08 1.18 1.37 1.54		
	80.0	353.15			1.73		
	35.0 50.0 65.0 80.0	308.15 323.15 338.15 353.15	96.9	0.022	1.13,1.15 1.33 1.50,1.52,1.53 1.71		
	35.0 50.0 65.0 80.0	308.15 323.15 338.15 353.15	87.5	0.096	1.07 1.27 1.44,1.45,1.48 1.64		
	25.0 35.0 50.0 65.0 80.0	298.15 308.15 323.15 338.15 353.15	77.9	0.13	0.93 1.03 1.20 1.35,1.39,1.40 1.49		
	25.0 35.0 50.0 65.0 80.0	298.15 308.15 323.15 338.15 353.15	59.0	0.42	0.78 0.87 0.98 1.16,1.18 1.31		
	25.0 35.0 50.0 65.0 80.0	298.15 308.15 323.15 338.15 353.15	40.1	0.36	0.61 0.66 0.77 0.92,0.95 1.10		
	25.0 35.0 50.0 65.0	298.15 308.15 323.15 338.15	20.2	0	0.58 0.60 0.69 0.80		
	25.0	298.15	0	0	0.80,0.802		

 $^{^{1}}$ c_{base} \equiv c_{C4}H₁₂N.OH/mol dm⁻³.

² See reference 2. Equivalent to a mole fraction of 1.45 x 10^{-5} .

102 Hydrogen Solubilities up to 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Braun, L. 2. Water; H₂O; [7732-18-5] Z. phys. Chem. 3. Propanoic acid; C₃H₆O₂; 1900, 33, 721-741 [79-09-4] VARIABLES: PREPARED BY: Temperature, concentration of acid C. L. Young EXPERIMENTAL VALUES: Wt. of acid Bunsen Wt. of acid Bunsen T/K coefficient, T/K per 100 g soln. per 100 g soln. coefficient, /g /g α 278.2 0.02366 288.2 6.500 0.01925 0.01929 9.763 2.634 0.02245 3.373 0.01908 0.02221 9.910 293.2 0 0.01905 5.267 0.02239 6.500 0.02181 2.634 0.01876 9.763 0.02120 3.373 0.01866 5.267 0.01842 9.910 0.02129 283.2 0.02213 6.500 0.01829 0.01788 0.02142 2.634 9.763 3.373 5.267 9.910 0.01782 0.02120 298.2 0.01750 0.02117 0.02093 6.500 2.634 0.01722 9.763 0.02042 3.373 0.01706 9.910 5.267 0.01705 0.02029 288.2 0 0.02059 6.500 0.01690 9.763 0.01638 2.634 0.02003 3.373 0.01987 9.910 0.01602 5.267 0.01983 N.B. The Bunsen coefficients at the lowest temperatures are thought to be considerably in error but the salting out parameters at the lower temperatures are probably more reliable (see water evaluation). AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: No details given. Ostwald method, using gas buret and pipet. Measurement of volume of gas before and after absorption. Vapor pressure of water was allowed

for by assuming Raoult's law. Solution was degassed. Concentration of acid was estimated by titration with base.

ESTIMATED ERROR:

 $\delta \alpha / \alpha = \pm 0.03$

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) D-Alanine; C₃H₇NO₂ or CH₃CH(NH₂)COOH; [338-69-2]

ORIGINAL MEASUREMENTS:

Hüfner, G.

Z. Physik. Chem. 1907, 57, 611-624.

VARIABLES:

T/K: H₂ P/kPa:

293.23 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature T/K	CC3H7NO2/mol dm-3	•	Absorbed Gas	Bunsen Coefficient
	293.26	0.0	mmHg	Volume ¹	$\frac{\alpha \times 10^2}{1.810^2}$
20.08	293.23	1.0	664.2	5.57	1.555

 $^{^1\,\}mathrm{Volume}$ of gas reduced to 273.15 K and 760 mmHg absorbed in 490.94 cm^3 solution at the stated pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, described in reference (1), was the Bunsen absorption type. It consisted of an absorption flask, which holds 409.94 cm³ of solvent, and gas burets.

The final partial pressure of the gas ranged between 662.5 and 688.1 mmHg. The author reported both the volume of gas absorbed at the final pressure in 409.94 cm³ of solvent reduced to 273.15 K and 760 mmHg, and the Bunsen coefficient, which was calculated assuming Henry's law.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Formed by the reaction of dilute sulfuric acid on zinc. The gas was washed with permanganate and caustic solutions and stored over mercury.
- (2) Water. Pure.
- (3) D-Alanine. Merck.

ESTIMATED ERROR:

 $\delta T/K = 0.01$

REFERENCES:

1. Hüfner, G.
Archiv. F. Anatomie und
Physiologie, Physiolog. Abtly.
1894, 5, 191.

²Average of three runs, see Hüfner's H₂ + H₂O data sheet.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Water; H₂O; [7732-18-5]
- 1,2,3-Propanetriol (Glycerol, Glycerine); C₃H₈O₃; [56-81-5]

ORIGINAL MEASUREMENTS:

Muller, C.

Z. Phys. Chem. 1912-13, 81,

483-503.

VARIABLES:

Concentration of component 3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of comp. (3) (wt-%)	Bunsen coefficient	Bunsen # coefficient at 288.2 K	Density of soln. at t/°C	t/°C
287.65	14.9	0.01654	0.01647	1.0366	14
286.15	22.8	0.01532	0.01510	1.0536	12.5
286.95	38	0.01226	0.01216	1.0966	14
287.65	43.5	0.01117	0.01110	1.1115	15
286.85	49.15	0.01019	0.01010	1.1268	14.5
288.05	51.5	0.01026	0.01025	1.1333	14.5
285.45	68	0.00822	0.00806	1.181	12.5
291.15	90.7	0.00853	0.00870	1.2386	18

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:

Volumetric method in which pressure was determined using a mercury manometer. Solution was degassed by boiling under reduced pressure. A considerable amount of water was removed by this process. Gas was saturated with water vapor before being admitted to absorption buret.

SOURCE AND PURITY OF MATERIALS:

- Prepared by reaction of acid on zinc, washed with caustic potash solution.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta P/P = \pm 0.001$; $\delta \alpha/\alpha = \pm 3\%$ (estimated by compiler).

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Druker, K; Moles, E. 2. Water; H₂O; [7732-18-5] Z. Physik. Chem. 3. 1,2,3-Propanetriol (Glycerol, Glycerin); C₃H₈O₃; [56-81-5] VARIABLES: Wt. fraction of 1,2,3-Propanetriol EXPERIMENTAL VALUES: ORIGINAL MEASUREMENTS: Druker, K; Moles, E. Z. Physik. Chem. 1910, 75, 405-436. PREPARED BY: C. L. Young

T/K	Wt. fraction of 1,2,3-Propanetriol	p/mmHg	p/kPa	Ostwald coefficient, L	Ratio density H ₂ O/ density soln.
298.2	0.0 0.040 0.105 0.220 0.498 0.505 0.526 0.670 0.800 0.820	760 716.3 736.1 684.3 709.9 730.1 672.2 741.1 708.0 665.5	101 95.50 98.14 91.23 94.65 97.34 89.62 98.81 94.39 88.73	0.01962 0.0186 0.0178 0.0154 0.0099 0.0097 0.0090 0.0067 0.0051	1.0 1.0101 1.0260 1.0542 1.1290 1.1300 1.1365 1.1752 1.2113
	0.880 0.950	662.3 741.8	88.30 98.90	0.0044 0.0034	1.2307 1.2502

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric method using an Ostwald type gas buret and pipet. Solvent degassed before being admitted to pipet. Density of solution determined using a Sprengel pyknometer.

SOURCE AND PURITY OF MATERIALS:

- 1. Electrolytically prepared from aqueous potassium hydroxide soln. Passed over hot platinum-asbestos to remove oxygen.
- 2. Distilled.
- "Pure" sample, purity about 98 mole per cent.

ESTIMATED ERROR:

 $\delta L/L = \pm 1-3\%$ for dil. soln.; $\pm 5-7\%$ in concentrated soln.

- 1. Hydrogen; H2; 1333-74-0
- 2. 2-Methyl-2-propanol or t-Butanol; C4H9OH; 75-65-0
- 3. Water; H₂O; 7732-18-5

ORIGINAL MEASUREMENTS:

Cargill, R.W.

J. Chem. Soc., Faraday Trans. I 1978, 74, 1444-1456

VARIABLES:

T/K : 277.5-334.6 P/kPa : 101.325 (1 atm) $C_4H_9OH/X_2 : 0.0-0.85$

PREPARED BY:

R.W. Cargill

EXPERIMENTAL VALUES:

Mol Fraction Alcohol/X2	T/K	104 T-1	log(S _O /cm ³ kg ⁻¹)	$S_{O}/cm^3 kg^{-1}$
0.85	281.4	35.55	1.910	81.3
0.85	289.2	34.59	1.932	85.5
0.85	298.7	33.49	1.968	92.9
0.85	309.2	32.35	1.997	99.3
0.85	320.3	31.23	2.026	106
0.85	332.8	30.06	2.054	113

avalues from reference 3.

The Solubility, S $_{\rm O}$, calculated as cm $^{\rm 3}$ gas at 273.15 K and Ar partial pressure of 101.325 kPa (1 atm) per kg of solvent.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

METHOD: Absorption of gas by a thin film of liquid. The Morrison and Billett (1) method was modified by replacing valve A with a constant flow pump, and by measuring the mass 2. 2-Methyl-2-propanol. Reagent grade, of the solvent leaving the absorption tube (instead of the volume) on a top-pan balance. 3. Water. Distilled then deionized.

APPARATUS/PROCEDURE: The solvent is degassed using the vapor pump principle (1). Each determination absorbs about 20 cm3 of gas in up to 500 cm³ of solvent, which was recycled. The density of the solvent was checked after each run, so that the exact composition of the solution could be determined (2).

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen. British Oxygen Co Gas 99.9 per cent pure, stored over saturated brine.
- (98 percent boils 82-83°C).

ESTIMATED ERROR:

 $\delta T/K = 0.1$

 $\delta P/mmHg = 0.5$

Solubility values reproducible within 0.5 percent (authors).

- 1. Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033; 1952, 3819.
- 2. International Critical Tables, Volume III, pp 112-118.
- 3. Morrison, T. J.; Billett, F. J. Chem. Soc. 1952, 3819

- 1. Hydrogen; H₂; 1333-74-0
- 2. 2-Methyl-2-propanol or \underline{t} -Butanol; C_4H_9OH ; 75-65-0
- 3. Water; H₂O; 7732-18-5

ORIGINAL MEASUREMENTS:

Cargill, R.W.

J. Chem. Soc., Faraday Trans. I 1978, 74, 1444-1456

EXPERIMENTAL VALUES:

Mol Fraction Alcohol/X₂	T/K	104 T-1	log(S _O /cm ³ kg ⁻¹)	So/cm3kg-1
0.072	278.2	35.96	1.271	18.7
0.072	286.7	34.90	1.265	18.4
0.072	296.8	33.70	1.282	19.1
0.072	306.1	32.68	1.301	20.0
0.072	320.7	31.19	1.333	21.5
0.072	331.7	30.16	1.374	23.7
0.10	280.7	35.64	1.300	20.0
0.10	285.7	35.02	1.316	20.7
0.10	298.3	33.54	1.342	22.0
0.10	299.6	33.38	1.336	21.7
0.10	308.2	32.46	1.359	22.9
0.10	318.4	31.42	1.387	24.4
0.10	319.7	31.29	1.391	24.6
0.10	332.8	30.06	1.459	28.8
0.14	278.0	35.98	1.373	23.6
0.14	286.9	34.87	1.408	25.6
0.14	299.5	33.40	1.444	27.8
0.14	307.5	32.53	1.475	29.9
0.14	322.1	31.06	1.520	33.1
0.14	333.9	29.96	1.559	36.2
0.31	278.1	35.97	1.625	42.2
0.31	287.3	34.82	1.657	45.4
0.31	296.6	33.72	1.677	47.5
0.31	308.4	32.44	1.715	51.9
0.31	321.8	31.08	1.755	56.9
0.31	333.9	29.96	1.803	63.5
0.53	277.5	36.05	1.786	61.1
0.53	287.3	34.82	1.808	64.3
0.53	297.2	33.66	1.836	68.6
0.53	308.7	32.41	1.867	73.6
0.53	320.7	31.19	1.903	80.0
0.53	334.6	29.90	1.954	90.0
0.71	279.2	35.83	1.849	70.6
0.71	289.8	34.52	1.870	74.1
0.71	303.2	33.01	1.930	85.1
0.71	319.5	31.30	1.977	94.8
0.71	332.8	30.06	2.023	105

- 1. Hydrogen; H₂; 1333-74-0
- 2. 2-Methyl-2-propanol or <u>t</u>-Butanol; C4H9OH; 75-65-0
- 3. Water; H₂O; 7732-18-5

ORIGINAL MEASUREMENTS:

Cargill, R.W.

J. Chem. Soc., Faraday Trans. I 1978, 74, 1444-1456

EXPERIMENTAL VALUES:

Wal Swanting				
Mol Fraction	T/K	104 T-1	log(S _O /cm ³ kg ⁻¹)	S _O /cm ³ kg ⁻¹
Alcohol/X2				
0.00	277.8	36.01	1.319	20.8
0.00	278.4	35.93	1.320	20.9
0.00	284.1	35.21	1.289	19.5
0.00	285.5	35.04	1.284	19.2ª
0.00	289.3	34.58	1.272	18.7ª
0.00	290.5	34.42	1,268	18.5 ^a
0.00	294.5	33.97	1.257	18.1
0.00	296.2	33.77	1.252	17.9 ^a
0.00	297.0	33.68	1.251	17.8
0.00	298.2	33.55	1.248	17.8 17.7 ^a
0.00	305.3	32.77	1.233	17.1
0.00	306.4	32.63	1.230	17.0a
0.00	318.2	31.44	1.214	16.4ª
				10.4-
0.00	320.5	31.20	1.212	16.3ª
0.00	327.6	30.53	1.206	16.2ª
0.00	332.4	30.09	1,212	16.3
0.00	333.5	29.99	1.206	16.1ª
0.00	338.7	29.54	1,208	16.1a
0.00	344.9	29.00	1.208	16.1ª
0.006	277.8	36.01	1.331	21.4
0.006	286.1	34.97	1.288	19.4
0.006	293.8	34.05	1.265	18.4
0.006	304.8	32.82	1.243	17.5
0.006				
	314.4	31.82	1.227	16.9
0.006	323.6	30.91	1.212	16.3
0.006	333.5	29.99	1.208	16.1
0.011	277 0	26.00	7 202	01 0
	277.9	36.00	1.323	21.0
0.011	285.2	35.08	1.291	19.5
0.011	294.8	33.93	1.259	18.2
0.011	304.7	32.83	1.236	17.2
0.011	313.2	31.94	1.226	16.8
0.011	324.1	30.86	1.218	16.5
0.011	333.9	29.97	1.223	16.7
0.029	278.3	35.94	1.291	19.5
0.029	285.8	35.01	1.275	18.8
0.029	294.9	33.92	1.246	17.6
0.029	303.2			
		32.99	1.236	17.2
0.029	319.0	31.36	1.229	16.9
0.029	333.4	30.00	1.240	17.4
0.046	270 2	25 02	1 250	17 0
0.046	279.2	35.83	1.250	17.8
0.046	285.2	35.08	1.244	17.5
0.046	294.9	33.92	1.236	17.2
0.046	303.7	32.96	1.231	17.0
0.046	313.9	31.87	1.256	18.0
0.046	324.1	30.86	1.273	18.8
0.046	333.4	30.00	1.290	19.5

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Muller, C.
2. Water; H ₂ O; [7732-18-5]	Z. Phys. Chem. <u>1912-13</u> , 81,
3. D-glucose (Grape sugar);	483-503.
C ₆ H ₁₂ O ₆ ; [50-99-7]	
VARIABLES:	PREPARED BY:
Concentration of component 3	C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of comp. (3) (wt-%)	Bunsen coefficient	Bunsen # coefficient at 293.2 K	Density of soln. at t/°C	t/°C
293.7	12.2	0.01595	0.01600	1.048	20.5
293.7	20.7	0.01445	0.01450	1.083	20.5
294.3	32.56	0.01243	0.01250	1.129	21
295.0	45.8	0.01000	0.01015	1.198	21.8
294.7	59.0	0.00775	0.00775	1.265	21

[#] given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric method in which pressure was determined using a mercury manometer. Solution was degassed by boiling under reduced pressure. A considerable amount of water was removed by this process. Gas was saturated with water vapor before being admitted to absorption buret.

SOURCE AND PURITY OF MATERIALS:

- Prepared by reaction of acid on zinc, washed with caustic potash solution.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$; $\delta P/P = \pm 0.001$; $\delta \alpha/\alpha = \pm 3\%$ (estimated by compiler).

(1) Hydrogen; H₂; [1333-74-0]

(2) Water; H₂O; [7732-18-5]

(3) D-Glucose; $C_6H_{12}O_6$; [50-99-7]

ORIGINAL MEASUREMENTS:

Hüfner, G.

Z. Physik. Chem. 1907, 57, 611-624.

VARIABLES:

293.15 - 293.50 T/K: H, P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature T/K	D-Gl g dm ⁻³	ucose mol dm ⁻³	Gas Pressure mmHg	Absorbed Gas Volume ¹	Bunsen Coefficient $\alpha \times 10^2$
20.11	293.26	0	0			1.810 ²
20.0	293.15	41.45	0.230	670.4	6.36	1.759
20.16 20.25	293.31 293.40	80.8 87.3	0.448 0.485	688.1 682.2	6.12 6.02	1.649 1.664 ³
20.35 20.28	293.50 293.43	166.2 174.0	0.923 0.966	670.6 670.2	5.60 5.48	1.514 ⁴ 1.516

¹ Volume of gas reduced to 273.15 K and 760 mmHg absorbed in 490.94 cm³ solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, described in reference (1), was the Bunsen absorption type. It consisted of an absorption flask, which holds 409.94 cm³ of solvent, and gas burets.

The final partial pressure of the gas ranged between 662.5 and 688.1 mmHg. The author reported both the volume of gas absorbed at the final pressure in 409.94 cm³ of solvent reduced to 273.15 K and 760 mmHg, and the Bunsen coefficient, which was calculated assuming Henry's law.

D-Glucose name Traubenzucker (grape sugar) in the paper.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Formed by the reaction of dilute sulfuric acid on zinc. The gas was washed with permanganate and caustic solutions and stored over mercury.
- (2) Water. Pure.
- (3) D-Glucose. Source not given.

ESTIMATED ERROR:

 $\delta T/K = 0.01$

REFERENCES:

1. Hüfner, G.
Archiv. F. Anatomie und Physiologie, Physiolog. Abtly. 1894, 5, 191.

²Average of three, see Hufner's H₂ + H₂O data sheet.

 $^{^{3}}$ Compiler calculated a value of 1.636 x 10^{-2} from data in the paper.

 $^{^4}$ Compiler calculated a value of 1.54 x 10 $^{-2}$ from data in the paper.

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Steiner, P. 2. Water; H₂O; [7732-18-5] Ann. der Phys. Chem. 3. β-D-Fructofuranosyl-α-D-glucopyranoside (Sucrose); C₁₂H₂₂O₁₁; [57-50-1] VARIABLES: PREPARED BY: Concentration of salt C. L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of salt /mol dm ⁻³	Density of soln. at 288.2 K /g cm ⁻³	Bunsen coefficient, α	Bunsen coefficient [#] at 288.2 K
288.2	0	0.999	0.01883	0.01883
287.31	0.520	1.0672	0.01571	0.01561
287.34	0.993	1.1286	0.01292	0.01284
286.95	1.699	1.2184	0.00900	0.00892
_				

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

METHOD/APPARATUS/PROCEDURE: Volumetric method using an Ostwald type gas buret and pipet. Solvent was degassed before being admitted to the pipet. Details in source. ESTIMATED ERROR: $\delta \alpha/\alpha = \pm 0.02$. REFERENCES:

- Hydrogen; H₂; [1333-74-0]
 Water; H₂O; [7732-18-5]
- 3. β -D-Fructofuranosyl α-D-Glucopyranoside (Sucrose); C12H22O3; [57-50-1]

ORIGINAL MEASUREMENTS:

Muller, C.

Z. Phys. Chem. 1912-13, 81, 483-503.

VARIABLES:

Concentration of component 3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

т/к	Conc. of comp. (3) (wt-%)	Bunsen coefficient	Bunsen # coefficient at 288.2 K	Density of soln. at t/°C	t/°C
288.4	5.04	0.01723	0.01726	1.019	15
284.8	14.70	0.01547	0.01510	1.060	11.6
285.2	20.26	0.01500	0.01462	1.084	11.8
285.9	29.86	0.01290	0.01257	1.128	13
285.0	31.74	0.01220	0.01185	1.138	12
286.5	39.65	0.01047	0.01033	1.175	13.5
285.8	42.94	0.00956	0.00939	1.195	12.5

given in original, method of calculation from Bunsen coefficient at experimental temperature not clear.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Volumetric method in which pressure was determined using a mercury manometer. Solution was degassed by boiling under reduced pressure. A considerable amount of water was removed by this process. Gas was saturated with water vapor before being admitted to absorption buret.

SOURCE AND PURITY OF MATERIALS:

- 1. Prepared by reaction of acid on zinc, washed with caustic potash solution.
- 2 and 3. No details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/P = \pm 0.001;$

 $\delta\alpha/\alpha = \pm 3\%$ (estimated by compiler).

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]
- (3) Serum albumin

ORIGINAL MEASUREMENTS:

Shkol'nikova, R. I.

Uch. Zp. Leningr. Gos. Univ., Ser. Khim. Nauk. 1959, Nr. 18, 64 - 86.

Chem. Abstr. 1961, 55, 25443b.

VARIABLES:

T/K: 283.15 - 313.15 P/kPa: 101.325 (1 atm) serum albumin/Wt %: 0.575 - 1.99

PREPARED BY:

A. L. Cramer H. L. Clever

EXPERIMENTAL VALUES:

T/K		serum alb	oumin/Wt %		
	0.575		1.	15	
	Bunsen	Ostwald	Bunsen	Ostwald	
	Coefficient	Coefficient	Coefficient	Coefficient	
	α x 10 ³	$L \times 10^3$	$\alpha \times 10^3$	$L \times 10^3$	
283.15			16.1	16.7	
	18.9	19.6			
288.15	18.3	19.3	15.4	16.2	
293.15	17.1	18.3	14.4	15.4	
298.15	16.7	18.2	13.9	15.2	
303.15	15.3	17.0	11.9	13.2	
308.15	14.5	16.4	11.6	13.1	
313.15	14.1	16.1	11.3	12.9	
					

T/K		serum alb	oumin/Wt %	
	1.	68	1.	99
	Bunsen	Ostwald	Bunsen	Ostwald
	Coefficient	Coefficient	Coefficient	Coefficient
	$\alpha \times 10^3$	1×10^3	$\alpha \times 10^3$	$L \times 10^3$
283.15	15.9	16.5	14.6	15.1
288.15	15.2	16.0	13.9	14.6
293.15	13.1	14.0	12.1	13.0
298.15	12.8	14.0	11.6	12.7
303.15	10.7	11.9	9.9	11.0
308.15	10.5	11.8	9.6	10.8
313.15	10.1	11.6	9.4	10.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure of Lannung were modified (1).

The author calculated the enthalpy of solution from the temperature coefficient of the Bunsen coefficient. It is 1590, 1760, 2210, 2370, and 2360 cal mol-1 in water, and in 0.575, 1.15, 1.68, and 1.99 wt % serum albumin respectively.

The values of the solubility of hydrogen in water were not given in the paper.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Stated to be 99.99 per cent.
- (2) Water. No information.
- (3) serum albumin. No information.

ESTIMATED ERROR:

REFERENCES:

1. Lannung, A. J. Am. Chem. Soc. 1930, 52, 68.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Findlay, A.; Shen, B.
2. Water; H ₂ O; [7732-18-5]	J. Chem. Soc. <u>1912</u> , 101,1459-68.
3. Dextrin (colloidal)	
VARIABLES:	PREPARED BY:
Concentration	C.L. Young
EXPERIMENTAL VALUES:	
Colubility of concentration	298.15 on of gas in liquid phase on of gas in gaseous phase.
Conc of dextrin Density of /10 ⁻² g cm ⁻³	solution S^+
710 g cm	
3.98 1.013	
5.59 1.019 8.12 1.029	
19.20 1.060	0.0174
${\it s}^{+}$ solubility independent of	pressure over range 1-2 atm.
	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Gas buret and absorption pipet. Manometer tube was of such a length as to allow measurements up to 2 x 10 ⁵ Pa (2 atm).	No details given.
	ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta S = \pm 1.5$ %.
	(estimated by compiler).
	REFERENCES:
1	1

	Organic Sc	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	,,,,,,,			1
COMPONENTS:		ORIGINA	AL MEASUREME	NTS:		
1. Hydrogen; H ₂ ; [1333-74-0]		- {	Findlay, A.; Shen, B.			
2. Water; H ₂ O; [7732		J. Chem. Soc. <u>1912</u> , 101, 1459-68		1, 1459-68.		
3. Gelatin (colloida:	1)	{				
					•	
VARIABLES:		PREPARI	ED BY:			
Pressure, concent	tration		C.1	. Young.		
EXPERIMENTAL VALUES:			15			
	•	= 298.		ionida mba		
Solubility, S , given	as concentr	ation of	gas in li gas in ga	seous ph	ase	
Conc. of gelatin /10 ⁻² g cm ⁻³	Density of solution	p ⁺ _{H2} /10 ⁵ Pa	S	p ⁺ H ₂ /10 ⁵ Pa	S	
1.53	1.002	1.004 1.336 1.664	0.0194 0.0193 0.0195	1.149 1.471 1.845	0.0188 0.0195 0.0194	
2.69	1.005	0.995 1.316 1.660	0.0189 0.0189 0.0189	1.157 1.468 1.840	0.0185 0.0190 0.0191	
4.72	1.011	1.004 1.332 1.673	0.0185 0.0186 0.0186	1.152 1.483 1.860	0.0181 0.0186 0.0185	
5.71	1.015	1.000 1.300 1.659	0.0182 0.0183 0.0181	1.155 1.464 1.844	0.0173 0.0184 0.0183	
+ partial pr	essure of hyd	rogen.				
	AIIXII.I A	RY INFORMA	TION			
ETHOD/APPARATUS/PROCEDURE:	-		AND PURITY	OF MATERIA	LS:	
Gas buret and absorption pipet. Manometer tube was of such a length as to allow measurements up to 2 x 10 ⁵ Pa (2 atm)			No detail	s given.		
		δT/K	TED ERROR: = ±0.1;δ. imated by			~
		REFERE				

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Water; H₂O; [7732-18-5] (3) Gelatin Chem. Abstr. 1961, 55, 25443b. VARIABLES: T/K: 283.15 - 313.15 P/kPa: 101.325 (1 atm) Gelatin/Wt %: 1, 5, 10 PRIGINAL MEASUREMENTS: Shkol'nikova, R. I. Uch. Zp. Leningr. Gos. Univ., Ser. Khim. Nauk. 1959, Nr. 18, 64 - 86. Chem. Abstr. 1961, 55, 25443b. PREPARED BY: A. L. Cramer H. L. Clever

EXPERIMENTAL VALUE	S:			
T/K	Gelatin	/Wt % 1	Gelatin	/Wt % 5
	Bunsen Coefficient	Ostwald Coefficient	Bunsen Coefficient	Ostwald Coefficient
283.15	$\frac{\alpha \times 10^3}{17.9}$	$\frac{\text{L} \times 10^3}{18.5}$	$\frac{\alpha \times 10^3}{15.2}$	L x 10 ³
288.15	16.1	16.9	14.3	14.8
293.15	14.4	15.5	13.0	14.0
298.15	13.1	14.3	11.0	12.9
303.15	11.6	12.9	10.5	11.6
308.15	10.6	12.3	9.8	11.6
313.15	10.2	11.7	9.3	10.7

T/K	Gelatin/Wt % 10		
	Bunsen Coefficient	Ostwald Coefficient	
	$\alpha \times 10^3$	L x 10 ³	
283.15	14.2	14.8	
288.15	13.2	13.8	
293.15	12.1	13.0	
298.15	11.0	12.1	
303.15	10.0	11.1	
308.15	9.1	10.3	
313.15	8.2	9.1	

313.15 8.2	9.1
The author calculated the enthalpy of temperature coefficient of the Bunser 3060, and 3240 cal mol-1 in water, an respectively.	coefficients. It is 1590, 3260,
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus and procedure of Lannung were modified (1).	(1) Hydrogen. Source not given. Stated to be 99.99 per cent.
	(2) Water. No information.
	(3) Gelatin. No information.
The values of the solubility of hydrogen in water were not given in the paper.	ESTIMATED ERROR: REFERENCES: 1. Lannung, A. J. Am. Chem. Soc. 1930, 52, 68.

COMPONENTS:	
	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Findlay, A.; Shen, B.
2. Water; H ₂ O; [7732-18-5]	J. Chem. Soc. 1912, 101, 1459-68.
3. Starch (colloidal)	
VARIABLES:	PREPARED BY:
Concentration	C.L. Young
Pypenyagan	
EXPERIMENTAL VALUES: T/K =	298.15
concentrat	ion of gas in liquid phase
Solubility, S, given as concentrat	ion of gas in gaseous phase
Conc. of starch Density of s	olution S ⁺
/10 ⁻² g cm ⁻³	51461611
2.01 1.005	0.0194
3.56 1.011 7.13 1.024	0.0189 0.0181
9.29 1.032	0.0182
a+	pressure over range 1-2 atm.
AUXILIARY	INFORMATION
AUXILIARY METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:
	

- Hydrogen; H₂; [1333-74-0] 1.
- 2. Phosphate buffer and human red cell ghosts in phosphate buffer.

ORIGINAL MEASUREMENTS:

Power, G.G.; Stegall, H.

J. Appl. Physiology, 1970, 29, 145-9

VARIABLES:

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

Bunsen coefficient T/K

s.D.* No. of measurements

Phosphate Buffer

310.15

0.00007

Ghosts suspension in phosphate buffer

310.15

0.01588

0.00006

5

* Standard deviation.

 α° ghost = (α ghosts suspension $-\alpha$ buffer)/g ghosts cm⁻³ $= 0.024 \pm 0.008$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

5 to 12 cm⁻³ samples placed in a stirrer cell and gas, saturated with water vapor passed through liquid for 30-60 mins. Samples of saturated liquid withdrawn and transferred to Van Slyke apparatus. Dissolved gas removed under reduced pressure. Red cell ghosts prepared by centrifugation of human blood and lysing the cells using phosphate buffer of pH 7.4. Ghost separated by high speed centrifugation. Washed with phosphate buffer contain- ESTIMATED ERROR: ing 0.01 M sodium nitrite.

SOURCE AND PURITY OF MATERIALS:

- Matheson sample, purity better than 99.7 mole per cent.

 $\delta T/K = \pm 0.1$

(1) Hydrogen; H₂; [1333-74-0]

(2) Alkanes

EVALUATOR:

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

USA

1980, September

CRITICAL EVALUATION:

The solubility of hydrogen at a partial pressure of 101.325 kPa (1 atm) in alkanes.

The data on the solubility of hydrogen in alkanes at hydrogen partial pressures less than 200 kPa are evaluated in this section. The hydrogen solubility data at hydrogen partial pressures greater than 200 kPa are compiled and evaluated in another part of the volume, which should be consulted along with this section. In general, a simple Henry's law treatment, uncorrected for non-idealality in either gas or liquid phase, of the solubility data measured at hydrogen partial pressures greater than 200 kPa, usually results in a mole fraction solubility at a hydrogen partial pressure of 101.325 kPa (1 atm) that is 50 to 100 per cent higher than the value actually measured at atmospheric pressure.

Most of the hydrogen solubility values at pressures less than 200 kPa were measured at a hydrogen partial pressure near 101.325 kPa (1 atm). The mole fraction solubility is calculated for a hydrogen partial pressure of 101.325 kPa (1 atm) from the experimental measurement, assuming that the gas is ideal, Henry's law is obeyed, and in some cases, that the Ostwald coefficient is independent of pressure. For most systems these assumptions are justified for the less than 200 kPa solubility experiments.

Hydrogen + Pentane [109-66-0]

Makranczy, Megyery-Balog, Rusz, and Patyi (1) report an Ostwald coefficient at 298.15 K which is equivalent to a mole fraction solubility of 6.7×10^{-4} . Frolich, Tauch, Hogan, and Peer (2) measured the hydrogen solubility in pentane at 298.15 K and pressures of 10 MPa and greater. A simple Henry's law treatment of the Frolich et~al. data gives a mole fraction solubility that is 50-70 per cent greater than the Makranczy et~al. value. The Makranczy et~al. values at 298.15 K have proven to be reliable for other systems. Thus their value is accepted as a tentative value.

Hydrogen + Hexane [110-54-3]

Four laboratories have reported values of the solubility of hydrogen in hexane at or near 101.325 kPa partial pressure of hydrogen. Guerry (3) reported values at 293.15 and 298.15 K, Waters, Mortimer, and Clements (4) reported solubility values at four temperatures between 263.15 and 293.15 K, Makranczy et al. (1) reported a value at 298.15 K, and Katayama and Nitta (5) reported values at five temperatures between 213.15 and 298.15 K.

The Waters $et~\alpha l$. data was extrapolated to obtain a solubility value at 298.15 K. That value, along with the 298.15 K values from the other three papers, has an arithmetic mean of 6.61 x 10^{-4} and has a standard deviation of 0.13. The values range from 6.43 to 6.99 x 10^{-4} .

It is the judgement of the evaluator that Katayama and Nitta used the most reliable method. The data from all four papers was treated by a linear regression with the Katayama and Nitta data given a weight of two. The 263.15 K value of Waters $et\ al.$ deviated over two standard deivations from the regression line. Both the 263.15 and 273.15 K values of Waters $et\ al.$ were discarded, and the following equation obtained on a linear regression of the remaining data with a weight of two to the Katayama and Nitta data and a weight of one to the data of the others.

The tentative equation for the temperature interval of 213.15 to 298.15 K is

$$\ln x_1 = -5.8952 - 4.2455/(T/100K)$$

with a standard error about the regression line of 2.34×10^{-5} .

From the equation, the temperature independent thermodynamic quantities are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 3.53 and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -49.0.

Table 1. Solubility of hydrogen in hexane at a hydrogen partial pressure of 101.325 kPa (1 atm).

Tentative mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
213.15	3.76	13.977
223.15	4.11	14.467
233.15	4.46	14.957
243.15	4.80	15.447
253.15	5.15	15.937
263.15	5.48	16.428
273.15	5.82	16.918
283.15	6.15	17.408

Hydrogen + Heptane [142-82-5]

Four laboratories have reported solubility measurements near a partial pressure of 101.325 kPa of hydrogen in heptane. The work of Cook, Hanson and Alder (7) is one of the first successful attempts to measure high accuracy, high precision gas solubility values. They report eleven measurements between temperatures of 243.15 and 328.15 K, which the evaluator believes to be of good accuracy.

The early value of Ijams (6) at 298.15 K is 14 per cent lower than the value of Cook et al. The solubility values reported at 298.15 K by Makranczy et al. (1) and by Guerry (3) agree well, but they are 4 per cent lower than the Cook et al. value.

The temperature of one solubility measurement made by Cook, Hanson and Alder is in question. In their paper (7) they give a temperature of 238.15 K (-35°C), but in Cook's thesis (8) the temperature is given as 243.15 K (-30°C). The latter value smooths the data better and appears to be the correct temperature.

The tentative equation for the temperature interval of 243.15 to 328.15 K is based entirely on the data of Cook $et\ al.$ (7). The equation is

$$\ln x_1 = -5.6689 - 4.8099/(T/100K)$$

with a standard error about the regression line of 4.60 x 10^{-6} .

From the equation the temperature independent thermodynamic quantities are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 4.00 and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ - 47.1.

Smoothed values of the mole fraction solubility and partial molar Gibbs energy of solution are in the following table.

Table 2. Solubility of hydrogen in heptane at a hydrogen partial pressure of 101.325 kPa (1 atm).

Tentative mole fraction solubility and partial molal Gibbs energy of solution are a function of temperature.

T/K	Mol Fraction	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
243.15	4.77	15.460
253.15	5.16	15.931
263.15	5.55	16.402
273.15	5.93	16.873
283.15	6.31	17.345
288.15	6.50	17.580
293.15	6.69	17.816
298.15	6.88	18.051
303.15	7.06	18.287
313.15	7.43	18.759
323.15	7.79	19.230

Hydrogen + Octane [111-65-9]

Cook, Hanson and Alder (7) report four solubility measurements between temperatures of 248.15 and 308.15 K. Makranczy, Megyery-Balog, Rusz, and Patyi (1) report one measurement of 298.15 K which is 6.3 per cent lower than the Cook $et\ al.$ value, and Ijams (6) reports one value of 298.15 K which is 1.4 per cent greater than the Cook $et\ al.$ value.

As discussed in connection with the hydrogen + heptane system, the Cook et al. data are considered the most reliable for this system. The tentative equation and smooth values are based entirely on their data.

Although a three constant equation will fit the Cook et al. data almost exactly, we are justified in using only a two constant equation. The linear regression of the data gives the tentative equation for the mole fraction solubility over the temperature interval of 248.15 to 308.15 K as

$$\ln x_1 = -5.6624 - 4.8438/(T/100K)$$

with a standard error about the regression line of 3.08 \times 10⁻⁶.

From the equation the temperature independent thermodynamic quantities are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 4.03 and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -47.1.

Smoothed values of the mole fraction solubility and partial molal Gibbs energy of solution are in Table 3.

Table 3. Solubility of hydrogen in octane at a hydrogen partial pressure of 101.325 kPa (1 atm).

Tentative mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	ΔG ₁ °/kJ mol ⁻¹
253.15	5.13	15.945
263.15	5.51	16.416
273.15	5.90	16.887
283.15	6.28	17.358
293.15	6.66	17.828
298.15	6.84	18.064
303.15	7.03	18.299
308.15	7.21	18.535

Hydrogen + 2,2,4-Trimethylpentane [540-84-1]

Cook, Hanson, and Alder (7) have reported data at a hydrogen partial pressure of 101.325 kPa (1 atm) on the system. Their data were carefully obtained, and are classed as tentative. Ijams (6) reports one solubility value of 298.15 K which is 4.3 per cent smaller than the Cook $et\ al.$ value.

A linear regression of the data of Cook $\it{et~al.}$ gives the equation for the mole fraction solubility over the temperature interval of 248.15 to 308.15 K

$$\ln x_1 = -5.6469 - 4.4889/(T/100K)$$

with a standard error about the regression line of 4.34×10^{-6} .

The enthalpy and entropy changes for transfer of one mole of gas from the gas phase at $101.325\ kPa$ (1 atm) to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 3.73 and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -46.9₅

The smoothed values of mole fraction solubility and partial molal Gibbs energy of solution are given in Table 4.

Table 4. Solubility of hydrogen in 2,2,4-trimethylpentane at a hydrogen partial pressure of 101.325 kPa (1 atm). Tentative mole fraction solubility and partial molar Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
253.15	5.99	15.618
263.15	6.41	16.087
273.15	6.82	16.557
283.15	7.23	17.026
293.15	7.63	17.496
298.15	7.83	17.730
303.15	8.03	17.965
308.15	8.22	18.200

Hydrogen + Nonane [111-84-2]

Thomsen and Gjaldbaek (9) report three solubility measurements at temperatures between 298.05 and 308.05 K. Makranczy $et\ al.(1)$ report one value at 298.15 K. Both data sets are classed as tentative, but the Thomsen and Gjaldbaek data at three temperatures were measured with higher precision. Thus the Thomsen and Gjaldbaek data are preferred. An equation and smoothed data table appears on their data sheet. The equation corresponds to temperature independent enthalpy and entropy changes for the transfer of hydrogen from the gas at 101.325 kPa (1 atm) to the infinitely dilute solution of

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 3.74 and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -47.9.

Hydrogen + Decane [124-18-5]

Both Ijams (6) and Makranczy $et\ al.$ (1) report a single value at 298.15 K. The values differ by nearly 20 per cent. The Makranczy value is classed as tentative and the Ijams value as doubtful.

- Hydrogen + Undecane [1120-21-4]
 - + Dodecane [112-40-3]
 - + Tridecane [629-50-5]
 - + Tetradecane [629-59-4]
 - + Pentadecane [629-62-9]

Makranczy, Megyery-Balog, Rusz, and Patyi (1) report one solubility value at $298.15~\mathrm{K}$ for each of the above five systems. The data are classed as tentative.

Hydrogen + Hexadecane [544-76-3]

Makranczy et al. (1) report one solubility value at 298.15 K. Cukor and Prausnitz (10) report eight values between the temperatures of 300 and 475 K. The Cukor and Prausnitz value at 300 K is 20 per cent greater than the Makranczy et al. value at 298.15 K. Although both results are classed as tentative, the Cukor and Prausnitz value is preferred.

The Cukor and Prausnitz data were fitted to a three constant equation by a linear regression. The equation for the mole fraction solubility at a hydrogen partial pressure of $101.325~\mathrm{kPa}$ (1 atm) over the 300 to 475 K temperature interval is

$$\ln x_1 = -11.01165 + 3.8183/(T/100K) + 2.4811 \ln (T/100K)$$

with a standard error around the regression line of 2.36×10^{-6} . The equation reproduces the Cukor and Prausnitz mole fraction values to within almost one part per thousand.

The equation results in the following values of the enthalpy, entropy, and heat capacity change for the transfer of one mole of hydrogen from the gas phase at 101.325 kPa hydrogen pressure to the infinitely dilute solution.

Table 5. Hydrogen + Hexadecane thermodynamics of transfer of one mole of hydrogen from gas at 101.325 kPa to infinitely dilute solution.

T/K	$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$	$\Delta \overline{S}_1^{\circ}/J K^{-1} mol^{-1}$	$\Delta \overline{C}_{p_1}^{\circ}/J K^{-1} mol^{-1}$
325	3.53	-46.6	20.6
400	5.08	-42.3	20.6
475	6.62	-38.8	20.6

Hydrogen + 2,6,10,15,19,23-Hexamethyltetracosane or Squalane [111-01-3]

Chappelow and Prausnitz (11) report eight values of the solubility of hydrogen in squalane over the temperature interval of 300 to 475 K which are classed as tentative. The mole fraction values at 101.325 kPa hydrogen partial pressure were fitted to a three constant equation by a linear regression. The equation is

$$\ln x_1 = -8.1089 + 0.07805/(T/100K) + 1.3623 \ln (T/100K)$$

with a standard error about the regression line of 3.15 x 10^{-6} . The equation reproduces the mole fraction values (see data sheet) to within two parts per thousand.

The equation results in the following values of the thermodynamic changes.

Table 6. Hydrogen + Squalane. Thermodynamic changes on transfer of one mole of hydrogen from the gas phase at 101.325 kPa (1 atm) to the infinitely dilute solution.

T/K	$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$	$\Delta \overline{S}_1^{\circ}/J K^{-1} mol^{-1}$	$\Delta \overline{C}_{p_1}^{\circ}/J K^{-1} mol^{-1}$
325	3.33	-43.6	11.3
400	4.47	-40.4	11.3
475	5.32	-38.4	11.3

References:

- Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. Hung. J. Ind. Chem. <u>1976</u>, 4, 269.
- Frolich, P. K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A. Ind. Eng. Chem. <u>1931</u>, 23, 548.
- Guerry, D. Jr. Ph.D. Thesis, Vanderbilt University, Nashville, TN 1944.
- Waters, J. A.; Mortimer, G. A.; Clements, H. E. J. Chem. Eng. Data <u>1970</u>, 15, 174, 462.
- Katayama, T.; Nitta, T.
 J. Chem. Eng. Data <u>1976</u>, 21, 194.
- Ijams, C. C. Ph.D. Thesis, Vanderbilt University, Nashville, TN 1941.
- Cook, M. W.; Hanson, D. N.; Alder, B. J. J. Chem. Phys. 1957, 26, 748.
- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- Thomsen, E. S.; Gjaldbaek, J. C. Acta Chem. Scand. 1963, 17, 127.
- Cukor, P. M.; Prausnitz, J. M. J. Phys. Chem. <u>1972</u>, 76, 598.
- Chappelow, C. C.; Prausnitz, J. M. Am. Inst. Chem. Eng. J. <u>1974</u>, 20, 1097.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Pentane; C₅H₁₂; [109-66-0]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson

H. L. Clever

EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	6.7	0.130	0.142

^{*}original datum

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Alkanes; C₆H₁₄ and C₇H₁₆ Ph.D. thesis, 1944 Vanderbilt University Nashville, TN Thesis Director, L. J. Bircher VARIABLES: T/K: 293.15, 298.15

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm)

H. L. Clever

EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient L			
Hexane; C ₆ H ₁₄ ; [110-54-3]						
293.15	6.41	0.110	0.118			
298.15	6.51	0.111	0.121			
Heptane; C ₇ H ₁₆ ; [142-82-5]						
293.15	6.37	0.0975	0.105			
298.15	6.63	0.101	0.110			

The Ostwald coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost complete recovery of the sample.

An improved temperature control system was used.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Alkanes. Distilled from sodium in air. In addition to the solubility data the thesis contains data of the refractive index, density, vapor pressure, and b.p.

SOURCE AND PURITY OF MATERIALS:

Hexane. Eastman Kodak Co. B.p. (760.3 mmHg) t/°C 68.85 - 68.90.

Heptane. B.p. (753.9 mmHg) t/°C 98.27 - 98.28 (corr.).

ESTIMATED ERROR:

 $\delta T/K = 0.05$

- Van Slyke, D. D.
 J. Biol. Chem. 1939, 130, 545.
- 2. Ijams, C. C. Ph.D. thesis, <u>1941</u> Vanderbilt University

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Hexane; C₆H₁₄; [110-54-3]

ORIGINAL MEASUREMENTS:

Waters, J. A.; Mortimer, G. A.; Clements, H. E.

J. Chem. Eng. Data 1970, 15, 174-176 and 462 (correction).

VARIABLES:

T/K: 263.15 - 293.15 H₂ P/kPa: 101.325 (1 atm) PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

Tempe t/ ^O C	rature T/K	c _{H2} /mo1 dm ⁻³ x 10 ³	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
-10	263.15	3.801	4.77	0.0852	0.0821
0	273.15	4.131	5.26	0.0926	0.0926
10	283.15	4.471	5.70	0.0991	0.1027
20	293.15	4.640	6.09	0.104	0.112

The mole fraction and Ostwald coefficient values were calculated from the authors data by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors reported two methods of solubility measurement. The hydrogen solubilities were measured by their method A.

The apparatus consisted of two glass bulbs connected by ¼" stainless steel tubing fitted with Hoke valves and a strain gage. The strain gage signal was measured by a potentiometer. The bulbs were immersed in an oil bath. The temperature was measured with a Pt resistance thermometer and Mueller bridge.

The solvent was degassed three times at liquid N_2 temperature. The solvent vapor pressure was measured in the apparatus. Gas in the second bulb at a known P and T was allowed into the bulb containing the solvent. The change in P was followed until equilibrium was reached. The gas uptake was calculated using Charles law. A correction was made for H_2 adsorption on the walls.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Minimum purity 99.50 per cent.
- (2) Hexane. Phillips Petroleum Co. Maximum impurities 0.5% benzene and 0.5% methyleyclopentane.

ESTIMATED ERROR:

 $\delta P/mmHg = 0.1$ $\delta T/K = 0.01$

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Katayama, T.; Nitta, T.
2. Hexane; C ₆ H ₁₄ ; [110-54-3]	J. Chem. Engng. Data. <u>1976</u> , 21,194-6
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
THE PARTY WATER	

EXPERIMENTAL VALUES:

T/K	Ostwald coefficient, L	Henry's Constant /atm	Mole fraction* of hydrogen in liquid, $x_{\rm H_2}$
298.15	0.130	1430	0.000699
273.15	0.105	1670	0.000599
253.15	0.0873	1920	0.000521
233.15	0.0710	2230	0.000448
213.15	0.0550	2690	0.000372

at a partial pressure of 1 atmosphere

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Volumetric apparatus with equilibrium cell of approximately 0.08 litres. Magnetic stirrer. Solvent carefully degassed. Equilibrium established in 1-1.5 hours. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Takachiho Chemical Industry Co. sample, purity 99.99 mole per cent.
- 2. Merck Uvasol spectral grade sample.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.12$ at T = 213.15K, ± 0.05 at other temperatures; $\&_{H_2} = \pm 1.5\%$

REFERENCES:

 Nitta, T.; Tatsuishi. A.;
 Katayama, T. J. Chem. Eng. Jpn. 1973, 6, 475.

Hydrogen; H₂: [1333-74-0] (1)

(2) Hexane; $C_{6}H_{14}$; [110-54-3]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	6.5	0.110	0.120

*original datum

 ${\tt Mol}$ fractions and Bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03 \text{ (authors)}$

REFERENCES:

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Alkanes; $C_7^H_{16}$, $C_8^H_{18}$, and $C_{10}^H_{22}$

ORIGINAL MEASUREMENTS:

Ijams, C. C.

Ph.D. thesis, <u>1941</u> Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient L
не	eptane; C7H16;	[142-82-5]	
298.15	5.90	0.0897	0.0979
Oc	tane; C ₈ H ₁₈ ;	[111-65-9]	
298.15	6.93	0.0950	0.1037
	2,4-Trimethylp 3 ^H 18; [540-84-1		octane;
298.15	7.48	0.1010	0.1102
De	ecane; C ₁₀ H ₂₂ ;	[124-18-5]	
298.15	5.37	0.0615	0.0671

The mole fraction and Ostwald coefficient values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified so that small solvent sample (2 cm³) could be used with almost 100 per cent recovery of the solvent.

An improved temperature control system was used.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Alkanes. Purified. Vapor pressure and boiling point also reported in the thesis.

ESTIMATED ERROR:

 $\delta T/K = 0.05$

REFERENCES:

 Van Slyke, D. D. J. Biol. Chem. <u>1939</u>, 130, 545.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Heptane; C₇H₁₆; [142-82-5]

ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

EXPERIMENTAL VALUES:

T/K		Solubii mol g ⁻¹		Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient L x 10 ²
238.154	4.797	4.71		4.804	7.80	6.94
248.15	4.978	4.9761		4.985	8.04	7.31
63.15	5.514	5.513 ¹		5.522	8.76	8.43
73.15	5.895	5.894¹		5.903	9.25	9.25
83.15	6.282	6.2811		6.290	9.74	10.09
85.25	6.354			6.363³	9.82	10.26
88.15	6.466	6.465 ¹		6.475³	9.96	10.51
298.15	6.865 6.871 6.875 6.872 6.871	6.866 ¹ 6.874 ¹ 6.871 ¹ av.		6.879	10.43	11.39
08.15	7.281 7.278 7.280 7.273 7.276 7.283 7.282 7.279	7.281 ¹ 7.274 ¹ 7.282 ¹ 7.281 ¹ av.	7.281 ² 7.274 ² 7.283 ² 7.282 ²	7.288	10.94	12 24
318.15		av.				12.34
328.15	7.70			7.713	11.43	13.31
	7.91			7.92 ³	11.59	13.92

Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: $\ln x_1 = -5.6689 - 4.8099/(T/100K)$

Standard error about the regression line = 4.60×10^{-6}

See the hydrogen + heptane evaluation for the recommended equation.

²Data from (2).

The paper gives the temperature as -35 °C (238.15 K), but reference (1) gives the temperature as -30 °C (243.15 K). The

³Values calculated by the compiler. higher temperature smooths the data better.

COMPONENTS: (1) Hydrogen; H ₂ ; [1333-74-0] (2) Heptane; C ₇ H ₁₆ ; [142-82-5]	ORIGINAL MEASUREMENTS: Cook, M. W.; Hanson, D. N.; Alder, B. J. J. Chem. Phys. <u>1957</u> , 26, 748 - 751.
VARIABLES: T/K: 243.15 - 328.15 P/kPa: 101.325 (1 atm)	PREPARED BY: P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

See preceeding page.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and (2) Heptane. Phillips Petroleum the assembly is shaken in an air bath. Co. Pure grade, 99+ mol per cent.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.
- Distilled, center portion used, b.p. 371.45K. Other solvent properties given in reference (1).

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$ (authors)

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

- (1) Hydrogen; H₂; [1333-74-0]
- Heptane; C7H16; [142-82-5]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson

H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	6.6	0.100	0.109

*original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

ORIGINAL MEASUREMENTS: COMPONENTS: Cook, M. W.; Hanson, D. N.; (1) Hydrogen; H₂; [1333-74-0] Alder, B. J. (2) Octane; C₈H₁₈; [111-65-9] J. Chem. Phys. 1957, 26, 748 - 751. VARIABLES: PREPARED BY: T/K: 248.15 - 308.15 P. L. Long P/kPa: 101.325 (1 atm) H. L. Clever

EXPERIMENTAL VALUES:

т/к	Solubility ¹ mol g ⁻¹ x 10 ⁶	Mol Fraction x ₁ × 10 ⁴	Bunsen Coefficient	Ostwald Coefficient L x 10 ²
248.15	4.331	4.947	7.17	6.52
273.15	5.139	5.869	8.28	8.28
298.15	5.984	6.832	9.37	10.22
308.15	6.343	7.241	9.81	11.07

1 Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler.

 $\ln x_1 = -8.5728 - 0.8677/(T/100K) + 1.4425 \ln (T/100K)$ Smoothed Data: Standard error about the regression line = 5.97×10^{-7}

For the recommended equation see the hydrogen + octane evaluation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and (2) Octane. the assembly is shaken in an air bath. Distilled

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is at attained. Mercury is used as the displacement fluid.

The solubility is calculated from the REFERENCES: initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.
- Eastman Kodak Co. Distilled, center portion used, b.p. 398.65K. Other solvent properties given in reference (1).

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Makranczy, J.; Megyery-Balog, K.; Rusz, L.; Patyi, L. (2) Octane; C₈H₁₈; [111-65-9] Hung. J. Ind. Chem. 1976, 4, 269-280. VARIABLES: T/K: 298.15 P/kPa: 101.325 (1 atm) PREPARED BY: S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient α	Ostwald Coefficient* L
298.15	6.4	0.088	0.096

^{*}original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 2,2,4-Trimethylpentane or isooctane; C₈H₁₈; [540-84-1]

ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748-751.

VARIABLES:

T/K: 283.15 - 318.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

T/K	Solubility ¹ mol g ⁻¹ x 10 ⁶	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
248.15	5.080	5.801	8.29	7.53
273.15	5.937	6.779	9.42	9.42
298.15	6.845	7.815	10.54	11.51
308.15	7.234	8.258	11.01	12.42

¹ Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler. Smoothed Data: $\ln x_1 = -9.2505 + 0.4341/(T/100K) + 1.7861 \ln (T/100K)$

Standard error around the regression line = 5.79×10^{-7}

T/K Mol Fraction	
$x_{1} \times 10^{4}$	
253.15 5.991	
263.15 6.379	
273.15 6.777	
283.15 7.186	
293.15 7.605	
298.15 7.820	
303.15 8.036	
308.15 8.255	

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.
- (2) 2,2,4-Trimethylpentane. Phillips Petroleum Co. Pure Grade, 99+ mol per cent. Distilled, center portion used, b.p. 372.35 K. Other solvent properties given in reference (1).

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$ (authors)

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Nonane; C₉H₂₀; [111-84-2]

ORIGINAL MEASUREMENTS:

Thomsen, E. S.; Gjaldbaek, J. C.

Acta Chem. Scand. 1963, 17, 127-133.

VARTABLES:

T/K: 298.05 - 308.05 Total P/kPa: 101.325 (1 atm)

PREPARED BY:

E. S. Thomsen

EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	- 104	Coefficient	Coefficient
	$x_1 \times 10^4$	2	2
	±	$\alpha \times 10^{2}$	L x 10 ²
298.05	6.87	8.58	9.36
298.15	6.98	8.71	9.51
308.05	7.27	8.98	10.1

The mole fraction and Ostwald solubility values were calculated by the compiler. Solubility values are for 101.325 (1 atm) partial pressure hydrogen assuming Henry's law is obeyed.

Smoothed Data: $ln x_1 = -5.7654 - 4.5010/(T/100K)$

Standard error about the regression line = 7.53×10^{-6}

T/K	Mol Fraction
	$x \times 10^4$
298.15	6.93
308.15	7.10
308.15	7.27

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as the confining liquid. The solvents were degassed in the apparatus. Details are in references 1 and 2.

The absorped volume of gas was calculated from the initial and final amounts, both saturated with solvent Vapor. The amount of solvent was determined by the weight of displaced mercury.

The saturation of the liquid with the gas was carried out close to atmospheric pressure. The solubility values were reported for one atmosphere gas pressure assuming Henry's law is obeyed.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Contained 0.02 per cent O₂ and 0.03 per cent N₂.
- (2) Nonane. Fluka "purum." Fractionated, distillation range 0.08 K.

ESTIMATED ERROR:

$$\delta T/K = 0.05$$

 $\delta x_1/x_1 = 0.015$

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

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	6.5	0.081	0.088

*original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

- (1) Hydrogen; H₂: [1333-74-0]
- (2) Decane; C₁₀H₂₂; [124-18-5]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson

H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	6.5	0.074	0.081

*original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03 \text{ (authors)}$

REFERENCES:

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

COMPONENTS: ORIGINAL MEASUREMENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Undecane; C₁₁H₂₄; [1120-21-4]

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	6.8	0.072	0.079

*original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03 \text{ (authors)}$

REFERENCES:

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

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0]

Dodecane; C₁₂H₂₆; [112-40-3] (2)

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	7.3	0.071	0.078

^{*}original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1) was

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

- Hydrogen; H₂; [1333-74-0] (1)
- Tridecane; C₁₃H₂₈; [629-50-5] (2)

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	7.4	0.068	0.074

*original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03 \text{ (authors)}$

REFERENCES:

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

- Hydrogen; H₂: [1333-74-0] (1)
- (2) Tetradecane; C₁₄H₃₀; [629-59-4]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bun Coeff
298.15	6.8	0.

Ostwald nsen ficient Coefficient* L α 0.059 0.064

*original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

- Hydrogen; H₂; [1333-74-0] (1)
- Pentadecane; C₁₅H₃₂; [629-62-9] (2)

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

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

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	7.0	0.057	0.062

*original datum

Mol fractions and busnen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03 \text{ (authors)}$

REFERENCES:

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

COMPONENTS: ORIGINAL MEASUREMENTS: Cukor, P.M.; Prausnitz, J.M. Hydrogen; H₂; [1333-74-0] J. Phys. Chem. 1972, 76,598-601. Hexadecane; C16H34; [544-76-3] VARIABLES: PREPARED BY: C.L. Young Temperature EXPERIMENTAL VALUES: Mole fraction of b Henry's Constant a T/K hydrogen in liquid, /atm $x_{\rm H_2}$ 300 1111 0.000900 0.000996 1004 325 0.00110 350 909 0.00121 375 825 400 749 0.00134 425 681 0.00147 0.00161 450 621 475 567 0.00176 Quoted in supplementary material for original paper. Calculated by compiler for a partial pressure b. of 1 atmosphere. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus similar to that described by Dymond and Hildebrand (1). Pressure measured with a null detector and precision No details given. gauge. Details in ref. (2). ESTIMATED ERROR: $\delta T/K = \pm 0.05$; $\delta x_{H_2} = \pm 2\%$. REFERENCES: 1. Dymond, J.; Hildebrand, J.H. Ind. Eng. Chem. Fundam. 1967,

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

10,638.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Hexadecane; C₁₆H₃₄; [544-76-3]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

S. A. Johnson H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient* L
298.15	7.2	0.055	0.060

^{*}original datum

Mol fractions and bunsen coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

Both components were analytical grade reagents of either Hungarian or foreign origin.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.03$ (authors)

REFERENCES:

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

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] 1. Chappelow, C.C.; Prausnitz, J.M. 2. Am. Inst. Chem. Engnrs. J. 1974, 20, 1097-2, 6, 10, 15, 19, 23 hexamethyltetracosane, (Squalane) 1104. $C_{30}H_{62}$; [111-01-3] VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: Mole fractionb of Henry's Constanta T/K hydrogen at 1 atm /atm partial pressure, $x_{\rm H_2}$ 300 726 0.001377 325 650 0.001538 350 589 0.001698 375 538 0.001859 400 494 0.002024 425 455 0.002198 450 421 0.002375 475 391 0.002558 Authors stated measurements were made at several pressures and values of solubility used were all within the Henry's-Law region. Calculated by compiler assuming linear relationship between mole fraction and pressure. AUXILIARY INFORMATION ... METHOD/APPARATUS/PROCEDURE. SOURCE AND PURITY OF MATERIALS: Volumetric apparatus similar to that described by Dymond and Hildebrand Solvent degassed, no other details (1). Pressure measured with a null given. detector and precision gauge. Details in ref. (2). ESTIMATED ERROR: $\delta T/K = \pm 0.1$; $\delta x_{H_2} = \pm 1$ %. (estimated by compiler). REFERENCES: 1. Dymond, J.; Hildebrand, J.H. Ind. Eng. Chem. Fundam. 1967, 6, 130.

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclohexane; C_6H_{12} ; [110-82-7]

EVALUATOR:

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

1980, September

CRITICAL EVALUATION:

Four laboratories have reported values of the solubility of hydrogen in cyclohexane at atmospheric pressure. Guerry (1) reported measurements at 293.15 and 298.15 K, Kruyer and Nobel (2) reported a value at 298.15 K, Dymond (3) reported four values over the 293.95 to 309.53 K temperature range, and Kraus and Gestrich (4) reported four values over the 283.15 to 313.15 K temperature range, which were presented on a graph.

It is the judgement of the evaluator that Dymond's measurements were carried out with more care and on better designed apparatus than the measurements of the others. Kruyer and Nobel's single value is 1.2 per cent less than Dymond's value, and the other data ranges 6 to 8 per cent below the values of Dymond.

A linear regression was applied to the data of Dymond to obtain the tentative equation

$$\ln x_1 = -5.6962 - 6.2403/(T/100K)$$

with a standard error about the regression line of 4.73×10^{-7} .

The temperature independent values of the thermodynamic changes in enthalpy and entropy for transfer of one mole of hydrogen from the gas at 101.325 kPa (1 atm) to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 5.19, and $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -47.4.

Smoothed values of the mole fraction solubility and Gibbs energy of solution are in the table.

Table 1. Solubility of hydrogen in cyclohexane at a hydrogen partial pressure of 101.325 kPa (1 atm). Tentative mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

т/к	Mol Fraction	ΔG ₁ °/kJ mo1 ⁻¹
293.15	4.00	19.07
298.15	4.14	19.31
303.15	4.29	19.54
308.15	4.43	19.78

References:

- 1. Guerry, D. J Ph.D. thesis, Vanderbilt University, Nashville, TN 1944.
- 2. Kruyer, S.; Nobel, A. P. P. Rec. Trav. Chim. 1961, 80, 1145.
- 3. Dymond, J. H. J. Phys. Chem. 1967, 71, 1829.
- 4. Krauss, W.; Gestrich, W. Chem. Tech. (Heidelberg) 1977, 6, 35.

ADDED NOTE:

Puri and Ruether (5) measured the solubility of hydrogen in mixtures of acetone and cyclohexane at 298.15 K and a total pressure of about 10^5 Pa. Their Ostwald coefficient value, measured for hydrogen + cyclohexane, converts to a mole fraction solubility of 4.24 x 10^{-4} at a hydrogen partial pressure of 101.325 kPa. The value is classed as tentative. The values of Dymond are still preferred.

5. Puri, P. S.; Ruether, J. A. Can. J. Chem. Eng. 1974, 52, 636.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclic hydrocarbons; $C_6^{H}_{10}$ and $C_6^{H}_{12}$

ORIGINAL MEASUREMENTS:

Guerry, D. Jr.

Ph.D. thesis, <u>1944</u> Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

VARIABLES:

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
СУ	clohexene; C6H	H ₁₀ ; [110-83-8]
293.15 298.15	3.35 3.42	0.0742 0.0753	0.0796 0.0822
Су	clohexane; C ₆ H	H ₁₂ ; [110-82-7	1
293.15 298.15	3.79 3.80	0.0787 0.0785	0.0845 0.0857

The Ostwald coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost complete recovery of the sample.

An improved temperature control system was used.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Hydrocarbons. Both were Eastman Kodak Co. products. They were purified by standard methods, and distilled from Na in a nitrogen atm.

SOURCE AND PURITY OF MATERIALS:

Cyclohexene. B.p. (756.6 mmHg) t/°C 82.35 - 82.50 (corr.).

Cyclohexane. B.p. (760.7 mmHg) t/°C 80.90 (corr.).

Data on density, refractive index and vapor pressure are in the thesis.

ESTIMATED ERROR:

 $\delta T/K = 0.05$

- Van Slyke, D. D.
 J. Biol. Chem. 1939, 130, 545.
- 2. Ijams, C. C. Ph.D. thesis, <u>1941</u> Vanderbilt University

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Kruyer, S.; Nobel, A.P.P.
2. Cyclohexane; C ₆ H ₁₂ ; [110-82-7]	Rec. Trav. Chim. <u>1961</u> , 80, 1145-56
VARIABLES:	PREPARED BY:
	C. L. Young
EXPERIMENTAL VALUES:	
T/K Ostwald coeffic	[a] ient, L Mole fraction of
	hydrogen, $x_{\rm H_2}$
298.15 0.092	0.000409
[a] Calculated by compiler for a par	rtial pressure of 101.325 kPa
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Technique consisted of saturating liquid with hydrogen in a spiral	1. Hydrogen and argon passed through molecular sieve 4A in liquid oxygen
adsorption tube and then stripping out the hydrogen with argon. The	and nitrogen trap respectively.
resulting argon-hydrogen mixture was analysed with a katharometer.	2. Distilled.
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.2; \delta L = \pm 3\%$
	REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclohexame; C_6H_{12} ; [110-82-7]

ORIGINAL MEASUREMENTS:

Dymond, J. H.

J. Phys. Chem. <u>1967</u>, 71, 1829-1831.

VARIABLES:

T/K: 293.95 - 309.53 P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.95	4.02	8.33	8.96
298.16	4.14	8.54	9.32
304.77	4.34	8.88	9.91
309.53	4.47	9.09	10.3

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: $\ln x_1 = -5.6962 - 6.2403/(T/100K)$

Standard error about the regression line = 4.73×10^{-7}

T/K	Mol Fraction $x_1 \times 10^4$
293.15	4.00
298.15	4.14
303.15	4.29
308.15	4.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Stuart Oxygen Co. Dried.
- (2) Cyclohexane. Matheson, Coleman and Bell chromatoquality reagent. Dried and fractionally frozen. m.p. 6.45°C.

ESTIMATED ERROR:

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Krauss, W.; Gestrich, W.
2. Cyclohexane; C_6H_{12} ; [110-82-7] Chem. Tech (Heidelberg), $\underline{19}$ 6, 35-37.	
VARIABLES:	PREPARED BY:
Temperature,	C.L. Young
EXPERIMENTAL VALUES:	
T/K Solubility*/ mol dm	bar ⁻¹ Mole fraction § of hydrogen in liquid, $^{\varpi}_{\mathrm{H}_2}$
283.15 0.0032 293.15 0.0034 303.15 0.0036	0.00035 0.00037 0.00040
<pre>313.15</pre>	0.00042
appear to be in error.	given in the original paper
<pre>\$ calculated by compiler for a</pre>	partial pressure of 101.325 kPa.
	INFORMATION
METHOD/APPARATUS/PROCEDURE: Stirred equilibrium cell. Volumetric apparatus in which	
a known volume of gas was added to a known volume of liquid and the equilibrium pressure measured.	SOURCE AND PURITY OF MATERIALS: No details given.
a known volume of liquid and the	No details given.
a known volume of liquid and the equilibrium pressure measured.	
a known volume of liquid and the equilibrium pressure measured.	No details given. ESTIMATED ERROR:

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. 2-Propanone, (Acetone); C

2-Propanone, (Acetone); C₃H₆O; [67-64-1]

Cyclohexane; C₆H₁₂; [110-82-7]

ORIGINAL MEASUREMENTS:

Puri, P.S.; Ruether, J.A.

Can. J. Chem. Eng. 1974 52, 636-640.

VARIABLES:

Liquid phase composition

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	Mole fraction of acetone in liquid,	Ostwald * coefficient, $_L$	
298.15	1.000	0.0943	
	0.8285	0.0929	
	0.7769	0.0900	
	0.5406	0.1028	
	0.3914	0.1058	
	0.2466	0.1030	
	0.0000	0.0953	

* total pressure approximately 105Pa.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

Volumetric apparatus similar to that described in ref. (1).

Degassed solution placed in calibrated dissolution vessel, gas saturated with solvent vapor introduced from a calibrated gas buret. Amount of gas dissolved determined from pressure and volume changes.

SOURCE AND PURITY OF MATERIALS:

- Liquid Carbonic Canadian Corp., sample purity 99.97 mole per cent.
- 2 & 3 Baker Reagent grade.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$; $\delta L = \pm 0.5$ % (estimated by compiler)

REFERENCES:

Ben-Naim, A.; Baer, S.
 Trans. Faraday. Soc. 1963, 59, 2735.

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Kruyer, S.; Nobel, A.P.P. 2. Benzene; C₆H₆; [71-43-2] Rec. Trav. Chim. 1961, 80, 1145-56 VARIABLES: PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	Ostwald coefficient, L	Mole fraction of hydrogen, $x_{\rm H_2}$
299.05	0.088	0.00036
312.75	0.095	0.00037
323.15	0.104	0.00040
333.15	0.110	0.00042

Liquid was an equimolar mixture of benzene and cyclohexane

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Technique consisted of saturating liquid with hydrogen in a spiral adsorption tube and then stripping out the hydrogen with argon. The resulting argon-hydrogen mixture was analysed with a katharometer.

SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen and argon psssed through molecular sieve 4A in liquid nitrogen and oxygen trap respectively.
- 2. and 3. Distilled.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \quad \delta L = \pm 3$ %

COMPONENTS: ORIGINAL MEASUREMENTS: Kruyer, S.; Nobel, A.P.P. Hydrogen; H₂; [1333-74-0] 1. Decahydronaphthalene [a] Rec. Trav. Chim. 1961, 80, 1145-56 2. [Decalin]; $\bar{C}_{10}H_{18}$; [91-17-8] VARIABLES: PREPARED BY: C. L. Young EXPERIMENTAL VALUES: [b] Ostwald coefficient, L Mole fraction of T/K hydrogen, $x_{\rm H}$, 0.000422 298.15 0.065 Probably contained about 15% cis-isomer [a] Calculated by compiler assuming a density of decalin (cis, transmixture) of 0.87 g cm 3 . Partial pressure of 101.325 kPa $\,$ [b] AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Hydrogen and argon passed through Technique consisted of saturating molecular sieve 4A in liquid oxygen liquid with hydrogen in a spiral adsorption tube and then stripping and nitrogen trap respectively. Out the hydrogen with argon. The resulting argon-hydrogen mixture was analysed with a katharometer. 2. "Chemically pure". ESTIMATED ERROR: $\delta T/K = \pm 0.2; \quad \delta L = \pm 3$ % REFERENCES:

1. Hydrogen; H ₂ ; [1333-74-0]	Krauss, W.; Gestrich, W.
2. Cis-decahydronaphthalene (Decalin); C10H18; [493-01-6]	ChemTech. (Heidelberg) 1977, 6, 35-37.
VARIABLES:	PREPARED BY:
Temperature	C. L. Young

T/K	Solubility *S/mol dm - 3 bar - 1	Mole fraction § of hydrogen in liquid, $^{x}{ m H}_{2}$
283.15	0.0021	0.000325
293.15	0.00225	0.000352
303.15	0.00235	0.000370
313.15	0.00250	0.000397
1		

- * Read off graph, the equations given in the original paper appear to be in error.
- \S Calculated by compiler for a partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: Stirred equilibrium cell. Volumetric apparatus in which a known volume of gas was added to a known volume of liquid and the equilibrium pressure measured. Details in source. ESTIMATED ERROR: $6T/K = \pm 0.05$; $6x_{H_2} = \pm 10^{-5}$ (estimated by compiler). REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:	
 Hydrogen; H₂; [1333-74-0] Trans-decahydronaphthalene (Decalin); C₁₀H₁₈; [493-02-7] 		Krauss, W.; Gestrich, W.; ChemTech. (Heidelberg) 1977, 6, 35-37.	
VARIABLES:		PREPARED BY:	
Temperature		C. L. Young	
EXPERIMENTAL VALUES: T/K Solubility *S/mol dm - 3 bar - 1		Mole fraction § of hydrogen in liquid, $^{x}_{ m H_{2}}$	
283.15	0.0022	0.00035	
293.15	0.0023	0.00037	
303.15	0.0025	0.00041	
313.15	0.0026	0.00043	

^{*} Read off graph, the equations given in the original paper appear to be in error.

AUXILIARY INFORMATION

ÆTHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Stirred equilibrium cell. Volumetric apparatus in which a known volume of gas was added to a known volume of liquid and the equilibrium pressure measured. Details in source.	No details given.
	ESTIMATED ERROR: $\delta T/K = \pm 0.05$; $\delta x_{\rm H_2} = \pm 10^{-5}$ (estimated by compiler). REFERENCES:

 $^{^{\}S}$ Calculated by compiler for a partial pressure of 101.325 kPa.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Cukor, P.M.; Prausnitz, J.M.
2. 1,1- Bicyclohexyl; C ₁₂ H ₂₂ ; [92-51-3]	J. Phys. Chem. <u>1972</u> ,76,598-601.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES:	
T/K Henry's Constant a	Mole fraction of b
/atm	hydrogen in liquid,
	<i>x</i> _{H₂}
300 2252	0.000444
325 2060	0.000485
350 1864 375 1669	0.000536 0.000599
400 1479	0.000676
425 1296	0.000772 0.000890
450 1124 475 964	0.001037
of 1 atmosphere.	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric apparatus similar to that described by Dymond and Hildebrand (1). Pressure measured with a null detector and precision gauge. Details in ref. (2).	No details given.
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.05; \ \delta x_{\rm H_2} = \pm 2\%.$
	REFERENCES:
	1. Dymond, J.; Hildebrand, J.H. Ind. Eng. Chem. Fundam. 1967, 6, 130.
	2. Cukor, P.M.; Prausnitz, J.M.; Ind. Eng. Chem. Fundam. 1971, 10, 638.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Benzene; C₆H₆; [71-43-2]

EVALUATOR:

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

1980, September

CRITICAL EVALUATION:

The solubility of hydrogen in benzene at a hydrogen partial pressure of 101.325 kPa (1 atm) over the temperature interval of 283.15 to 338.15 K.

Eight laboratories have reported solubility values on the hydrogen + benzene system at hydrogen partial pressures near 101.325 kPa (1 atm). Another six laboratories have reported solubility values of hydrogen partial pressures greater than 200 kPa which are compiled and evaluated in another part of the volume.

The atmospheric pressure measurements were:

Just (1) values of 293.15 and 298.15 K, Horiuti (2) four values between 280.15 and 335.95 K, Maxted and Moon (3) five values between 273.65 [sic] and 313.15 K, Cook $et\ al.$ (4) five values between 283.15 and 318.15 K, Kruyer and Nobel (5) a value of 298.15 K, deWet (6) three values between 291.65 and 304.55 K, and Krauss and Gestrich (7) four values between 283.15 and 313.15 K, and Puri and Ruether (8) one value at 298.15 K.

It is generally accepted by workers in gas solubility that the measurements of Horiuti (2), and of Cook, Hanson, and Alder (4) were carried out with exceptional care and accuracy.

Linear regressions were made of two arrangements of the mole fraction solubility data from the papers above. Both data sets were fitted to two and to three constant equations.

The first data arrangement was to use all of the data except the mole fraction solubility at 273.65 K of Maxted and Moon (3). Benzene freezes near 278.7 K, thus that temperature appears to be in error. The second data arrangement was to use just the nine data points of Horiuti (2) and Cook $et\ al.$ (4).

The three constant equations could not be justified for either of the two data arrangements. There was no significant change in the standard error about the regression line between the two and three constant equations.

When all of the data were used, only the 298.15 K value of Just (1) fell more than two standard deviations from the regression line. It was omitted and all of the remaining data were fitted by a linear regression to a two constant equation.

The two constant equations obtained from the two data arrangements were essentially identical except that the equation from all of the data had a standard error about the regression line of 8.10×10^{-6} and the Horiuti and the Cook et al. data had a standard deviation of 2.89×10^{-6} . The two equations gave the same values of smoothed mole fraction solubilities at 5 degree intervals from 283.15 to 338.15 K to three digits.

The recommended equation for the mole fraction solubility over the temperature interval of 283.15 to 338.15 K is

$$\ln x_1 = -5.5284 - 8.1390/(T/100K)$$

with a standard error about the regression line of 2.89 \times 10⁻⁶.

The temperature independent thermodynamic changes from the equation for the transfer of one mole of hydrogen gas from the gas phase at 101.325 $\rm kpa$ to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 6.767, and $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -45.96.

 $^{
m Values}$ of the mole fraction solubility and partial molal Gibbs energy of solution are in Table 1.

Table 1. Solubility of hydrogen in benzene at a hydrogen partial pressure of 101.325 kPa (1 atm).

Recommended mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	ΔG°/kJ mol ⁻¹
283.15 288.15 293.15 298.15 303.15 308.15 313.15 318.15 323.15	2.242 2.357 2.473 2.591 2.710 2.831 2.953 3.076 3.200 3.326	19.782 20.012 20.242 20.471 20.701 20.931 21.161 21.391 21.621 21.850
328.15 333.15 338.15	3.326 3.452 3.579	22.080 22.310

References:

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342.
- Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125.
- 3. Maxted, E. B.; Moon, C. H. Trans. Faraday Soc. 1936, 32, 769.
- 4. Cook, M. W.; Hanson, D. M.; Alder, B. J. J. Chem. Phys. 1957, 26, 748.
- 5. Kruyer, S.; Nobel, A. P. P. Rec. Trav. Chim. 1961, 80, 1145.
- 6. deWet, W. J. J. S. Afr. Chem. Inst. 1964, 17, 9.
- 7. Krauss, W.; Gestrich, W. Chem. Tech. (Heidelberg) 1977, 6, 35.
- 8. Puri, P. S.; Ruether, J. A. Can. J. Chem. Eng. 1974, 52, 636.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Benzene; C₆H₆; [71-43-2] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	2.61	6.589	7.071
298.15	2.76	6.926	7.560

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Benzene. No information.

ESTIMATED ERROR:

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

- 1. Timofejew, W. Z. Physik. Chem. 1890, 6, 141.
- 2. Steiner, Ann. Phys. (Leipzig) 1894, 52, 275.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Benzene; C₆H₆; [71-43-2] Sci. pap. Inst. Phys. Chem. Res.

Sci. pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125-256.

VARIABLES: PREPARED BY:

T/K: 280.15 - 335.95 M. E. Derrick P/kPa: 101.325 (1 atm) H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen Coefficient	Ostwald Coefficient
	$x_1 \times 10^4$	$\alpha \times 10^2$	L x 10 ²
280.15	2.170	5.56	5.85
296.05	2.570	6.46	7.00
314.45	2.982	7.33	8.44
335.95	3.570	8.545	10.51

The mole fraction and Bunsen coefficient values were calculated by the compiler.

Smoothed Data: $\ln x_1 = -5.4671 - 8.3096/(T/100K)$

Standard error about the regression line = 2.32×10^{-6}

See hydrogen + benzene evaluation for the recommended equation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret, a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption pipet.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by electrolysis.
- (2) Benzene. Merck. Extra pure, free from sulfur sample refluxed with sodium amalgam. Boiling point 80.18°C (760 mmHg).

ESTIMATED ERROR:

$$\delta T/K = 0.05$$

 $\delta x_1/x_1 = 0.005$

COMPONENTS -		IODIOTALLA AGRAGADA A	
COMPONENTS:		ORIGINAL MEASUREMENTS:	
1. Hydrogen; H ₂ ; [1333-74		Maxted, E.B., Moon, C.H.,	
2. Benzene, C ₆ H ₆ ; [71-43-	-2]	Trans. Faraday Soc. <u>1936</u> , 32,769-75.	
'ARIABLES:		PREPARED BY:	
Temperature		C.L. Young	
EXPERIMENTAL VALUES:			
T/K Bunsen coefficien α		Mole fraction of hydrogen, $x_{\rm H_2}$	
273.65 0.052 281.45 0.057 294.35 0.062 303.75 0.067 313.15 0.072		0.000204 0.000224 0.000248 0.000270 0.000296	
Farcial pressu		en = 1 atm = 101.325 kPa.	
VE my		INFORMATION .	
METHOD:/APPARATUS/PROCEDURI		SOURCE AND PURITY OF MATERIALS;	
Volumetric apparatus with absorption cell. Details	rocking in source.	Electrolytic grade. Degassed, high purity sample, no other details given.	
		ESTIMATED ERROR:	
		$\delta T/K = \pm 0.2; \ \delta x_{H} = \pm 1\%.$	
		(estimated by compiler)	
		REFERENCES:	

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Cook, M. W.; Hanson, D. N.; Alder, B. J. (2) Benzene; C₆H₆; [71-43-2] J. Chem. Phys. 1957, 26, 748 - 751. VARIABLES: PREPARED BY: T/K: 283.15 - 318.15 P/kPa: 101.325 (1 atm) P. L. Long

PARTED TARRANTAL MATTER.

EXPERIMENTAL VALU	JES:			
T/K	Solubility 1 mol g-1 x 106	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
283.15	2.884	2.253	5.75	5.96
288.25	3.030 3.024 3.027 av.	2.364 ²	6.00	6.33
298.15	3.306 3.301 <u>3.303</u> 3.303 av.	2.578	6.46	7.05
308.15	3.595 3.582 3.596 3.591	2.805	6.95	7.84
318.15	3.89 3.88 3.88 ₅ av.	3.034 ²	7.42	8.64

¹ Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: $\ln x_1 = -5.6949 - 7.6547/(T/100K)$

Standard error about the regression line = 1.86×10^{-7} See the hydrogen + benzene evaluation for the recommended equation

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is decassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degasse ESTIMATED ERROR: solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

SOURCE AND PURITY OF MATERIALS:

(1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.

H. L. Clever

(2) Benzene. Baker and Adamson Reagent Grade. Distilled, used center cut, boiling point 353.15 K. Other solvent properties given in reference 1.

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. <u>1957</u>, 28, 370.

²Values calculated by compiler from data in (1).

COMPONENTS:		ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ;	[1333-74-0]	Kruyer, S.; Nobel, A.P.P.
2. Benzene; C ₆ H ₆ ;	; [71-43-2]	Rec. Trav. Chim. 1961, 80, 1145-56
VARIABLES:		PREPARED BY:
		C. L. Young
EXPERIMENTAL VALUES:		<u> </u>
T/K	Ostwald coeffi	[a] cient, L Mole fraction of hydrogen, x H ₂
298.15	0.071	0.000258
[a] Calculated by	compiler for a pa	artial pressure of 101.325 kPa
[a] Calculated by		artial pressure of 101.325 kPa INFORMATION
[a] Calculated by	AUXILIARY	
	AUXILIARY RE: of saturating in a spiral then stripping h argon. The ogen mixture was	INFORMATION
METHOD/APPARATUS/PROCEDUL Technique consisted liquid with hydrogen adsorption tube and Out the hydrogen wit resulting argon-hydr	AUXILIARY RE: of saturating in a spiral then stripping h argon. The ogen mixture was	INFORMATION SOURCE AND PURITY OF MATERIALS: 1. Hydrogen and argon passed through molecular sieve 4A in liquid oxygen and nitrogen trap respectively. 2. Distilled. ESTIMATED ERROR:
METHOD/APPARATUS/PROCEDUL Technique consisted liquid with hydrogen adsorption tube and Out the hydrogen wit resulting argon-hydr	AUXILIARY RE: of saturating in a spiral then stripping h argon. The ogen mixture was	INFORMATION SOURCE AND PURITY OF MATERIALS: 1. Hydrogen and argon passed through molecular sieve 4A in liquid oxygen and nitrogen trap respectively. 2. Distilled.
METHOD/APPARATUS/PROCEDUL Technique consisted liquid with hydrogen adsorption tube and Out the hydrogen wit resulting argon-hydr	AUXILIARY RE: of saturating in a spiral then stripping h argon. The ogen mixture was	INFORMATION SOURCE AND PURITY OF MATERIALS: 1. Hydrogen and argon passed through molecular sieve 4A in liquid oxygen and nitrogen trap respectively. 2. Distilled. ESTIMATED ERROR:

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] de Wet, W. J. (2) Benzene; C₆H₆; [71-43-2] J. S. Afr. Chem. Inst. 1964, 17, 9 - 13. VARIABLES: T/K: 291.65 - 304.55 P/kPa: 101.325 (1 atm) PREPARED BY: P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
291.65 298.15 304.55	2.52 2.65 2.86	6.36 6.65 7.11	6.79 7.26 7.93

The mole fraction and Ostwald coefficient values were calculated by the compiler.

Smoothed Data: $\ln x_1 = -5.3098 - 8.6944/(T/100K)$

Standard error about the regression line = 3.24×10^{-6}

See the evaluation of the hydrogen + benzene system for the recommended equation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is a modification of that used by Morrison and Billett (1) and others (2). The degassed solvent is saturated with gas as it flows down a glass helix containing the gas. The amount of solvent passed down the helix was such that 10 to 25 cm³ of gas was absorbed.

Degassing. The solvent is placed in a large continuously evacuated bulb until the solvent boils freely without further release of dissolved gases.

Saturation. The solvent is flowed in a thin film down the glass helix containing the gas. The volume of gas absorbed is measured on an attached buret system.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Gas from commercial cylinders purified over activated charcoal at liquid air temperature. Impurities estimated to be less than 0.3 per cent.
- (2) Benzene. Source not given. Distilled immediately before use.

ESTIMATED ERROR:

 $\delta T/K = 0.05$

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033; Ibid. 1952, 3819.
- Clever, H. L.; Battino, R.; Saylor, J. H.; Gross, P. M. J. Phys. Chem. <u>1957</u>, 61, 1078.

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Krauss, W.; Gestrich, W. 2. Benzene; C₆H₆; [71-43-2] Chem.-Tech. (Heidelberg), 1977, 6, 35-37. VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: Solubility S/ mol dm-3 bar-1 Mole fraction of T/K hydrogen in liquid, $x_{\rm H_2}$ 283.15 0.00235 0.000209 293.15 0.00265 0.000235 303.15 0.000260 0.00285 313.15 0.00310 0.000286 * read off graph, the equations given in the original paper appear to be in error. § calculated by compiler for a partial pressure of 101.325 kPa. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Stirred equilibrium cell. No details given. Volumetric apparatus in which a known volume of gas was added to a known volume of liquid and the equilibrium pressure measured. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05$; $\delta x_{\rm H_2} = 5 \times 10^{-6}$ (estimated by compiler) REFERENCES:

COMP	ONENTS:	ORIGINAL MEASUREMENTS:
1.	Hydrogen; H ₂ ; [1333-74-0]	Puri, P.S.; Ruether, J.A.
2.	2-Propanone, (Acetone); C ₃ H ₆ O; [67-64-1]	Can. J. Chem. Eng. <u>1974</u> , 52, 636-640.
3.	Benzene; C ₆ H ₆ ; [71-43-2]	
VARI	ABLES:	PREPARED BY:
	Liquid phase composition	C.L. Young

EXPERIMENTAL V	1.	AL	U.	ES	:
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T/K	Mole fraction of acetone in liquid	Ostwald * coefficient, L	
298.15	1.000	0.0943 0.0919	
	0.6381	0.0952	
	0.4255 0.2233	0.0890 0.0847	
	0.0000	0.0756	

* total pressure approximately 10⁵Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus similar to that described in ref. (1).

Degassed solution placed in calibrated dissolution vessel, gas saturated with solvent vapor introduced from calibrated gas buret. Amount of gas dissolved determined from pressure and volume changes.

SOURCE AND PURITY OF MATERIALS:

- Liquid Carbonic Canadian Corp. sample purity 99.97 mole per cent.
- 2.& 3.Baker reagent grade.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$; $\delta L = \pm 0.5$ %. (estimated by compiler)

REFERENCES:

Ben-Naim, A.; Baer, S. Trans. Faraday Soc. <u>1963</u> 59, 2735.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Methylbenzene or toluene; C7H8; [108-88-3]

EVALUATOR:

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

1980, September

CRITICAL EVALUATION:

Six laboratories have reported on the solubility of hydrogen in methylbenzene at a hydrogen partial pressure near 101.325 kPa. Just (1) reported two values at 293.15 and 298.15 K, Cook, Hanson, and Alder (2) reported four values between temperatures of 258.15 and 308.15 K, Saylor and Battino (3) reported one value at 298.15 K, deWet (4) reported three values between temperatures of 291.25 and 305.25 K, Waters, Mortimer and Clements (5) reported four values between temperatures of 263.15 and 293.15 K, and Krauss and Gestrich (6) reported four values between temperatures of 283.15 and 313.15 K.

Comparison of the mole fraction solubility values at 101.325 kPa shows that the data falls into three ranges. The data of Just and of deWet agree and are greater than the other workers. The results of Cook et al. and of Saylor and Battino agree within 0.4 per cent and are of intermediate value. The data of Waters et al. and of Krauss and Gestrich agree within 3 to 5 per cent and are the low set of values.

All of the data are classed as tentative, but the data of Cook $et \ \alpha l$. are preferred by the evaluator because of their well designed apparatus, and self-consistent results. The values below are based on a linear regression of the Cook $et\ al.$ mole fraction solubility data.

The equation for use between 258.15 and 308.15 K is

$$\ln x_1 = -6.0373 - 6.0307/(T/100K)$$

which has a standard error about the regression line of 7.17 x 10^{-7} .

The changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 5.01 and $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -50.2.

Smoothed values of the mole fraction solubility and Gibbs energy of solution are in Table 1.

The solubility of hydrogen in methylbenzene Table 1. at a hydrogen partial pressure of 101.325 Mole fraction solubility and the partial molar Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction 10 4 x 1	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
258.15	2.31	17.972
268.15	2.52	18.474
278.15	2.73	18.976
288.15	2.94	19.478
298.15	3.15	19.980
308.15	3.37	20.482

References:

- Just, G. Z. Phys. Chem. 1901, 37, 342.
- 2. Cook, M. W.; Hanson, D. N.; Alder, B. J. J. Chem. Phys. 1957, 26, 748.
- 3.
- Saylor, J. H.; Battino, R. J. Phys. Chem. 1958, 62, 1334. deWet, W. J. J. S. Afr. Chem. Inst. 1964, 17, 9. 4. 5.
- Water, J. A.; Mortimer, G. A.; Clements, H. E. J. Chem. Eng. Data 1970, 15, 174.
- 6. Krauss, W.; Gestrich, W. Chem.-Tech. (Heidelberg) 1977, 6, 35.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Hydrogen; H ₂ ; [1333-74-0]	Just, G.	
(2) Methylbenzene or toluene; C ₇ H ₈ ; [108-88-3]	Z. Phys. Chem. <u>1901</u> , 37, 342 - 367.	
VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm)	PREPARED BY: M. E. Derrick H. L. Clever	

EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	3.70	7.812	8.384
298.15	3.82	8.010	8.742

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Methylbenzene. No information.

ESTIMATED ERROR:

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

- Timofejew, W.
 Physik. Chem. 1890, 6, 141.
- Steiner,
 Ann. Phys. (Leipzig) 1894, 52,
 275.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Methylbenzene or toluene; C7H8; [108-88-3]

ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748-751.

VARIABLES:

T/K: 258.15 - 308.15 P/kPa: 101.325 (1 atm) 258.15 - 308.15

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

T/K	Solubility ¹ mol g ⁻¹ x 10 ⁶	Mol Fraction x 1 × 10 ⁴	Bunsen Coefficient \alpha \times 10^2	Ostwald Coefficient L x 10 ²
258.15	2.507	2.311	5.06	4.78
273.15	2.844	2.621	5.65	5.65
298.15	3.438 3.436 3.437 av.	3.167	6.64	7.25
308.15	3.685 3.685 3.685 av.	3.369	6.99	7.89

Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: $\ln x_1 = -6.0373 - 6.0307/(T/100K)$

Standard error about the regression line = 7.17×10^{-7}

See the hydrogen + methylbenzene evaluation for the recommended equation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. are attached to a mounting plate, and (2) Methylbenzene. Baker and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.
- Adamson Reagent Grade. Distilled, center portion used, b.p. 383.65K. Other solvent properties given in reference (1).

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$ (authors)

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Methylbenzene or toluene; C_7H_8 ; [108-88-3]

ORIGINAL MEASUREMENTS:

Saylor, J. H.; Battino, R.

J. Phys. Chem. <u>1958</u>, 62, 1334 - 1337.

VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Т/К	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
298.15	3.18	6.67	7.28

The mole fraction and Bunsen coefficient values were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was degassed (2) by evacuating the space above it, shaking, and then passing it as a fine mist into another evacuated container. The degassed solvent was saturated with gas as it passed down a glass helix in a thin film. The glass helix contained the gas and solvent vapor at a total pressure of one atm (1). The volume of the liquid and the volume of the gas absorbed were determined in a system of burets.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. No information given.
- (2) Methylbenzene. Malinckrodt reagent grade. Shaken with conc. H₂SO₄, water washed, dried over Drierite, distilled. Boiling point 110.40 - 110.60 °C.

ESTIMATED ERROR:

 $\delta T/K = 0.03$ $\delta P/mmHg = 3$ $\delta x_1/x_1 = 0.04 \text{ (authors)}$

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033; ibid, 1952, 3819.
- 2. Baldwin, R. R.; Daniel, S. G. J. Appl. Chem. 1952, 2, 161

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Methylbenzene or toluene; C_7H_8 ; [108-88-3]

ORIGINAL MEASUREMENTS:

de Wet, W. J.

J. S. Afr. Chem. Inst. 1964, 17, 9 - 13.

VARIABLES:

compiler.

T/K: 291.25 - 305.25 P/kPa: 101.325 (1 atm)

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES: T/K Mol Fraction Bunsen Ostwald Coefficient $x_1 \times 10^4$ $\alpha \times 10^2$ L $\times 10^2$ 291.25 3.60 7.62 8.12

291.25 3.60 7.62 8.12 298.45 3.79 7.95 8.69 305.25 3.98 8.29 9.26

The mole fraction and Ostwald coefficient values were calculated by the

Smoothed Data: $\ln x_1 = -5.7429 - 6.3694/(T/100K)$

Standard error about regression line = 4.19×10^{-7}

See the evaluation of hydrogen + methylbenzene for the recommended equation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is a modification of that used by Morrison and Billett (1) and others (2). The degassed solvent is saturated with gas as it flows down a glass helix containing the gas The amount of solvent passed down the helix was such that 10 to 25 cm³ of gas was absorbed.

Degassing. The solvent is placed in a large continously evacuated bulb until the solvent boils freely without further release of dissolved gases.

Saturation. The solvent is flowed in a thin film down the glass helix containing the gas. The volume of gas absorbed is measured on an attached buret system.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Gas from commercial cylinders purified over activated charcoal at liquid air temperature. Impurities estimated to be less than 0.3 per cent.
- (2) Methylbenzene. Source not given. Distilled immediately before use.

ESTIMATED ERROR:

 $\delta T/K = 0.05$

- Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033; Ibid. 1952, 3819.
- Clever, H. L.; Battino, R.;
 Saylor, J. H.; Gross, P. M.
 J. Phys. Chem. 1957, 61, 1078.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Methylbenzene or toluene; C_7H_8 ; [108-88-3]

ORIGINAL MEASUREMENTS:

Waters, J. A.; Mortimer, G. A.; Clements, H. E.

J. Chem. Eng. Data 1970, 15, 174-176 and 462 (correction).

VARIABLES:

T/K: 263.15 - 293.15 H₂ P/kPa: 101.325 (1 atm)

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature	c _{H2} /mol dm ⁻³	Mol Fraction	Bunsen Coefficient	Ostwald Coefficient
t/°C	T/K	x 10 ³	$x_1 \times 10^4$	α	L
-10	263.15	2.164	2.23	0.0485	0.0467
0	273.15	2.396		0.0537	0.0537
10	283.15	2.538	2.67	0.0569	0.0590
20	293.15	2.708	2.88	0.0607	0.0651

The mole fraction and Ostwald coefficient values were calculated from the authors data by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors reported two methods of solubility measurement. The hydrogen solubilities were measured by their method A.

The apparatus consisted of two glass bulbs connected by 4" stainless steel tubing fitted with Hoke valves and a strain gage. The strain gage signal was measured by a potentiometer. The bulbs were immersed in an oil bath. The temperature was measured with a Pt resistance thermometer and Mueller bridge.

The solvent was degassed three times at liquid $\rm N_2$ temperature. The solvent vapor pressure was measured in the apparatus. Gas in the second bulb at a known P and T was allowed into the bulb containing the solvent. The change in P was followed until equilibrium was reached. The gas uptake was calculated using Charles law. A correction was made for $\rm H_2$ adsorption on the walls.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Minimum purity 99.50 per cent.
- (2) Methylbenzene. Fisher Co. Spectrophotometric grade.

ESTIMATED ERROR:

 $\delta P/mmHg = 0.1$ $\delta T/K = 0.01$

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Krauss, W.; Gestrich, W. 2. Methylbenzene (Toluene); Chem.-Tech. (Heidelberg), 1977, 6, C7H8; [108-88-3] 35-37. VARIABLES: PREPARED BY: C.L. Young Temperature, EXPERIMENTAL VALUES: Solubility */ mol dm-3 bar-1 Mole fraction of T/K hydrogen in liquid, $x_{\rm H_2}$ 283.15 0.0026 0.00028 293.15 0.00275 0.000295 0.0029 0.000315 303.15 313.15 0.00305 0.000335 * read off graph, the equations given in the original paper appear to be in error. § calculated by compiler for a partial pressure of 101.325 kPa. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Stirred equilibrium cell. Volumetric apparatus in which a known volume of gas was added to No details given. a known volume of liquid and the equilibrium pressure measured. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05; \ \delta x_{H_2} = \pm 10^{-5}$ (estimated by compiler) REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1,3-Dimethylbenzene (m-Xylene);
 C₈H₁₀; [108-38-3]

ORIGINAL MEASUREMENTS:

de Wet, W. J.

J. S. Afr. Chem. Inst. 1964, 17, 9 - 13.

VARIABLES:

T/K: 291.15 - 305.25 P/kPa: 101.325 (1 atm)

PREPARED BY:

P. L. Long H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
291.15	3.96	7.25	7.73
298.45	4.14	7.52	8.22
305.25	4.36	7.87	8.79

The mole fraction and Ostwald coefficient values were calculated by the compiler.

Smoothed Data: $ln x_1 = -5.7584 - 6.0492/(T/100K)$

Standard error about the regression line = 2.21×10^{-6}

T/K	Mol Fraction $x_1 \times 10^4$
	$\frac{x_1 \times 10^{\circ}}{}$
288.15	3.87
293.15	4.01
298.15	4.15
303.15	4.29
308.15	4.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is a modification of that used by Morrison and Billett (1) and others (2). The degassed solvent is saturated with gas as it flows down a glass helix containing the gas. The amount of solvent passed down the helix was such that 10 to 25 cm³ of gas was absorbed.

Degassing. The solvent is placed in a large continuously evacuated bulb until the solvent boils freely without further release of dissolved gases.

Saturation. The solvent is flowed in a thin film down the glass helix containing the gas. The volume of gas absorbed is measured on an attached buret system.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Gas from commercial cylinders purified over activated charcoal at liquid air temperature. Impurities estimated to be less than 0.3 per cent.
- (2) 1,3-Dimethylbenzene (m-Xylene). Source not given. Distilled immediately before use.

ESTIMATED ERROR:

 $\delta T/K = 0.05$

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033; Ibid. <u>1952</u>, 3819.
- Clever, H. L.; Battino, R.;
 Saylor, J. H.; Gross, P. M.
 J. Phys. Chem. <u>1957</u>, 61, 1078.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Dimethylbenzene or xylene; C₈H₁₀; [1330-20-7] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	3.99	7.300	7.834
298.15	4.12	7.499	8.185

The compiler assumed the dimethylbenzene was a mixture of 40 per cent 1,3-dimethylbenzene, and 20 per cent each of 1,2-dimethylbenzene, 1,4-dimethylbenzene, and ethylbenzene. See Riddick, J. A.; Bunger, W. B. Organic Solvents 3rd Ed., Wiley-Interscience, New York, 1970, p. 614.

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Dimethylbenzene. No information.

ESTIMATED ERROR:

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

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

- (1) Hydrogen; H₂; [1333-74-0]

EVALUATOR:

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

1980, September

CRITICAL EVALUATION:

The system has often been used as a model system in hydrogenation studies. In spite of the importance of the system, the solubility of hydrogen in $\alpha\text{-methylstyrene}$ is not known with good accuracy. The solubility measurements from three laboratories do not show good agreement.

Polejes (1,2) reports eighteen solubility measurements at atmospheric pressure over the 286.15 to 315.85 K temperature interval in his thesis, and he has published a graph showing the hydrogen solubility obeys Henry's law at 299.8 K (80°F) and hydrogen partial pressures up to 4.83 MPa (700 psia). Ma (3,4) reports eight measurements at atmospheric pressure over the 303.15 to 333.15 K temperature interval in his thesis and he has published the data in a graph showing the solubility of hydrogen in α -methylstyrene and its hydrogenation product cumene and in a 60 per cent α -methylstyrene 40 per cent cumene mixture. Herskowitz, Morita, and Smith (5) report thirty five solubility measurements at atmospheric pressure over the 287.95 to 346.65 K temperature range. Polejes' values are the lowest, and Ma's values are the highest. The range between low and high values as a per cent of the median value of Herskowitz et al. is 30 per cent at 303 K and is 40 per cent at 333 K.

In addition to the measurements above there are two other sets of solubility measurements referenced in the literature which were not available to the <code>solubility series</code>. Ma (3) and Sherwood and Farkas (6) reference solubility data of Farkas which apparently were never published. It is probably safe to assume the data of Farkas have been superseded by those of Ma, since both sets of measurements were made in the same laboratory. Herskowitz <code>et al</code>. reference unpublished data in the Ph.D. thesis of Ali (7), which they state shows a solubility maximum at 328 K (58°C). An attempt to obtain a copy of the Ali data for the <code>solubility series</code> was not successful.

In the opinion of the evaluator there is not enough evidence to justify rejection of any of the three available data sets. The three sets of data are classed as doubtful, but the data of Herskowitz $et\ al$. are preferred for use. Herskowitz $et\ al$. give a smoothing equation for their data as a function of temperature with the solubility in mole cm⁻³. The equation is on their data sheet. If the data of Ali (7) are published they may settle the uncertainty about the system.

References:

- Polejes, J. D. Ph.D. Thesis, University of Wisconsin, Madison, WI, 1959.
- Johnson, D. L.; Saito, H.; Polejes, J. D.; Hougen, O. A. A. I. Chem. Eng. J. 1957, 3, 411.
- Ma, Y. H. Sc.D. Thesis, Massachusetts Institute of Technology, Cambridge, MA, 1967.
- Satterfield, C. N.; Ma, Y. H.; Sherwood, T. K. I. Chem. Eng. Symp. Ser. 1968, No. 28, 22.
- Herskowitz, M.; Morita, S.; Smith, J. M. J. Chem. Eng. Data <u>1978</u>, 23, 227.
- Sherwood, T. K.; Farkas, E. J. Chem. Eng. Sci. 1966, 21, 573.
- Ali, J. K. Ph.D. Thesis, University of Birmingham, Birmingham, UK, 1974.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) (1-Methylethenyl)benzene or α -methylstyrene; C_9H_{10} ; [98-83-9]

ORIGINAL MEASUREMENTS:

Polejes, J. D. Ph. D. thesis, 1959 University of Wisconsin

Distr. Abstr. 1959, 19, 3261.

Thesis Director O. A. Hougen

VARIABLES:

T/K: 286.15 - 315.85 P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempe	rature T/K	Mol Fraction $x_1 \times 10^4$	c _{H2} /mol cm ⁻³ x 10 ⁶
13.0	286.15	2.72	2.11
13.9	287.05	2.73	2.12
18.1	291.25	2.80	2.16
19.0	292.15	2.78	2.14
20.4	293.55	2.78	2.14
25.0	298.15	2.89	2.22
28.0	301.15	2.90	2.22
30.5	303.65	2.95	2.25
31.8	304.95	3.03	2.31
34.0	307.15	2.97	2.26
34.2	307.35	3.01	2.29
35.0	308.15	2.94	2.23
37.5	310.65	2.93	2.22
38.0	311.15	3.06	2.32
40.4	313.55	3.14	2.37
42.0	315.15	3.12	2.35
42.5	315.65	3.11	2.34
42.7	315.85	3.03	2.28

Data read from a large scale figure in the thesis.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a water jacketed flask with magnetic stirrer, a vacuum system, and a gas supply and (2) α-Methylstyrene. gas buret.

The solvent was degassed by pumping for twice the time for gas bubble evolution to cease. A measured volume of gas was brought into contact with the solvent, the solvent was stirred until there was no more gas uptake.

There was no mention as to whether or not the gas was presaturated with sovent vapor. The amount of solvent was determined by weight.

The mole fraction solubility was fitted to an equation linear in temperature.

Reference 1 shows a figure of hydrogen solubility in α -methylstyrene at 80 °F (299.82 K). The solubility of hydrogen (dm³ H_2 (273.15 K, 1 atm)dm Obeys Warris 122 was to 2 hydrogen obeys Henry's law up to a hydrogen partial pressure of 700 psia. Data for the figure is not in the thesis.

SOURCE AND PURITY OF MATERIALS:

- 1) Hydrogen.

The compiler had a copy of the gas solubility part of the thesis, pp 132 - 139. The materials were not described in that part of the thesis.

ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.05$$

REFERENCES:

1. Johnson, D. L.; Saito, H.; Polejes, J. D.; Hougen, O. A. A. I. Chem. Eng. J. 1957, 3, 411.

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Ma, Y. H. Sc. D. thesis, 1967 (2) (1-Methylethenyl)benzene or Massachusetts Institute of Technology α-methylstyrene; C₉H₁₀; Satterfield, C. N.; Ma, Y. H.; Sherwood, T. K. I. Chem. E. Symp. Ser. 1968, No. 28, [98-83-9] VARIABLES: PREPARED BY: T/K: 303.15 - 333.15 P/kPa: 101.325 (1 atm)

EXPERIMENTAL VALUES:

Temperature		Henry's Constant	$C_{\rm H_2}/\rm mol~cm^{-3}~x~10^6$	Mol Fraction
t/°C	T/K	cm³ atm mol-1 H2		x ₁ × 10 4
30	303.15	3.37 x 10 ⁵ 3.42 x 10 ⁵	2.97 2.92	3.89 3.83
40	313.15	2.97×10^{5} 3.03×10^{5}	3.37 3.30	4.46 4.37
50	323.15	2.82 x 10 ⁵ 2.83 x 10 ⁵ 2.87 x 10 ⁵	3.55 3.53 3.48	4.74 4.72 4.65
60	333.15	2.75×10^5	3.64	4.91

The compiler read the Henry's constant values from a large scale graph in the thesis. The same graph appears in the cited paper as figure 2.

Henry's law was of the form $p/\text{atm} = \text{K c}_{\text{H}_2}/\text{mol H}_2 \text{ cm}^{-3} \text{ solvent.}$

The values of the concentration of hydrogen and mole fraction hydrogen at one atm partial pressure were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a waterjacketted flask with a magnetic stirrer, a vacuum system, a gas supply, (2) α -Methylstyrene. and a monometer system to maintain constant pressure.

Between 150 and 200 cm3 of solvent is degassed in the flask by stirring and vacuum pumping for three to four times the time for gas bubble evolution to cease.

Gas is admitted to 1 atm total pressure and maintained at 1 atm while the gas dissolves.

The saturated liquid is sampled four times at $15\ \mathrm{m}$ intervals with a gas tight syringe. Twenty microliter samples of liquid are analyzed for hydrogen in a gas chromatograph with a seven foot 5 A molecular sieve packed column. The column is kept at 100 °C, the carrier gas is nitrogen, and a thermal conductivity detector is used. The apparatus is calibrated with samples of known H2 concentration

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen.

The compiler had a copy of the gas solubility part of the thesis, pp. 72 - 77, and 99. The materials were not described on those pages.

H. L. Clever

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

 $\delta x_1/x_1 = 0.05$

- (1) Hydrogen; H₂; [1333-74-0]
- (2) (1-Methylethenyl)benzene or α -methylstyrene; C_9H_{10} ; [98-83-9]

ORIGINAL MEASUREMENTS:

Herskowitz, M.; Morita, S.; Smith, J. M.

J. Chem. Eng. Data 1978, 23, 227-228.

VARIABLES: T/K: 287.95 - 346.65 P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

	rature	Hydro	gen So	lubili	ty, c _H	2/mol	$cm^{-3} \times 10^{6}$		
t/°C	T/K					· 4		Av.	Std.Dev.
14.8	287.95	2.39	2.43	2.45	2.43			2.425	0.025
33.8	306.95	2.74	2.74	2.78	2.78	2.70		2.748	0.033
41.0	314.15	2.79	2.86	2.82	2.83	2.88		2.836	0.035
48.5	321.65	3.08	3.10	3.06	3.06	3.08	3.04	3.070	0.021
58.5	331.65	3.09	3.12	3.09	3.16	3.11	3.09	3.110	0.028
65.5	338.65	3.18	3.17	3.16	3.16	3.16		3.166	0.009
73.5	346.65	3.29	3.26	3.24	3.27			3.265	0.021

The authors applied a linear regression to their data to obtain the equation $c_{\rm H_2/mol\ cm^{-3}} = (2.26 + 0.0145 t/^{\circ}C) \times 10^{-6}$

for the solubility of hydrogen in α-methyl styrene at a hydrogen partial pressure of 101.325 kPa (1 atm) between the temperatures of 15 and 74 $^{\circ}$ C with a stanard deviation of 0.064 x 10⁻⁶. The compiler calculated the average solubilities in the table below.

-				
	T/K	Mol Fraction	n Bunsen	Ostwald
		4	Coefficient	Coefficient
		$x_1 \times 10^4$	α	L
	287.95	3.13	0.0544	0.0573
	306.95	3.61	0.0616	0.0692
	314.15	3.76	0.0636	0.0731
	321.65	4.10	0.0688	0.0810
	331.65	4.19	0.0697	0.0846
	338.65	4.30	0.0710	0.0880
	346.65	4.47	0.0732	0.0929

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was saturated with H2 at atmospheric pressure by bubbling the gas through the solvent for at least 10 hours. Saturation was approached from both under- and oversaturation.

The saturated solution samples were analyzed on a gas chromatograph. Thirty microliter samples of H2 saturated solvent were analyzed for H₂ in a gas chromatograph using a 6 m long, 0.63 cm OD diameter column Packed with 20-40 mesh 5A molecular sieve particles, with nitrogen as the Carrier gas. The apparatus was calibrated with a hydrogen + nitrogen mixture of known composition.

Other solvent names: Isopropenylbenzene 2-Phenyl-1-propene

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Liquid Carbonic Corp. Stated purity 99.99 per cent.
- (2) (1-Methylethenyl)benzene. Dow Chemical Co. Stated purity was 99.2 per cent.

ESTIMATED ERROR:

 $\delta T/K = 0.1$ $\delta c/c = 0.03$

- (1) Hydrogen; H₂; [1333-74-0]
- (2) (1-Methylethyl)-benzene or cumene; C₉H₁₂; [98-82-8]

ORIGINAL MEASUREMENTS:

Ma, Y. H.

Sc. D. thesis, <u>1967</u>

Massachusetts Institute of Technology

Satterfield, C. N.; Ma, Y. H.; Sherwood, T. K.

I. Chem. E. Symp. Ser. 1968, No. 28, 22 - 29.

VARIABLES:

T/K: 303.15 - 333.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temp	erature	Henry's Constant	$C_{\rm H_2}/\rm mol~cm^{-3}~x~10^6$	Mol Fraction
t/°C	T/K	cm³ atm mol-1 H ₂		x_1 × 10 4
25	298.15	3.12×10^{5} 3.10×10^{5}	3.21 3.16	4.50 4.43
30	303.15	2.90×10^{5}	3.45	4.86
40	313.15	2.65×10^{5} 2.68×10^{5}	3.77 3.73	5.36 5.31
50	323.15	2.53×10^{5} 2.58×10^{5}	3.95 3.88	5.68 5.58
60	333.15	2.44 x 10 ⁵	4.10	5.95

The compiler read the Henry's constant values from a large scale graph in the thesis. The same graph appears in the cited paper as figure 2.

Henry's law was of the form $p/atm = K c_{H_2}/mol H_2 cm^{-3}$ solvent.

The values of the concentration of hydrogen and mole fraction hydrogen at one atm partial pressure were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The apparatus consists of a waterjacketted flask with a magnetic stirrer, a vacuum system, a gas

stirrer, a vacuum system, a gas supply, and a monometer system to maintain constant pressure. Between 150 and 200 cm³ of solvent

Between 150 and 200 cm³ of solvent is degassed in the flask by stirring and vacuum pumping for three to four times the time for gas bubble evolution to cease.

Gas is admitted to 1 atm total pressure and maintained at 1 atm while the gas dissolves.

The saturated liquid is sampled four times at 15 m intervals with a gas tight syringe. Twenty microliter samples of liquid are analyzed for hydrogen in a gas chromatograph with a seven foot 5 A molecular sieve packed column. The column is kept at 100°C, the carrier gas is nitrogen, and a thermal conductivity detector is used. The apparatus is calibrated with samples of known H₂ concentration.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen.
- (2) Cumene.

The compiler had a copy of the gas solubility part of the thesis, pp. 72 - 77, and 99. The materials were not described on those pages.

ESTIMATED ERROR:

 $\delta T/K = 0.1$ $\delta x_1/x_1 = 0.05$

- (1) Hydrogen; H₂; [1333-74-0]
- (2) (1-Methylethenyl)benzene or α-methylstyrene; C₉H₁₀; [98-83-9]; 60 vol %.
- (3) (1-Methylethyl)-benzene or cumene; C₉H₁₂; [98-82-8]; 40 vol %.

ORIGINAL MEASUREMENTS:

Ma, Y. H.

Sc. D. thesis, 1967

Massachusetts Institute of Technology

Satterfield, C. N.; Ma, Y. H.; Sherwood, T. K.

I. Chem. E. Symp. Ser. 1968, No. 28, 22 - 29.

VARIABLES:

303.15 - 333.15 T/K: P/kPa: 101.325 (1 atm)

Cumene/vol %: 40

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Tempe	erature T/K	Henry's Constant cm ³ atm mol ⁻¹ H ₂	C _{H2} /mol cm ⁻³ x 10 ⁶	Mol Fraction $x_1 \times 10^4$
30	303.15	3.04 x 10 ⁵ 3.07 x 10 ⁵	3.29 3.26	4.43 4.39
40	313.15	2.79×10^{5} 2.84×10^{5}	3.58 3.52	4.87 4.79
50	323.15	2.63×10^{5}	3.80	5.23
60	333.15	2.59×10^{5}	3.86	5.36

The compiler read the Henry's constant values from a large scale graph in the thesis. The same graph appears in the cited paper as figure 2.

Henry's law was of the form $p/atm = K c_{H_2}/mol H_2 cm^{-3}$ solvent.

The values of the concentration of hydrogen and mole fraction hydrogen at one atm partial pressure were calculated by the compiler.

The solvent is 60 vol $% \alpha$ -methylystyrene, 40 vol $% \alpha$ -cumene. Assuming no volume change on mixing the solution is 0.617 mole fraction α -methylstyrene.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus consists of a waterjacketted flask with a magnetic stirrer, a vacuum system, a gas supply, (2) α -Methylstyrene. and a monometer system to maintain constant pressure.

Between 150 and 200 cm3 of solvent is degassed in the flask by stirring and vacuum pumping for three to four times the time for gas bubble evolution to cease.

Gas is admitted to 1 atm total pressure and maintained at 1 atm while the gas dissolves.

The saturated liquid is sampled four times at 15 m intervals with a gas tight syringe. Twenty microliter samples of liquid are analyzed for hydrogen in a gas chromatograph with a seven foot 5 A molecular sieve Packed column. The column is kept at 100°C, the carrier gas is nitrogen, and a thermal conductivity detector is used. The apparatus is calibrated with samples of known H2 concentration.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen.
- (3) Cumene.

The compiler had a copy of the gas solubility part of the thesis, pp. 72 - 77, and 99. The materials were not described on those pages.

ESTIMATED ERROR:

$$\delta T/K = 0.1$$

$$\delta x_1/x_1 = 0.05$$

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Cukor, P.M.; Prausnitz, J.M.
<pre>2. Benzene, 1,1'-methylenebis-, (Diphenylmethane); C₁₃H₁₂; [101-81-5]</pre>	J. Phys. Chem. <u>1972</u> , 76,598-601.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES:	1
	.a b
T/K Henry's Consta /atm	int ^a Mole fraction of ^b hydrogen in liquid
/ d clii	w _{H2}
	112
300 3464 325 3020	0.0002886 0.0003311
350 2644	0.0003782
375 2322	0.0004306
400 2048 425 1813	0.0004882 0.0005515
450 1610	0.0006211
475 1436	0.0006963
a. Quoted in supplementa paper.	ary material for original
	er for a partial pressure
of 1 atmosphere.	it for a partial pressure
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric apparatus similar to	
that described by Dymond and	
Hildebrand (1). Pressure measured	No details given.
with a null detector and precision gauge. Details in ref. (2)	
J	
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.05; \ \delta x_{H_2} = \pm 2\%.$
	REFERENCES:
	1. Dymond, J.; Hildebrand, J.H. Ind. Eng. Chem. Fundam. 1967, 6, 130.
	2. Cukor, P.M.; Prausnitz, J.M. Ind. Eng. Chem. Fundam. 1971,10, 638.

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Krauss, W.; Gestrich, W. 1. 1,2,3,4- Tetrahydronaphthalene, 2. Chem. Tech. (Heidelberg), 1977, 6, 35-37. $(Tetralin); C_{10}H_{12}; [119-62-2]$ VARIABLES: PREPARED BY: C.L. Young Temperature EXPERIMENTAL VALUES: Mole fraction of Solubility */ mol dm-3 bar-1 T/K hydrogen in liquid, $x_{\rm H_2}$ 0.0014 0.00019 283.15 293.15 0.00165 0.000225 0.000254 303.15 0.00185 313.15 0.00200 0.000277 read off graph, the equations given in the original paper appear to be in error. § calculated by compiler for a partial pressure of 101.325 kPa. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Stirred equilibrium cell. Volumetric apparatus in which a known volume of gas was added No details given. to a known volume of liquid and the equilibrium pressure measured. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.05$; $\delta x_{H_2} = \pm 10^{-5}$ (estimated by compiler) REFERENCES:

COMPONENTS:

(1) Hydrogen; H₂; [1333-74-0]

(2) Alcohols

EVALUATOR:

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

1980, September

CRITICAL EVALUATION:

An Evaluation of the Mole Fraction Solubility of Hydrogen in Alcohols at a Hydrogen Partial Pressure of 101.325 kPa (1 atm).

The solubility of hydrogen in alcohols from papers that report the solubility at 200 kPa pressure or less is evaluated in this section. For the compilation and evaluation of the solubility of hydrogen in alcohols from paper that report the solubility at pressures greater than 200 kPa see a later section of the volume.

Most of the solubility measurements evaluated in this section were made at a total pressure near 101.325 kPa (1 atm). Mole fraction solubility values were calculated at a hydrogen partial pressure of 101.325 kPa assuming the gas to be ideal, Henry's law to be obeyed, and the Ostwald coefficient to be independent of pressure. The assumptions probably introduce errors that are less than the experimental error of the solubility measurement.

Hydrogen + Methanol [67-56-1]

Just (1) reported solubility measurements at 293.15 and 298.15 K and Katayama and Nitta (2) reported five measurements between the temperatures of 213.15 and 298.15 K. At 298.15 K Just's mole fraction solubility is 3 per cent greater than Katayama and Nitta's. Although both sets of data are classed as tentative the thermodynamic changes and smoothed solubility values below are based on a linear regression of the Katayama and Nitta data.

The equation for use over the 213.15 to 298.15 K range is

$$\ln x_1 = -7.3644 - 4.0838/(T/100K)$$

with a standard error about the regression line of 8.45×10^{-7} .

The temperature independent thermodynamic changes for the transfer of one mole of hydrogen from the gas at a hydrogen partial pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 3.395 and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -61.2.

The smoothed solubility values and the Gibbs energy of solution are given in Table 1.

Table 1. Solubility of hydrogen in methanol at a hydrogen partial pressure of 101.325 kPa. Tentative values of mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	ΔG°/kJ mol ⁻¹
213.15 223.15 233.15 243.15 253.15 263.15 273.15	0.932 1.016 1.10 1.18 1.26 1.34	16.447 17.059 17.671 18.283 18.896 19.508 20.120
283.15 288.15 293.15 298.15	1.50 1.5 1.57 1.61	20.733 21.039 21.345 21.651

The single datum of Makranczy et al. (7) is several per cent lower than the smoothed solubility values and is classified as doubtful. Hydrogen + Ethanol [64-17-5]

There are five papers on the solubility of hydrogen in ethanol. The early work of Carius (3) is mostly of historical interest. Only his solubility value at 274.15 K agrees with the results of modern day work. His values at the other temperatures up to 296.85 K are low and show an incorrect sign of the temperature coefficient of solubility. The data should be rejected. Just's (1) two values of 293.15 and 298.15 K are about five per cent greater than modern values and are classed as doubtful.

The measurements of Maxted and Moon (4), Katayama and Nitta (2), and Cargill (5) are in good agreement. The total of nineteen solubility values over the 213.15 to 333.15 K temperature interval from the three papers were combined in a linear regression to obtain the equation

$$\ln x_1 = -7.0155 - 4.3918/(T/100K)$$

with a standard error about the regression line is 2.04×10^{-6} . A three constant equation shows no improvement in the standard error.

The temperature independent thermodynamic changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at a partial pressure of 101.325 to the infinitely dilute solution are

$$\Delta \overline{H}_{?}^{\circ}/kJ \text{ mol}^{-1}$$
 3.65, and $\Delta \overline{S}_{?}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -58.3.

The smoothed values of mole fraction solubility and Gibbs energy of solution are in Table 2.

Table 2. The solubility of hydrogen in ethanol at a hydrogen partial pressure of 101.325 kPa.

The recommended mole fraction solubility and partial molar Gibbs energy of solution as a function of temperature.

T/K	Mole Fraction* 10 4x 1	ΔGγ/kJ mol ⁻¹
213.15 223.15 233.15 243.15 253.15 263.15 273.15	1.14 ₅ 1.25 1.36 ₅ 1.47 ₅ 1.58 ₅ 1.69 1.80	16.084 16.668 17.251 17.834 18.417 19.001
283.15 288.15 293.15 298.15 303.15	1.905 1.955 2.005 2.065 2.11	20.167 20.459 20.751 21.042 21.334
313.15 323.15 333.15	2.21 2.30 2.40 ⁵	21.917 22.501 23.084

 $^{^{\}star}$ Mole fraction values rounded to 0.005 x 10 $^{-\star}$

The single datum of Makranczy $et\ al.$ (7) is several per cent lower than the smoothed solubility values and is classified as doubtful.

Hydrogen + 1-Propanol [71-23-8]

Katayama and Nitta (2) have reported solubility measurements on the hydrogen + 1-propanol system. A linear regression of their five measurements over the 213.15 to 298.15 K temperature interval gives the equation

$$\ln x_1 = -6.9745 - 4.1646/(T/100K)$$

With a standard deviation about the regression line of 2.17 x 10^{-6} .

The single datum of Makranczy $et\ al.$ (7) is in reasonable agreement with the data in table 3.

The temperature independent thermodynamic changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at a hydrogen partial pressure of 101.325 to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 3.46, and $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -58.0.

The smoothed values of mole fraction solubility and Gibbs energy of solution are in Table 3.

Table 3. The solubility of hydrogen in 1-propanol at a hydrogen partial pressure of 101.325 kPa. Tentative values of the mole fraction solubility and partial molar Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \bar{G}_1^{\circ}/kJ \text{ mol}^{-1}$
213.15	1.33	15.823
223.15	1.45	16.403
233.15	1.57	16.983
243.15	1.69	17.562
253.15	1.81	18.142
263.15	1.92	18.722
273.15	2.04	19.302
283.15	2.15	19.882
288.15	2.20	20.172
293.15	2.26	20.462
298.15	2.31	20.752

Hydrogen + 2-Propanol [67-63-0]

Puri and Ruether (6) measured the solubility of hydrogen in mixtures of acetone and 2-propanol at 298.15 K and a total pressure of approximately $10^5 \mathrm{Pa}$. Their Ostwald coefficient measured for hydrogen and pure 2-propanol converts to a mole fraction solubility at 101.325 kPa of 2.66 x 10^{-4} . The value is classed as tentative.

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

Katayama and Nitta (2) report five solubility measurements over the 213.15 to 298.15 K temperature interval, and Makranczy, Rusz, and Balog-Megyery (7) report one measurement at 298.15 K. The two values at 298.15 K agree within 1.5 per cent. The data are classed as tentative.

The six measurements from the two papers were combined in a linear regression to obtain the equation for the 213.15 to 298.15 K temperature interval of

$$\ln x_1 = -6.9350 - 3.8994/(T/100K)$$

with a standard error about the regression line of 2.65×10^{-6} .

The temperature independent thermodynamic changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas phase at a hydrogen partial pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 3.24, and $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$ -57.7.

The smoothed values of the mole fraction solubility and the partial molar Gibbs energy of solution are in Table 4.

Table 4. Solubility of hydrogen in 1-butanol at a hydrogen partial pressure of 101.325 kPa. Tentative values of the mole fraction solubility and partial molar Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction 10 4 x 1	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
213.15 223.15 233.15 243.15 253.15 263.15 273.15	1.57 1.70 1.83 1.96 2.09 2.22 2.34	15.528 16.104 16.681 17.258 17.834 18.411
283.15 288.15 293.15 298.15	2.46 2.52 2.58 2.64	19.564 19.852 20.141 20.429

Hydrogen + 1-Pentanol [71-41-0]

Just (1) has reported solubility measurements on the hydrogen + 1-pentanol system. On comparison of Just's two values of 293.15 and 298.15 K with the solubility of hydrogen in alcohols of similar molecular weight, Just's values appear to be smaller than expected. The values are classed as doubtful.

The datum of Makranczy et al. (7) appears to be more in line with data on both lower and higher alcohols and is classified as tentative.

Hydrogen + 1-Hexanol [111-27-3]

The value of Makranczy $et \ al.$ (7) for this system appears to be in line with data on both lower and higher alcohols and is classified as tentative.

Hydrogen + 1-Heptanol [111-70-6] Hydrogen + 1-Octanol [111-87-5]

The mole fraction solubility data at 298.15 K of Makranczy $et\ al.$ (7) are considerably lower than those of Ijams (8). The former are classified as tentative and the latter as doubtful.

Hydrogen + 1-Nonanol [143-08-8] Hydrogen + 1-Decanol [112-30-1] Hydrogen + 1-Undecanol [112-42-5] Hydrogen + 1-Dodecanol [112-53-8]

Makranczy et al. (7) measured the solubility of hydrogen at 298.15 K in each of the above systems. The results are classified as tentative.

Hydrogen + Cyclohexanol [108-93-0]

Cauquil (9) and Kruyer and Nobel (10) each report one value of the solubility of hydrogen in this system. There is a twofold difference in the two values with the Cauquil value being the higher value. Both Values are classed as doubtful. However, comparison of the trends in the solubility of helium and neon in cyclohexanol and aliphatic alcohols of similar molecular weight definitely indicate the lower value of Kruyer and Nobel should be preferred.

References:

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342.
- 2. Katayama, T.; Nitta, T. *J. Chem. Engng. Data.* <u>1976</u>, *21*, 194.
- 3. Carius, L. Justus Liebigs Ann. Chem. 1855, 94, 129.
- 4. Maxted, E. B.; Moon, C. H. Trans. Faraday Soc. 1936, 32, 769.
- 5. Cargill, R. W. J. Chem. Soc., Faraday Trans. I 1978, 74, 1444.
- 6. Puri, P. S.; Ruether, J. A. Can. J. Chem. Eng. 1974, 52, 636.
- Makranczy, J.; Rusz, L.; Balog-Megyery, K. Hung. J. Ind. Chem. 1979, 7, 41.
- 8. Ijams, C. C. Ph.D. Thesis, Vanderbilt University, Nashville, TN, 1941.
- 9. Cauquil, G. J. Chim. Phys. 1927, 24, 53.
- 10. Kruyer, S.; Nobel, A. P. P. Rec. Trav. Chim. 1961, 80, 1145.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Methanol; CH₃OH; [67-56-1] Z. Phys. Chem. 1901, 37, 342 - 367.

VARIABLES:

T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²	
293.15	1.52	8.401	9.016	
298.15	1.57	8.657	9.449	

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Methanol. No information.

ESTIMATED ERROR:

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

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

COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Katayama, T.; Nitta, T. 2. Methanol; CH₄O; [67-56-1] J. Chem.Engng.Data.1976, 21,194-6 VARIABLES: PREPARED BY: Temperature C.L. Young

T/K	Ostwald coefficient,L	Henry's Constant /atm	Mole fraction * of hydrogen in liquid, $^x{\rm H}_2$
298.15	0.0975	6160	0.000162
273.15	0.0973	7110	0.000141
		· -	
253.15	0.0675	7960	0.000126
233.15	0.0557	9090	0.000110
213.15	0.0442	10710	0.0000934

^{*} at a partial pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Volumetric apparatus with equilibrium cell of approximately 0.08 litres. Magnetic stirrer. Solvent carefully degassed. Equilibrium established in 1-1.5 hours. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Takachiho Chemical Industry Co. sample, purity 99.99 mole per cent.
- Nakarai Chemicals sample, purity
 99.9 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.12$ at 213.15K, ± 0.05 at other temperatures, $\delta x_{H_2} = \pm 1.5\%$

REFERENCES:

1. Nitta, T.; Tatsuishi. A.;

Katayama, T. J. Chem. Eng. Jpn. 1973,

6,475.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Makranczy, J.; Rusz, L.; Balog-Megyery, K.
2. Methanol; CH ₄ O; [67-56-1]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6
!	
VARIABLES:	PREPARED BY:
	C.L. Young
EXPERIMENTAL VALUES:	
T/K P^+ /kPa Ostwald coe	efficient Mole fraction of hydrogen*, $x_{ m H_2}$
298.15 101.3 0.09	17 0.000153
* calculated by compi	ler
+ partial pressure of	hydrogen
	•
_	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1) was used.	No details given.
	ESTIMATED ERROR:
	$\delta x_{\rm H_2} = \pm 3\%$
	DEEE DEMCKS.
	REFERENCES: 1. Bodor, E.; Bor, Gy.; Mohai, B.;
	Sipos, G. Veszpremi Vegyip. Egy. Kozl.
	1957, 1, 55. Chem. Abstr. 1961, 55, 3175h
	01.0m. ND001. 1001, 00, 31/311

COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Carius, L. (2) Ethanol; C₂H₆O; [64-17-5] Justus Liebigs Ann. Chem. 1855, 94, 129 - 166. Also known as Ann. Chem. Pharm. VARIABLES: PREPARED BY: 274.15- 296.85 101.325 (1 atm) T/K: P/kPa: M. E. Derrick H. L. Clever EXPERIMENTAL

L	VALUES:				
		T/K	Mol Fraction	Bunsen	Ostwald
			_	Coefficient	Coefficient
			$x_1 \times 10^4$	$\alpha \times 10^2$	$L \times 10^2$
		274.15	1.764	6.916	6.941
		278.15	1.754	6.847	6.972
		284.55	1.752	6.765	7.05
		287.55	1.741	6.726	7.08
		293.05	1.736	6.668	7.15
		296.85	1.734	6.633	7.21

The mole fraction and Ostwald coefficient values were calculated by the compiler.

The values above are not recommended. The value at 274.15 K agrees well with the recent work of Katayama and Nitta (See data sheet). The other values appear to be low and of the wrong temperature coefficient.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and method of Bunsen (1) were used.

The apparatus consists of an absorption tube sealed at the low end with a rubber plate, and a water jacket.

The gas is placed in the absorption tube, and its pressure, temperature, and volume determined. The solvent is added, and the system shaken until the volume no longer changes. Final temperature, pressure and volume measurements are made.

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared from the reaction of zinc and dilute sulfuric acid.
- (2) Ethanol. Absolute alcohol. Specific gravity 0.792 at 20 °C.

ESTIMATED ERROR:

REFERENCES:

1. Bunsen, R. W.

Justus Liebigs Ann. Chem. 1855,
93, 1.

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0]

(2) Ethanol; C₂H₆O; [64-17-5]

ORIGINAL MEASUREMENTS:

Just, G.

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

VARIABLES:

T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²	
293.15	2.09	8.032	8.620	
298.15	2.14	8.186	8.935	

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Ethanol. No information.

ESTIMATED ERROR:

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

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

196	Hydrogen Solubilities up to 200kPa		
COMPONENTS: 1. Hydrogen; H ₂ ; [1333-74-0] 2. Ethanol; C ₂ H ₆ O; [64-17-5]		ORIGINAL MEASUREMENTS: Maxted, E.B.; Moon, C.H.; Trans. Faraday Soc. 1936, 32, 769-75.	
VARIABLES:		DDEDARED BY	
Temperature		PREPARED BY: C.L. Young	
EXPERIMENTAL VALUES:		L	
т/к	Bunsen coefficier a	Mole fraction of hydrogen, $x_{ m H_2}$	
273.75 283.15 293.45 298.15 303.15 313.15 313.95 323.15	283.15 0.0737 0.000190 293.45 0.0769 0.000200 298.15 0.0784 0.000205 303.15 0.0802 0.000211 313.15 0.0840 0.000223 313.95 0.0839 0.000223		
	AUXILIARY	INFORMATION	
METHOD: /APPARATUS PROCEDUR	Æ:	SOURCE AND PURITY OF MATERIALS:	
Volumetric apparatus with rocking absorption cell. Details in source.		 Electrolytic grade. Degassed, high purity sample, no 	

Degassed, high purity sample, no other details given.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \delta x_{H_2} = \pm 1%.$

(estimated by compiler.)

Organic Compounds Containing Oxygen 197 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-75-0] Katayama, T.; Nitta, T. J. Chem. Engng. Data. 1976, 21, 194-6. Ethanol; C₂H₆O; [64-17-5] VARIABLES: PREPARED BY: C.L. Young. Temperature. EXPERIMENTAL VALUES:

т/к	Ostwald coefficient, L	Henry's Constant /atm	Mole fraction of hydrogen in liquid, $^{\omega}_{ m H_2}$
			
293.15	0.0852	4900	0.000204
273.15	0.0696	5640	0.000177
253.15	0.0580	6400	0.000156
233.15	0.0480	7270	0.000138
213.15	0.0372	8750	0.000114

* at a partial pressure of 1 atmosphere.

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Volumetric apparatus with equilibrium cell of approximately 0.08 litres. Magnetic stirrer. Solvent carefully degassed. Equilibrium established in 1-1.5 hours. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

- 1. Takachiho Chemical Industry Co. sample, purity 99.99 mole per cent.
- 2. Nakarai Chemicals sample, purity 99.9 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.12$ at 213.15K, \pm 0.05 at other temperatures; $\delta x_{\rm H_2} = \pm 1.5\%$

REFERENCES:

1.Nitta, T.; Tatsuishi, A.; Katayama, T.; J. Chem. Eng. Jpn. 1973, 6,475.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Ethanol; C₂H₆O; [64-17-5]

ORIGINAL MEASUREMENTS:

Cargill, R. W.

J. Chem. Soc., Faraday Trans. I 1978, 74, 1444 - 1456.

VARIABLES:

T/K: 278.9 - 333.2 P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

T/K	104 T-1	S _O /cm³kg ⁻¹	Mol Fraction	Bunsen	Ostwald
			x ₁ _x 10 ⁴	Coefficient a x 10 ²	Coefficien L x 10 ²
278.9	35.87	91.6	1.88	7.34	7.49
289.2	34.59	96.4	1.98	7.64	8.09
299.2	33.43	100	2.055	7.84	8.59
309.2	32.35	106	2.18	8.2	9.3
320.2	31.24	111	2.28	8.5	10.0
333.2	30.02	115	2.36	8.7	10.6

The mole fraction, Bunsen coefficient, and Ostwald coefficient values were calculated by the compiler.

The solubility, $S_{\text{O}},$ calculated as $\text{cm}^3\,(273.15~\text{K},~101.325~\text{kPa}~(1~\text{atm}))$ hydrogen per kg of solvent.

AUXILIARY INFORMATION .

METHOD/APPARATUS/PROCEDURE:

Absorption of gas by a thin film of liquid. The Morrison and Billett (1) method was modified by replacing valve A with a constant flow pump and by measuring the mass of the solvent leaving the absorption tube (instead of the volume) on a top-pan balance.

The solvent is degassed using the vapor pump principle (1). Each determination absorbs about 20 cm³ of gas in up to 500 cm³ of solvent.

SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. British Oxygen Co. Gas 99.9 per cent pure, stored over saturated brine.
- (2) Ethanol. Absolute alcohol. Sample was 0.98 mole fraction alcohol, 0.02 mole fraction water.(ea. 0.8 wt per cent water).

ESTIMATED ERROR:

T/K = 0.1 P/mmHq = 0.5

Solubilities reproducible within 0.5 per cent.

REFERENCES:

Morrison, T. J.; Billett, F. J. Chem. Soc. 1948, 2033; 1952, 3819.

COMPONENTS:	ORIGINAL MEASUREMENTS:			
1. Hydrogen; H ₂ ; [1333-74-0	Makranczy, J.; Rusz, L.;			
2. Ethanol; C ₂ H ₆ O; [64-17-5]	Balog-Megyery, K.			
2. Hendholy 621160, [61 1, 6]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6.			
VARIABLES:	PREPARED BY:			
Į ,	C.L. Young			
EXPERIMENTAL VALUES:				
T/K P ⁺ /kPa Ostwald coef:	ficient Mole fraction of hydrogen*, $x_{ m H_2}$			
298.15 101.3 0.0768	0.000184			
258.13 101.3	0.000104			
* calculated by compi	ler			
+ partial pressure of				
partial pressure or	nyarogen.			
	j			
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
Volumetric method. The apparatus of] We start and			
Bodor, Bor, Mohai, and Sipos (1) was used.	No details given.			
	ESTIMATED ERROR:			
	$\delta x_{\rm H_2} = \pm 3\%$			
	Н2			
	REFERENCES:			
	1. Bodor, E.; Bor, Gy.; Mohai, B.;			
	Sipos, G. Veszpremi Vegyip. Egy. Kozl.			
	1957, 1, 55. Chem. Abstr. 1961, 55,3175h.			

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Katayama, T.; Nitta, T.
2. l-Propanol; C ₃ H ₈ O; [71-23-8]	J. Chem. Engng. Data. 1976,21,194-6
VARIABLES: Temperature	PREPARED BY: C.L. Young
DVDEDTMENTAL WAY HEE.	

EXPERIMENTAL VALUES:

T/K	Ostwald coefficient, L	Henry's Constant /atm	Mole fraction* of hydrogen in liquid, $^{x}{ m H}_{2}$
298.15	0.0763	4270	0.000234
273.15	0.0615	4970	0.000201
253.15	0.0520	5550	0.000180
233.15	0.0426	6360	0.000157
213.15	0.0336	7510	0.000133

^{*} at a partial pressure of 1 atmosphere

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

Volumetric apparatus with equilibrium cell of approximately 0.08 litres. Magnetic stirrer. Solvent carefully degassed. Equilibrium established in 1-1.5 hours. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

- Takachiho Chemical Industry Co. sample, purity 99.99 mole per cent.
- Nakarai Chemicals sample, distilled, purity 99.9 mole per cent.

ESTIMATED ERROR:

 δ T/K = ±0.12 at 213.15K; ±0.05 at other temperatures; $\delta x_{\rm H_2}$ = ±1.5%

REFERENCES:

Nitta, T.; Tatsuishi. A.;
 Katayama, T. J. Chem. Eng. Jpn. 1973,
 6,475.

COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Makranczy, J.; Rusz, L.; Balog-Megyery, K. 2. 1-Propanol; C₃H₈O; [71-23-8] Hung. J. Ind. Chem. 1979, 7, 41-6. VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: P⁺/kPa Ostwald coefficient Mole fraction of T/K hydrogen*, $x_{\rm H_2}$ 298.15 101.3 0.0742 0.000228 calculated by compiler partial pressure of hydrogen AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric method. The apparatus of No details given. Bodor, Bor, Mohai, and Sipos (1) was used. ESTIMATED ERROR: $\delta x_{\rm H_2} = \pm 3\%$ REFERENCES: Bodor, E.; Bor, Gy.; Mohai, B.; Sipos, G. Veszpremi Vegyip. Egy. Kozl. 1957, 1, 55, Chem. Abstr. 1961, 55, 3175h

COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen, H_2 ; [1333-74-0]] Katayama, T.; Nitta, T. 2. 1-Butanol; C4H10O; [71-36-3] J. Chem. Engng. Data. 1976, 21, 194-6 VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: T/K Ostwald Henry's Constant Mole fraction* of coefficient,L hydrogen in liquid, /atm $x_{\rm H_2}$

3750

4320

4770

5530

6340

AUXILIARY INFORMATION

METHOD /APPARATUS/PROCEDURE:

298.15

273.15

253.15

233.15

213.15

Volumetric apparatus with equilibrium cell of approximately 0.08 litres. Magnetic stirrer. Solvent carefully degassed. Equilibrium established in 1-1.5 hours. Details in ref. (1).

0.0709

0.0577

0.0493

0.0398

0.0324

SOURCE AND PURITY OF MATERIALS:

1. Takachiho Chemical Industry Co. sample, purity 99.99 mole per cent.

0.000267

0.000231

0.000210

0.000181

0.000158

2. Nakarai Chemicals sample, distilled, purity 99.9 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.12$ at 213.15K; \pm 0.05 at other temperature; $\delta x_{\rm H_2} = \pm 1.5$ %

REFERENCES:

1. Nitta, T.; Tatsuishi. A.; Katayama, T. J. Chem. Eng. Jpn. <u>1973</u>,6, 475.

^{*} at a partial pressure of 1 atmosphere

COMPONENTS:			
1. Hydrogen; H ₂ ; [1333-74-0]	ORIGINAL MEASUREMENTS: Makranczy, J.; Rusz, L.; Balog-		
	Megyery, K.		
2. 1-Butanol; C ₄ H ₁₀ O; [71-36-3]	Hung. J. Ind. Chem. <u>1979</u> , 7, 41-6.		
VARIABLES:			
VARIABLES:	PREPARED BY: C.L. Young.		
EXPERIMENTAL VALUES:			
T/K P ⁺ /kPa Ostwald coe	fficient Mole fraction of hydrogen*, $x_{ m H_2}$		
298.15 101.3 0.069	9 0.000263		
* calculated by comp	iler		
+ partial pressure o	f hydrogen		
	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	INFORMATION SOURCE AND PURITY OF MATERIALS:		
METHOD/APPARATUS/PROCEDURE: Volumetric method. The apparatus of Bodor, Bor, Mohai, and Sipos (1)	SOURCE AND PURITY OF MATERIALS:		

COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) 1-Pentanol; C₅H₁₂O; [71-41-0] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	1.59	3.292	3.533
298.15	1.65	3.397	3.708

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

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

SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) 1-Pentanol. No information.

ESTIMATED ERROR:

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

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

COMPONENTS:			ORIGINAL MEA	SUREMENTS:
1. Hydrogen;	Hydrogen; H ₂ ; [1333-74-0]		Makranczy, J.; Rusz, L.; Balog-Megyery, K.	
2. 1-Pentanol	e. 1-Pentanol; C ₅ H ₁₂ O; [71-41-0] or			
			Hung. J.	Ind. Chem. <u>1979</u> , 7, 41-6.
1-Hexanol;	C ₆ H ₁₄ O; [111-27-3]		
ARIABLES:			PREPARED BY:	
				C.L. Young
~~~~				
XPERIMENTAL VALUI	ES:			
T/K	P ⁺ /kPa	Ostwald coe	efficient	Mole fraction of hydrogen*, $x_{\rm H_2}$
		1-Per	ntanol	
298.15	101.3	0.060		0.000268
		a	-	
298.15	101.3	1-He>	kanol Ro	0.000301
2,0.13	TOT. 2	0.036		0.00001
	* calcula	ated by compi	ller	
	+ partial	l pressure of	hydrogen	
		AUXILIARY	INFORMATION	
ETHOD/APPARATUS/I	PROCEDURE:			PURITY OF MATERIALS:
701				7 1 1 1 1 m 1 1 m
Volumetric met of Bodor, Bor,	nod. The a Mohai, and	apparatus 1 Sipos (1)	No	details given.
as used.				
			1	
	•			
			ESTIMATED E	
			$\delta x_{\mathrm{I}}$	H ₂ = ±3%
			REFERENCES:	
			l. Bodor Sipos Veszpi	E.; Bor, Gy.; Mohai, B.;

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Aliphatic alcohols;  $C_7^H_{16}^O$  and  $C_8^H_{18}^O$

### ORIGINAL MEASUREMENTS:

Ijams, C. C.

Ph.D. thesis, <u>1941</u> Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

### VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

### PREPARED BY:

H.L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
1-	Heptanol; C7H1	6 ⁰ ; [111-70-6]	1
298.15	3.85	0.0607	0.0663
1-	Octanol; C ₈ H ₁₈	0; [111-87-5]	
298.15	3.92	0.0555	0.0606

The mole fraction and Ostwald coefficient values were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified so that small solvent sample (2 cm³) could be used with almost 100 per cent recovery of the solvent.

An improved temperature control system was used.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Aliphatic alcohols. Purified. Vapor pressure and boiling point also reported in the thesis.

### ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

### REFERENCES:

Van Slyke, D. D.
 J. Biol. Chem. 1939, 130, 545.

	NENTS:		ORIGINAL MEASUREMENTS:
1.	Hydrogen;	H ₂ ; [1333-74-0]	Makranczy, J.; Rusz, L.; Balog-Megyery, K.
2.	l-Heptano	l; C ₇ H ₁₆ O; [111-70-6] or	Hung. J. Ind. Chem. 1979, 7, 41-6
	1-Octanol	; C ₈ H ₁₈ O; [111-87-5]	
ARI	ABLES:		PREPARED BY: C.L. Young
			C.D. Todaig
XPE	RIMENTAL VALU	ES:	<u> </u>
	т/к	P ⁺ /kPa Ostwald co	efficient Mole fraction of hydrogen*, $x_{\rm H_2}$
		1-Нер	tanol
	298.15	101.3 0.05	0.000316
		1-0ct	anol
	298.15	101.3 0.05	0.000332
		* calculated by comp	iler
		+ partial pressure o	E hydrogen.
			INFORMATION
метн	OD/APPARATUS,	AUXILIARY	
Vol Bod	umetric me	AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:
Vol Bod	umetric me or, Bor, M	AUXILIARY PROCEDURE: thod. The apparatus of	INFORMATION SOURCE AND PURITY OF MATERIALS:
Vol Bod	umetric me or, Bor, M	AUXILIARY PROCEDURE: thod. The apparatus of	INFORMATION SOURCE AND PURITY OF MATERIALS:
Vol Bod	umetric me or, Bor, M	AUXILIARY PROCEDURE: thod. The apparatus of	INFORMATION SOURCE AND PURITY OF MATERIALS:
Vol Bod	umetric me or, Bor, M	AUXILIARY PROCEDURE: thod. The apparatus of	INFORMATION  SOURCE AND PURITY OF MATERIALS:  No details given.

### 208 Hydrogen Solubilities up to 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Makranczy, J.; Rusz, L.; Balog-Megyery, K. 2. 1-Nonanol; $C_9H_{20}O$ ; [143-08-8] Hung. J. Ind. Chem. 1979, 7, 41-6 or 1-Decanol; C₁₀H₂₂O; [112-30-1] VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: P⁺∕kPa Mole fraction of T/K Ostwald coefficient hydrogen*, $x_{\rm H_2}$ 1-Nonanol 0.000343 0.0480 298.15 101.3 1-Decanol 0.000358 0.0458 298.15 101.3 * calculated by compiler + partial pressure of hydrogen AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric method. The apparatus No details given. of Bodor, Bor, Mohai, and Sipos (1) was used.

ESTIMATED ERROR:

$$\delta x_{\rm H_2} = \pm 3\%$$

### REFERENCES:

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

### Organic Compounds Containing Oxygen COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Makranczy, J.; Rusz, L.; Balog-Megyery, K. 2. 1-Undecanol; C₁₁H₂₄0; [112-42-5] Hung. J. Ind. Chem. 1979, 7, 41-6. 1-Dodecanol; C₁₂H₂₆O; [112-53-8] VARIABLES: PREPARED BY: C.L. Young EXPERIMENTAL VALUES: T/K $P^+/kPa$ Mole fraction of Ostwald hydrogen*, $x_{\rm H_2}$ coefficient 1-Undecanol 298.15 101.3 0.000362 0.0426 1-Dodecanol 298.15 101.3 0.000370 0.0404 * calculated by compiler + partial pressure of hydrogen AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE:

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

### SOURCE AND PURITY OF MATERIALS:

No details given.

### ESTIMATED ERROR:

$$\delta x_{\rm H_2} = \pm 38$$

### REFERENCES:

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

(1) Hydrogen; H₂; [1333-74-0]

(2) Cyclohexanol; C₆H₁₂O; [108-93-0]

ORIGINAL MEASUREMENTS:

Cauquil, G.

J. Chim. Phys. 1927, 24, 53 - 55.

VARIABLES:

PREPARED BY:

T/K: 299.15 P/kPa: 101 - 102 (760-6 (760 - 766 mmHg) P. L. Long H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient L
299.15	3.5	0.075	0.082
	3.6	0.076	0.083

The author reported what the compiler believes is an Ostwald coefficient. The compiler calculated the mole fraction and Bunsen coefficient values.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a flask and a mercury leveling bulb to control the pressure.

The solvent volume was measured, the gas introduced over the solvent, The gas absorbed was found by differnce between the initial and final gas volume.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. No information.
- (2) Cyclohexanol. Source not given. Distilled.

ESTIMATED ERROR:

 $\delta L/L = 0.10$  (compiler)

COMP	COMPONENTS:		ORIGINAL MEASUREMENTS:	
1.	Hydrogen; H,; [13	33-74-0]	Kruyer, S.; Nobel, A.P.P.	
	-		Rec. Trav. Chim. 1961, 80, 1145-56	
/ARI	ABLES:		PREPARED BY:	
			C. L. Young	
XPE	RIMENTAL VALUES:	<del></del>	[a]	
	T/K O	stwald coeffic		
	298.15	0.039	0.000168	
[a]	Calculated by com	piler for a pa	rtial pressure of 101.325 kPa	
[a]	outediated by com		rtial pressure of 101.325 kPa  INFORMATION	
METH	OD/APPARATUS/PROCEDURE:	AUXILIARY	<u> </u>	
METH Tec liq ads out	outediated by com	AUXILIARY saturating a spiral n stripping rgon. The	INFORMATION	
METH Tec liq ads out	OD/APPARATUS/PROCEDURE:  chnique consisted of uid with hydrogen in orption tube and the the hydrogen with a ulting area.	AUXILIARY saturating a spiral n stripping rgon. The	INFORMATION  SOURCE AND PURITY OF MATERIALS:  1. Hydrogen and argon passed through molecular sieve 4A in liquid oxygen and nitrogen trap respectively.	

### 212 Hydrogen Solubilities up to 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Puri, P.S.; Ruether, J.A. 2-Propanone, (Acetone); C3H6O; [67 - 64 - 1]Can. J. Chem. Eng. 1974, 52, 636-640 З. 2-Propanol; C₃H₈O; [67-63-0] VARIABLES: PREPARED BY: Liquid phase composition C.L. Young EXPERIMENTAL VALUES: T/K Mole fraction of Ostwald acetone in liquid, coefficient, L298.15 1.000 0.0943 0.736 0.1016 0.655 0.1038 0.486 0.1038 0.351 0.1023 0.122 0.0920 0.000 0.0845 total pressure approximately 105Pa. AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus similar to that 1. Liquid Carbonic Canadian Corp. described in ref. (1). Degassed sample purity 99.97 mole per cent. solution placed in calibrated dissolution vessel, gas saturated with 2. and 3. Baker Reagent grade.

solvent vapor introduced from calibrated gas buret. Amount of gas dissolved determined from pressure and volume changes.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.01; \delta L = \pm 0.5%.$ (estimated by compiler).

### REFERENCES:

1. Ben-Naim, A.; Baer, S. Trans. Faraday. Soc. 1963, 59, 2735.

COMPONENTS: (1) Hydrogen; H ₂ ; [1333-74-0] (2) Ethers	EVALUATOR:  H. L. Clever Department of Chemistry Emory University Atlanta, GA 30322 USA 1980, September
-------------------------------------------------------------------	---------------------------------------------------------------------------------------------------------

CRITICAL EVALUATION:

An Evaluation of the Mole Fraction Solubility of Hydrogen in Ethers at a Hydrogen Partial Pressure of 101.325 kPa (1 atm).

Most of the solubility measurements evaluated in this section were carried out at a total pressure near 101.325 kPa. The mole fraction solubility values at a hydrogen partial pressure of 101.325 kPa were calculated on the assumption that the following statements are true. The gas is ideal, Henry's law is obeyed, and the Ostwald coefficient is independent of Pressure. The assumptions introduce errors that are probably smaller than the experimental errors of the solubility measurements.

Hydrogen + 1,1'-Oxybisethane or diethyl ether [60-29-7]

Christoff (1) made one measurement at 273.15 K, and Horiuti (2) made six measurements between the temperatures of 192.55 and 294.25 K of the solubility of hydrogen in diethyl ether. Horiuti's value of the mole fraction solubility at 273.15 K is 6.1 per cent greater than Christoff's value.

Both authors work is classed as tentative. However, the work of Horiuti is preferred. Horiuti's mole fraction solubility values show a definite curvature on a log  $x_1$  vs. 1/T plot.

Although the observed curvature may be due to a systematic error in the measurement related to the relatively large vapor pressure of the solvent, the evaluator choses to believe the effect is real and has treated Horiuti's data by a linear regression to obtain the three constant tentative equation for use between 193.15 and 298.15 K.

$$\ln x_1 = -10.3539 + 1.2545/(T/100K) + 2.3384 \ln (T/100K)$$

with a standard error about the regression line of  $4.32 \times 10^{-6}$ .

The three constant equation gives temperature dependent values of the thermodynamic changes of enthalpy and entropy for the transfer of one mole of hydrogen from the gas phase at a partial pressure of 101.325 kPa to the infinitely dilute solution. Values of the thermodynamic changes at several temperatures are given in Table 1. Smoothed values of the mole fraction solubility and the partial molar Gibbs energy of solution as a function of temperature are given in Table 2.

Table 1. Hydrogen + diethyl ether. Changes in enthalpy, entropy and heat capacity for the transfer of one mole of hydrogen from the gas at a partial pressure of 101.325 kPa to the infinitely dilute solution at several temperatures.

T/K	$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$	$\Delta \overline{s}_1^{\circ}/J K^{-1} mol^{-1}$	$\Delta \overline{C}_{p_1}^{\circ}/J K^{-1} mol^{-1}$
223.15	3.30	-51.0	19.4
248.15	3.78	-49.0	19.4
273.15	4.27	-47.1	19.4
298.15	4.75	-45.4	19.4

Table 2.	The solubility of hydrogen in diethyl ether at a hydrogen partial pressure of 101.325.
	Tentative values of the mole fraction
	solubility and partial molar Gibbs energy
	of solution as a function of temperature.

		· · · · · · · · · · · · · · · · · · ·
T/K	Mol Fraction 10 x 1	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
193.15	2.84	13.112
203.15	3.10	13.646
213.15	3.37	14.170
223.15	3.65	14.685
233.15	3.95	15.191
243.15	4.26	15.688
253.15	4.59	16.178
263.15	4.93	16.660
273.15	5.29	17.135
278.15	5.47	17.370
283.15	5.66	17.602
288.15	5.85	17.834
293.15	6.05	18.063
298.15	6.24	18.291

Hydrogen + 1,1'-Oxybispropane or dipropyl ether [111-43-3]

Guerry (3) measured the solubility at temperatures of 293.15 and 298.15 K. The results are classed as tentative.

Hydrogen + 1,4-Dioxane [123-91-1]

Guerry (3) measured the solubility at temperatures of 293.15 and 298.15 K. Krauss and Gestrich (4) measured the solubility at four temperatures between 283.15 and 313.15 K. The mole fraction value of Guerry is 6.5 per cent larger than the Krauss and Gestrich value at 293.15 K. Both sets of data are classed as tentative. However, the tentative equation and smoothed data below are based on a linear regression of only the data of Krauss and Gestrich. The equation for use from 283.15 to 313.15 K is

$$\ln x_1 = -5.7347 - 8.6743/(T/100K)$$

with a standard error about the regression line of  $2.96 \times 10^{-6}$ .

The temperature independent values for the thermodynamic changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at a partial pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 7.21 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -47.7.

Smoothed values of the solubility and partial molar Gibbs energy of solution are in Table 3.

Table 3. Solubility of hydrogen in 1,4-dioxane at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molar Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
283.15 293.15 298.15	1.51 1.68 1.76	20.713 21.190 21.428
303.15 313.15	1.85	21.666 22.143

Hydrogen + Tetrahydrofuran [109-99-9] + 2,3-Dihydropyran [22512-65-6]

+ Tetrahydro-2H-pyran [142-68-7]

Guerry (3) measured the solubility at temperatures of 293.15 and 298.15 K in each of these systems. The results are classed as tentative.

### References:

- 1. Christoff, A. Z. Phys. Chem. 1912, 79, 456.
- 2. Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125.
- 3. Guerry, D. Jr. Ph.D. thesis, Vanderbilt University, Nashville, TN  $\frac{1944}{}$ .
- 4. Krauss, W.; Gestrich, W. Chem.-Tech. (Heidelberg) 1977, 6, 35.

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Christoff, A. (2) 1,1'-Oxybisethane or diethyl Z. Phys. Chem. 1912, 79, 456 - 460. ether; $C_4H_{10}O$ ; [60-29-7]**VARIABLES:** PREPARED BY: T/K: 273.15 M. E. Derrick P/kPa: Atmospheric H. L. Clever

### EXPERIMENTAL VALUES:

т/к	Mole Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
273.15	5.01	11.15	11.15

The author measured the Ostwald coefficient. The total pressure was corrected for the vapor pressure of the solvent at the temperature of the measurement. The compiler calculated the mole fraction and Bunsen coefficient values.

The value is 6.2 per cent lower that the value reported by Horiuti at 273.15 K. The Horiuti value is preferred.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus is a modified Ostwald apparatus described by Just (1), and modified by Skirrow (2). The apparatus consists of a thermostated gas buret and absorption flask.

The modification involves the use of vapor free gas in the gas buret. A correction is made for the vapor pressure of the liquid. A steel capillary tube with a stopcock, which prevents the gas and the liquid vapor ESTIMATED ERROR: mixing in the buret, is used to connect the absorption flask and the buret.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by the reaction of zinc and dilute sulfuric acid.
- (2) Diethyl ether. Merck (Darmstadt). Stated to be pure and anhydrous.

 $\delta L/L = 0.05$ 

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342.
- 2. Skirrow, F. W. Z. Phys. Chem. 1902, 41, 139.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1,1'-Oxybisethane or diethyl ether;  $C_4H_{10}O$ ; [60-29-7]

### ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125 - 256.

### VARIABLES:

T/K: 192.55 - 294.25 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

EXPERIMENTAL	VALUES •			
	T/K	Mol Fraction	Bunsen	Ostwald
		$x_1 \times 10^4$	Coefficient $\alpha \times 10^2$	Coefficient L x 10 ²
	192.55	2.84	7.06	4.98
	213.25	3.34	8.10	6.32
	233.15	3.98	9.37	8.00
	252.05	4.53	10.4	9.64
	273.15	5.335	11.88	11.88
	294.25	6.060	13.08	14.09

The mole fraction and Bunsen coefficient values were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -10.3539 + 1.2545/(T/100K) + 2.3384 \ln (T/100K)$ 

Standard error about the regression line =  $4.32 \times 10^{-6}$ 

T/K	Mol Fraction
	$x_1 \times 10^4$
193.15	2.84
203.15	3.10
213.15	3.37
223.15	3.65
233.15	3.95
243.15	4.26

T/K	Mol Fraction
	$x_1 \times 10^4$
253.15	4.59
263.15	4.93
273.15	5.29
283.15	5.66
293.15	6.05
298.15	6.24

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of Water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. ESTIMATED ERROR: The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption Pipet.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by electrolysis.
- (2) 1,1'-Oxybisethane. Merck's "for analysis". Stored over sodium amalgam and distilled before use. Constant boiling within 0.01 degree.

$$\delta T/K = 0.05$$
  
 $\delta x_1/x_1 = 0.01$ 

### COMPONENTS: 0 (1) Hydrogen; H₂; [1333-74-0]

(2) 1,1'-Oxybispropane or dipropyl ether; C₆H₁ 40; [111-43-3]

ORIGINAL MEASUREMENTS:

Guerry, D. Jr.

Ph.D. thesis, <u>1944</u> Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

VARIABLES:

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

### **EXPERIMENTAL VALUES:**

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient α	Ostwald Coefficient L	•
293.15	6.15	0.101	0.108	
298.15	6.43	0.105	0.115	

The Ostwald coefficients were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost complete recovery of the sample.

An improved temperature control system was used.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Dipropyl ether. Eastman Kodak Co. Refluxed four hours over Na, then distilled from Na in a N₂ atm. B.p. (746.2 mmHg) t/°C 89.03 - 89.28 (corr.). Refractive index, density, and vapor pressure data are in the thesis.

### ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

- Van Slyke, D. D.
   J. Biol. Chem. <u>1939</u>, 130, 545.
- 2. Ijams, C. C.
  Ph.D. thesis, <u>1941</u>
  Vanderbilt University

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclic ethers:  $C_4H_8O$ ,  $C_4H_8O_2$ ;  $C_5H_8O$ , and  $C_5H_{10}O$

### ORIGINAL MEASUREMENTS:

Guerry, D. Jr.

Ph. D. thesis, <u>1944</u> Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

### VARIABLES:

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
Te	trahydrofuran;	C4H80; [109-	99-9]
293.15 298.15	2.60 2.74	0.0719 0.0752	0.0771 0.0821
1,	4-Dioxane; C ₄ H	₈ 0 ₂ ; [123-91-	1]
293.15 298.15	1.79 1.93	0.0471 0.0502	0.0505 0.0548
2,	3-Dihydropyran	; с ₅ н ₈ 0; [255	12-65-6]
293.15 298.15	2.68 2.64	0.0662 0.0648	0.0710 0.0707
Те	trahydro-2H-py	ran; C ₅ H ₁₀ O;	[142-68-7]
293.15 298.15	3.12 3.24	0.0718 0.0742	0.0770 0.0810

The Ostwald coefficients were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus was a modified Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost 100 per cent recovery of the sample.

An improved temperature control system was used.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Cyclic ethers. The ethers were fractionally distilled from over Na in a nitrogen atmosphere. In addition to the solubility data the thesis contains measured values of refractive index, density, vapor pressure and b.p.

Tetrahydrofuran. Eastman Kodak Co. B.p. (752.7 mmHg) t/°C 65.50 - 65.54.

1,4-Dioxane. Eastman Kodak Co. B.p.(743.7 mmHg) t/°C 100.81-100.82.

Dihydro-2H-pyran. Prepared from tetrahydrofurfuryl alcohol. B.p. (743.6 mmHg) t/°C 84.81 - 84.89.

Tetrahydro-2H-pyran. Prepared by catalytic reduction of dihydro-2H-pyran. B.p.(750.6 mmHg) t/°C 87.51 - 87.52. All b. p. are corrected.

### ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

- Van Slyke, D. D.
   J. Biol. Chem. 1939, 130, 545.
- Ijams, C. C. Ph. D. thesis, <u>1941</u> Vanderbilt University

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]	Krauss, W.; Gestrich, W.		
2. 1,4-Dioxane; C ₄ H ₈ O ₂ ; [123-91-1]	Chem Tech. (Heidelberg), <u>1977</u> 6, 35-37.		
VARIABLES: Temperature	PREPARED BY: C.L. Young		
EXPERIMENTAL VALUES:			
T/K Solubility*/ mol d	Mole fraction of hydrogen in liquid,  **H2***  **H2***  **H2***  **H2***  **H2***  **H2***  **H2***  **H2***  **H2**  **H2**		
283.15 0.00175 293.15 0.00195 303.15 0.00215 313.15 0.0023	0.000150 0.000168 0.000188 0.00020		
§ calculated by compiler for a	partial pressure of 101.325 kPa.		
AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:		
Stirred equilibrium cell. Volumetric apparatus in which a known volume of gas was added to a known volume of liquid and the equilibrium pressure measured. Details in source.	No details given.		
	ESTIMATED ERROR: $\delta T/K = \pm 0.05; \ \delta x_{\rm H_2} = \pm 10^{-5}$ (estimated by compiler) $REFERENCES:$		

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 2-Propanone or acetone; C₃H₆O; [67-64-1]

### **EVALUATOR:**

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

1980, September

### CRITICAL EVALUATION:

Three laboratories have reported measurements of the solubility of hydrogen in acetone at pressures near 101.325 kPa. Just (1) measured the solubility at 293.15 and 298.15 K, Horiuti (2) made seven measurements over the temperature interval of 191.25 to 313.15 K, and Puri and Ruether (3) measured the Ostwald coefficient of solubility at 298.15 K and a total pressure of approximately  $10^5$  Pa.

The Just mole fraction solubility values are about 25 per cent less than Horiuti's values, and the Puri and Ruether value is 5.3 per cent less than Horiuti's smoothed value at 298.15 K. The Just values are rejected, and the Horiuti, and Puri and Ruether values are classed as tentative. However, the values of Horiuti are preferred.

A linear regression was made of Horiuti's mole fraction solubility values. A three constant equation appears to be justified, although as with the hydrogen + diethyl ether system, this may be due to an error in the measurement connected with the relatively large solvent vapor pressure. The tentative equation for use over the 193.15 to 313.15 K temperature interval is

$$\ln x_1 = -9.5956 - 1.1902/(T/100K) + 1.7267 \ln (T/100K)$$

with a standard error about the regression line of 2.40  $\times$  10⁻⁶.

Several values of the temperature dependent enthalpy and entropy changes for the transfer of one mole of hydrogen gas at a partial pressure of lol.325 kPa to the infinitely dilute solution are given in Table 1.

Smoothed values of the mole fraction solubility and partial molar Gibbs energy of solution are given in Table 2.

Table 1. Hydrogen + Acetone. Changes in enthalpy and entropy on transfer of mole of hydrogen from the gas at 101.325 kPa to the infinitely dilute solution.

$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$	$\Delta \overline{S}_1^{\circ}/J K^{-1} mol^{-1}$	$\Delta \overline{C}_{p_1}^{\circ}/J K^{-1} mol^{-1}$
3.76	-55.6	14.4
4.19	-53.9	14.4
4.55	-52.4	14.4
4.91	-51.0	14.4
5.27	-49.7	14.4
	3.76 4.19 4.55 4.91	3.76 -55.6 4.19 -53.9 4.55 -52.4 4.91 -51.0

Table 2. The solubility of hydrogen in acetone at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molar Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	ΔG°/kJ mo1 ⁻¹
193.15 203.15 213.15 223.15 233.15 243.15 253.15 263.15	1.14 1.29 1.44 1.60 1.76 1.93 2.11 2.30	14.574 15.130 15.679 16.221 16.757 17.287 17.811 18.329
273.15 283.15 288.15	2.49 2.70 2.80	19.349 19.600
293.15 298.15 303.15	2.90 3.01 3.12	19.851 20.100 20.348
313.15	3.34	20.841

### References:

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342.
- Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn.) 1931/32, 17, 125.
- 3. Puri, P. S.; Ruether, J. A. Can. J. Chem. Eng. 1974, 52, 636.

### COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) 2-Propanone or acetone; C₃H₆O; [67-64-1] ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367.

### VARIABLES:

T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	2.14	6.548	7.027
298.15	2.31	7.000	7.641

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

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

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

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

### SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) 2-Propanone. No information.

### ESTIMATED ERROR:

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

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 2-Propanone or acetone; C₃H₆O; [67-64-1]

### ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125 - 256.

### **VARIABLES:**

T/K: 191.25 - 313.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	$x_1 \times 10^4$	Coefficient	Coefficient
	_	$\alpha \times 10^{2}$	L x 10"
191.25	1.12	3.90	2.73
212.45	1.42	4.83	3.76
232.55	1.77	5.85	4.98
252.25	2.07	6.69	6.18
273.15	2.50	7.83	7.83
294.05	2.95	8.99	9.68
313.15	3.320	9.865	11.31

The mole fraction and Bunsen coefficient values were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -9.5956 - 1.1902/(T/100K) + 1.7267 \ln (T/100K)$ Standard error about the regression line = 2.40 x 10⁻⁶

T/K	Mol Fraction
	$x_1 \times 10^4$
193.15	1.14
203.15	1.29
213.15	1.44
223.15	1.60
233.15	1.76
243.15	1.93
253.15	2.11

_	T/K	Mol Fraction
		$x_1 \times 10^4$
	263.15	2.30
	273.15	2.49
	283.15	2.70
	293.15	2.90
	298.15	3.01
	303.15	3.12
	313.15	3.34

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret, a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption pipet.

### SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by electrolysis.
- (2) 2-Propanone. Nippon Pure Chem. Co. or Merck. Extra pure grade, recrystallized with sodium sulfite. Stored over calcium chloride then fractionated. Boiling point 56.09°C (760 mmHg).

### ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
 $\delta x_1/x_1 = 0.01$ 

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclohexanone; C₆H₁₀O; [108-94-1]

### ORIGINAL MEASUREMENTS:

Guerry, D. Jr.

Ph.D. thesis, 1944 Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

VARIABLES:

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

т/к	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
293.15	2.16	0.0467	0.0501
298.15	2.23	0.0480	0.0524

The Ostwald coefficients were calculated by the compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost complete recovery of the sample.

An improved temperature control system was used.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Cyclohexanone. Eastman Kodak Co. Purified, distilled, b.p. (754.5 mmHg) t/°C 155.19. Refractive index, density, and vapor pressure data are in the thesis.

### ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

- 1. Van Slyke, D. D. J. Biol. Chem. 1939, 130, 545.
- 2. Ijams, C. C. Ph.D. thesis, 1941 Vanderbilt University

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Kruyer, S.; Nobel, A.P.P.
2. Phenol; C ₆ H ₆ O; [108-95-2]	Rec. Trav. Chim. 1961, 80, 1145-56
VARIABLES:	PREPARED BY:
	C. L. Young
EXPERIMENTAL VALUES:	
	[a]
T/K Ostwald coeffic	ient,L Mole fraction of hydrogen, $x_{ m H_2}$
	2
298.15 0.033	0.000122
[a] Calculated by compiler for a pa	rtial pressure of 101.325 kPa
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Technique consisted of saturating	1. Hydrogen and argon passed
liquid with hydrogen in a spiral adsorption tube and then stripping	through molecular sieve 4A in liquid oxygen and nitrogen trap respectively.
out the hydrogen with argon. The	
resulting argon-hydrogen mixture was analysed with a katharometer.	2. "Chemically pure".
	ESTIMATED ERROR: $\delta T/K = \pm 0.2$ ; $\delta L = \pm 3%$
	01/K = 10.2; OH - 136
	REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Acetic acid; C₂H₄O₂; [64-19-7]

### **EVALUATOR:**

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

1980, September

### CRITICAL EVALUATION:

The solubility of hydrogen in acetic acid was measured at 293.15 and 298.15 K by Just (1) and between 291.75 and 347.95 K by Maxted and Moon (2). The mole fraction solubility values from the two laboratories show some scatter, but in general agree within one to two per cent.

A linear regression was applied to the total of 14 solubility measurements to obtain the tentative equation for use between 289.75 (the melting point of acetic acid) and 348.15 K.

$$\ln x_1 = -6.7248 - 6.2238/(T/100K)$$

with a standard error about the regression line of 1.88  $\times$  10⁻⁶.

The temperature independent thermodynamic changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at a pressure of  $101.325~\mathrm{kPa}$  to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 5.17 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -55.9.

The smoothed values of the mole fraction solubility and partial molal  ${\tt Gibbs}$  energy of solution are in Table 1.

Table 1. The solubility of hydrogen in acetic acid at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K		Mol Fraction 10 ⁴ x ₁	∆G ₁ °/kJ mol ⁻¹
289.75 293.15 298.15 303.15 308.15 313.15 318.15 323.15 323.15 333.15 338.15	(m.p.)	1.40 1.44 1.49 1.54 1.59 1.65 1.70 1.75 1.80 1.85	21.375 21.565 21.845 22.124 -22.404 22.684 22.963 23.242 23.522 23.801 24.081 24.361
348.15		2.01	24.640

### References:

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342.
- 2. Maxted, E. B.; Moon, C. H. Trans. Faraday Soc. 1936, 32, 769.

## COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Acetic Acid; C₂H₄O₂; [64-19-7] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	1.47	5.751	6.172
298.15	1.49	5.799	6.330

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

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

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

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

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Acetic acid. No information.

### ESTIMATED ERROR:

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

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Maxted, E.B.; Moon, C.H.;
2. Acetic acid; C ₂ H ₄ O ₂ ; [64-19-7]	Trans. Faraday, Soc. <u>1936</u> , 32,769-75.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young

Bunsen coefficient, a	Mole fraction of hydrogen, $x_{\rm H_2}$
0.0558	0.000142
0.0596	0.000154
0.0620	0.000161
0.0649	0.000170
0.0676	0.000179
0.0714	0.000191
0.0742	0.000201
0.0566	0.000145
0.0594	0.000153
0.0669	0.000176
0.0547	0.000140
0.0590	0.000152
	coefficient, α  0.0558 0.0596 0.0620 0.0649 0.0676 0.0714 0.0742 0.0566 0.0594 0.0669 0.0547

 $^{\star}\mathrm{and}\, **\,$  minor modification of apparatus used, details in source. Partial pressure of hydrogen = 1 atm = 101.325 kPa.

AUXILIARY	INFORMATION
METHOD:/APPARATUS/PROCEDURE:  Volumetric apparatus with rocking absorption cell. Details in source.	SOURCE AND PURITY OF MATERIALS:  1. Electrolytic grade.  2. Degassed, high purity sample, no other details given.
	ESTIMATED ERROR: $\delta T/K = \pm 0.2;  \delta x_{\rm H_2} = \pm 1 \text{%}.$ (estimated by compiler.) REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Hydrogen; H ₂ ; [1333-74-0] (2) Esters	H. L. Clever Department of Chemistry Emory University Atlanta, GA 30322 USA
	1980, September

CRITICAL EVALUATION:

An Evaluation of the Mole Fraction Solubility of Hydrogen in Esters at a Hydrogen Partial Pressure of 101.325 kPa (1 atm).

Most of the solubility measurements evaluated in this section were carried out at a total pressure near 101.325 kPa. The mole fraction solubility values at a hydrogen partial pressure of 101.325 kPa were calculated on the assumption that the following statements are true. The gas is ideal, Henry's law is obeyed, and the Ostwald coefficient is independent of pressure. The assumptions introduce errors that are probably smaller than the experimental errors of the solubility measurement.

Hydrogen + Acetic acid, methyl ester or methyl acetate [79-20-9]

Horiuti (2) measured seven values of the solubility over the 194.65 to 313.15 K temperature interval. There are no other measurements. The work of Horiuti generally has proved to be reliable. The tentative equation for the 193.15 to 313.15 K temperature range was obtained by a linear regression of his data.

$$\ln x_1 = -6.1832 - 5.7501/(T/100K)$$

with a standard error about the regression line of  $3.00 \times 10^{-6}$ .

The temperature independent values of changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas phase at a pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 4.78 and  $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -51.4.

Smoothed values of the mole fraction solubility at a hydrogen partial pressure of  $101.325\ kPa$  are given on the data sheet.

Hydrogen + Acetic acid, ethyl ester or ethyl acetate [141-78-6]

Just (1) reported solubility values at 293.15 and 298.15 K. Maxted and Moon (3) reported five values over the 273.65 to 312.95 K temperature interval.

Several of the solubility values appear to be inaccurate. The most likely inaccurate values are the 293.15 K value of Just, and either the 273.65 or the 312.95 K value of Maxted and Moon. Linear regressions were made of several combinations of the data. Thermodynamic values of changes in enthalpy and entropy were consistent with other hydrogen + solvent systems when the 293.15 K value of Just and the 273.65 K value of Maxted and Moon were omitted.

The tentative equation for use between 273.15 and 313.15 K is

$$\ln x_1 = -5.8144 - 6.4228/(T/100K)$$

with a standard error about the regression line of 3.77  $\times$  10⁻⁶.

The temperature independent changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at a pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 5.34 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -48.3.

The smoothed solubility data and partial molal Gibbs energy of solution are in Table  $\ 1$  .

Table 1 . The solubility of hydrogen in ethyl acetate at a hydrogen partial pressure of 101.325 kPa. Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
273.15	2.84	18.545
278.15	2.96	18.787
283.15	3.09	19.028
288.15	3.21	19.270
293.15	3.34	19.512
298.15	3.46	19.754
303.15	3.59	19.995
308.15	3.71	20.237
313.15	3.84	20.479

Only Just (1) has reported solubility measurements on the above systems. His solubility values at 293.15 and 298.15 K are classed as tentative.

### References:

- 1. Just, G. Z. Phys. Chem. 1901, 37, 342.
- 2. Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn.) 1931/32, 17, 125.
- 3. Maxted, E. B.; Moon, C. H. Trans. Faraday Soc. 1936, 32, 769.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Acetic acid methyl ester or methyl acetate;  $C_3H_6O_2$ ; [79-20-9] (Jpn) 1931/32, 17, 125 - 256.

### ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. pap. Inst. Phys. Chem. Res.

### VARIABLES:

T/K: 194.65 - 313.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	$x_1 \times 10^4$	Coefficient	Coefficient
	$x_1 \times 10^{\circ}$	2	2
	<u>.</u>	$\alpha \times 10^{-2}$	L x 10
194.65	1.09	3.49	2.49
212.85	1.39	4.34	3.38
233.05	1.72	5.24	4.47
253.05	2.09	6.24	5.78
273.15	2.52	7.30	7.30
294.05	2.93	8.28	8.91
313.15	3.333	9.168	10.51

The mole fraction and Bunsen coefficient values were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -6.1832 - 5.7501/(T/100K)$ 

Standard error about the regression line =  $3.00 \times 10^{-6}$ 

T/K	Mol Fraction	
	$x_1 \times 10^4$	
193.15	1.05	
203.15	1.22	
213.15	1.39	
223.15	1.57	
233.15	1.75	
243.15	1.94	
253.15	2.13	

T/K	Mol Fraction
	$x_1 \times 10^4$
263.15	2.32
273.15	2.51
283.15	2.71
293.15	2.90
298.15	3.00
303.15	3.10
313,15	3.29

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret, (1) Hydrogen. Prepared by a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption pipet.

### SOURCE AND PURITY OF MATERIALS:

- electrolysis.
- (2) Acetic acid, methyl ester. Merck. Extra pure grade treated with phosphorous pentoxide several times and distilled several times. Boiling point, 57.12°C (760 mmHg).

### ESTIMATED ERROR:

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Acetic acid ethyl ester or ethyl acetate; C₄H₈O₂; [141-78-6]

### ORIGINAL MEASUREMENTS:

Just, G.

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

### VARIABLES:

T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald Coefficient
	$x_1 \times 10^4$	$\alpha \times 10^2$	L x 10 ²
293.15 298.15	3.20 3.43	7.340 7.802	7.877 8.516

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

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

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

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

### SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Acetic Acid ethyl ester. No information.

### ESTIMATED ERROR:

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

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

### 234 Hydrogen Solubilities up to 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Maxted, E.B.; Moon, C.H.; 2. Acetic acid, ethyl ester (Ethyl Trans. Faraday Soc. 1936, 32,769-75 Acetate); C₄H₈O₂; [141-78-6] VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: T/K Bunsen Mole fraction of hydrogen, $x_{\rm H_2}$ coefficient, α 0.0708 273.65 0.000301 283.15 0.0724 0.000312 0.000333 294.15 0.0761 303.15 0.0808 0.000358 312.95 0.0863 0.000387 Partial pressure of hydrogen = 1 atm = 101.325 kPa. AUXILIARY INFORMATION METHOD: /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus with rocking 1. Electrolytic grade. absorption cell. Details in source. 2.

# METHOD:/APPARATUS/PROCEDURE: Volumetric apparatus with rocking absorption cell. Details in source. 1. Electrolytic grade. 2. Degassed, high purity sample, no other details given. ESTIMATED ERROR: $\delta T/K = \pm 0.2; \ \delta x_{H_2} = \pm 1 \%.$ (estimated by compiler.) REFERENCES:

## COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Acetic acid 2-methylpropyl ester or isobutyl acetate; C₆H₁₁O₂; [110-19-0] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15 298.15	5.13 5.33	8.653 8.940	9.287 9.758

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

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

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

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

### SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Acetic acid 2-methylpropyl ester. No information.

### ESTIMATED ERROR:

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

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

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Acetic acid pentyl ester or amyl acetate; C₇H₁₄O₂; [628-63-7] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) T/K: Components: ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	4.60	6.925	7.432
298.15	4.73	7.089	7.738

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

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

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

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

# SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Acetic acid pentyl ester. No information.

# ESTIMATED ERROR:

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

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

COMPONENTS:	EVALUATOR:	
(1) Hydrogen; H ₂ ; [1333-74-0] (2) Halocarbons	H. L. Clever Department of Chemistry Emory University Atlanta, GA 30322 USA 1980, September	

### CRITICAL EVALUATION:

An Evaluation of the Mole Fraction Solubility of Hydrogen in Halocarbons at a Hydrogen Partial Pressure of 101.325 kPa (1 atm).

Most of the solubility measurements evaluated in this section were made at a total pressure near 101.325 kPa. Mole fraction solubility values were calculated at a hydrogen partial pressure of 101.325 kPa with at least two of the following three assumptions. The gas is ideal, Henry's law is obeyed, and the Ostwald coefficient is independent of pressure. The assumptions introduce errors that are probably less than the experimental error of the solubility measurement.

Hydrogen + Hexadecafluoroheptane or Perfluoroheptane [335-57-9]

Gjaldbaek (1) reported four solubility measurements between the temperatures of 297.88 and 321.90 K. Cook, Hanson, and Alder (2) reported a total 14 measurements at six temperatures between 248.15 and 323.15 K.

Both sets of data are classed as tentative. The two data sets accord well except for Gjaldbaek's values near 321 K which are 8 per cent greater than the smoothed curve through the Cook  $et\ al.$  data.

The tentative equation for the 248.15 K to 323.15 K temperature interval was obtained by a linear regression of all of the data of Cook  $et\ al.$  and the two values near 298 K of Gjaldbaek.

$$\ln x_1 = -4.7741 - 5.3211/(T/100K)$$

with a standard error about the regression line of 1.98 x  $10^{-5}$ .

The temperature independent values of the changes in enthalpy and entropy for the transfer of one mole of hydrogen in the gas at 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 4.42 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -39.7.

The smoothed values of solubility and the partial molal Gibbs energy are given in Table 1. A three constant equation would reproduce the experimental data more closely, but it does not appear justified because of the two solubility measurements between 321 and 322 K that were not used in the linear regression. The evaluator has preferred the data of Cook  $et\ al.$  because it has generally proven to be reliable.

Table 1. The solubility of hydrogen in perfluoroheptane at a hydrogen partial pressure of 101.325 kPa. The tentative mole fraction solubility and the partial molal Gibbs energy of solution as a function of temperature.

т/к	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
248.15	9.89	14.274
258.15	10.75	14.671
268.15	11.61	15.068
278.15	12.47	15.465
288.15	13.32	15.862
293.15	13.75	16.060
298.15	14.18	16.259
303.15	14.60	16.457
313.15	15.44	16.854
323.15	16.27	17.251

Hydrogen + Tetrachloromethane [56-23-5]

The solubility of hydrogen in tetrachloromethane has been measured at two laboratories. Horiuti (3) made four measurements between 273.15 and 332.15 K. Cook, Hanson, and Alder (2) made three solubility measurements between the temperatures of 273.15 and 308.15 K. The work of both laboratories is generally reliable and both data sets are classed as tentative. The poorest agreement between the two data sets is at 273.15 K where the experimental values differ by 5.4 per cent with Horiuti's measurement the greater value.

When the two data sets are smoothed by a Gibbs energy equation linear in temperature the two laboratories have the same value of solubility at about 283 K. Above 283 K the Horiuti values are greater by about 2.7 per cent.

A linear regression of all of the data from both laboratories showed the 273.15 K solubility of Horiuti to deviate the most from the regression line. Although the deviation was less than 2 standard deviations an arbitrary decision was made to reject the value. A second linear regression of the remaining six values gave the tentative equation for use over the 273.15 to 333.15 K range.

$$\ln x_1 = -5.6661 - 7.0762/(T/100K)$$

with a standard error about the regression line of 3.95  $\times$  10⁻⁶.

The temperature independent values for the changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at a pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 5.88 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -47.1.

Smoothed values of the solubility and partial molal  $Gibbs\ energy\ of\ solution\ are\ in\ Table\ 2.$ 

Table 2. The solubility of hydrogen in tetrachloromethane at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction ¹ 10 ⁴ x ₁	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
273.15	2.595	18.751
283.15	2.845	19.223
293.15	3.095	19.694
298.15	,3.225	19.929
303.15	3.355	20.165
313.15	3.615	20.636
323.15	3.875	21.107
333.15	4.140	21.578

¹ Mole fractions rounded to nearest  $0.005 \times 10^{-4}$ .

Hydrogen + Trichloromethane [67-66-3]

Only Maxted and Moon (4) have measured the solubility of hydrogen in trichloromethane. Their values are classed as tentative. A linear regression of the four solubility values gives the tentative equation for use over the temperature range of 273.15 to 298.15 K of

$$\ln x_1 = -7.1710 - 3.7486/(T/100K)$$

with a standard error about the regression line of  $3.57 \times 10^{-6}$ .

The temperature independent values of the changes in enthalpy and entropy on transfer of one mole of hydrogen from the gas phase at  $101.325~\mathrm{kPa}$  to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 3.12 and  $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -59.6.

Smoothed values of the solubility and the partial molal Gibbs energy of solution are in Table 3.

Table 3. The solubility of hydrogen in trichloromethane at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction 10 ⁴ x ₁	ΔG°/kJ mol ⁻¹
273.15	1.97	19.374
278.15	1.99	19.708
283.15	2.02	20.025
288.15	2.07	20.324
293.15	2.13	20.606
298.15	2.20	20.872

Hydrogen + 1,2-Dichloroethane [107-06-2]

Only Waters, Mortimer, and Clements (5) have measured the solubility of hydrogen in 1,2-dichloroethane. Their four solubility values, classed as tentative, were put through a linear regression to obtain the equation for use over the 263.15 to 298.15 K temperature range.

$$\ln x_1 = -5.5837 - 9.1168/(T/100K)$$

with a standard error about the regression line of 1.89 x  $10^{-6}$ .

The temperature independent values of the changes of enthalpy and entropy for the transfer of one mole hydrogen from the gas phase at a partial pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 7.58 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -46.4.

The smoothed values of solubility and the partial molal Gibbs energy of solution are in Table 4.

Table 4. The solubility of hydrogen in 1,2-dichloroethane at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
263.15	1.18	19.797
273.15	1.335	20.261
283.15	1.50	20.725
288.15	1.59	20.957
293.15	1.68	21.189
298.15	1.77	21.422

Hydrogen + 1,1,2,2-Tetrachloroethane [79-34-5]

Only deWet (6) has measured the solubility of hydrogen in 1,1,2,2-tetrachloroethane. A linear regression applied to his three tentative solubility values gives the equation for the 288.15 to 308.15 K temperature interval of

$$\ln x_1 = -6.5798 - 3.6640/(T/100K)$$

with a standard error about the regression line of  $3.51 \times 10^{-6}$ .

The values of the temperature independent changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas phase at a partial pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 3.05 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -54.7.

The smoothed solubility values and partial molal Gibbs energy of solution are in Table 5.

Table 5. The solubility of hydrogen in 1,1,2,2-tetrachloroethane at a hydrogen partial pressure of 101.325 kPa. Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

т/к	Mol Fraction	ΔG°/kJ mol ⁻¹
288.15	3.89	18.810
293.15	3.98	19.084
298.15	4.06	19.357
303.15	4.14	19.631
308.15	4.23	19.904

Hydrogen + 1-Chlorohexane [544-10-5]

Guerry (7) has measured the solubility of hydrogen in 1-chlorohexane at the temperatures of 293.15 and 298.15 K. The values are classed as tentative.

Hydrogen + Chlorobenzene [108-90-7]

Horiuti (3) measured the solubility of hydrogen in chlorobenzene at seven temperatures between 232.25 and 353.95 K. His values of solubility are the only ones for the system and they are classed as tentative.

A graph of the data of Horiuti as  $\ln x_1 vs.\ 1/T$  shows a systematic deviation from linearity. Linear regressions for a two constant and a three constant equation show a four fold improvement in the standard error. Thus, the tentative equation for use over the 233.15 to 353.15 K temperature range is the three constant equation

$$\ln x_1 = -10.0240 - 0.7256/(T/100K) + 1.8288 \ln (T/100K)$$

with a standard error about the regression line of  $1.44 \times 10^{-6}$ .

The three constant equation gives temperature dependent values of the changes of enthalpy and entropy for the transfer of one mole of hydrogen from the gas phase at  $101.325~\mathrm{kPa}$  partial pressure to the infinitely dilute solution. Values of the thermodynamic changes at several temperatures are given in Table 6.

Table	6.	Thermodynamic changes for the dissolution
		of hydrogen in chlorobenzene as a function
		of temperature.

T/K	$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$	$\Delta \overline{S}_1^{\circ}/J K^{-1} mol^{-1}$	$\Delta \overline{C}_{P_1}^{\circ}/J K^{-1} mol^{-1}$
233.15	4.15	-55-3	15.2
273.15	4.76	-52.9	15.2
298.15	5.14	-51.5	15.2
323.15	5.52	-50.3	15.2
353.15	5.97	-49.0	15.2

Smoothed values of the solubility and partial molal Gibbs energy of solution are in Table 7.

Table 7. The solubility of hydrogen in chlorobenzene at a partial pressure of hydrogen of 101.325 kPa. Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
233.15	1.53	17.034
243.15	1.67	17.583
253.15	1.82	18.126
263.15	1.97	18.663
273.15	2.13	19.195
283.15	2.30	19.721
288.15	2.39	19.982
293.15	2.47	20.241
298.15	2.56	20.499
303.15	2.65	20.756
313.15	2.84	21.267
323.15	3.02	21.772
333.15	3.22	22.273
343.15	3.42	22.769
353.15	3.63	23.261

Linford and Hildebrand (8) report values of the solubility at seven temperatures between 276.85 and 301.75 K. The data are classed as tentative. A linear regression of the data gives the equation for use over the temperature interval of 273.15 to 303.15 K of

$$\ln x_1 = -5.3371 - 5.9346/(T/100K)$$

with a standard error about the regression line of  $2.88 \times 10^{-6}$ .

The temperature independent values of the changes in enthalpy and entropy On transfer of one mole of hydrogen from the gas phase at a partial pressure of 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1}$$
 4.93 and  $\Delta \overline{S}_1^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -44.4.

There is a table of smoothed mole fraction solubility values on the data sheet.

The authors also report the solubility of hydrogen in several mixtures of benzene + 1,1,2-trichloro-1,2,2-trifluoroethane.

# Hydrogen + 1-Bromoheptane [629-04-9]

Ijams (9) measured one value of the solubility at a temperature of 298.15 K. The value is classed as tentative.

# References:

- 1. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.
- Cook, M. W.; Hanson, D. N.; Alder, B. J. J. Chem. Phys. 1957, 26, 748.
- Horiuti, J. Sci. Pap. Inst. Phys. Chem. Res. (Jpn.) 1931/32, 17, 125.
- 4. Maxted, E. B.; Moon, C. H. Trans. Faraday Soc. 1936, , 769.
- Waters, J. A.; Mortimer, G. A.; Clements, H. E. J. Chem. Eng. Data <u>1970</u>, 15, 174.
- 6. deWet, W. J. J. S. Afr. Chem. Inst. <u>1964</u>, 17, 9.
- Guerry, D. Jr. Ph.D. thesis, Vanderbilt University, Nashville, TN, 1944.
- 8. Linford, R. G.; Hildebrand, J. H. Trans. Faraday Soc. 1970, 66, 577.
- Ijams, C. C. Ph.D. thesis, Vanderbilt University, Nashville, TN, 1941.

### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Cook, M. W.; Hanson, D. N.; Alder, B. J. (2) Hexadecafluoroheptane or per-J. Chem. Phys. 1957, 26, 748-751. fluoroheptane; C7F16; [335-57-91 VARIABLES. PREPARED BY: T/K: 248.15 - 323.15 P. L. Long

EXPERIMENTAL		s:
	K K	S

P/kPa:

T/K	solubility ¹ mol g ⁻¹ x 10 ⁶	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
248.15	2.589	10.037	10.45	9.49
273.15	3.077	11.927	12.15	12.15
285.25	3.333 <u>3.334</u> 3.333 ₅ av.	12.922	13.03	13.60
298.15	3.613 3.616 3.615 <u>3.614</u> 3.614 ₅ av.	14.007	13.96	15.24
308.15	3.853 3.849 3.849 <u>3.850</u> 3.850	14.920	14.74	16.63
323.15	4.29 <u>4.30</u> 4.29 ₅ av.	16.64²	16.21	19.18

Data from (1).

101.325 (1 atm)

The Bunsen and Ostwald coefficients were calculated by the compiler.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

(1) Hydrogen. Matheson Co. spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.

H. L. Clever

(2) Hexadecafluoroheptane. Source not given. Distilled, center portion used, b.p. 355.65K. Other solvent properties given in reference (1).

## ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$  (authors)

# REFERENCES:

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

 $\ln x_1 = -12.1850 + 4.9152/(T/100K) + 3.6328 \ln (T/100)$ Smoothed Data:

Standard error about the regression line =  $9.85 \times 10^{-6}$ See the hydrogen + hexadecafluoroheptane evaluation for the recommended equation.

²Mole fraction value calculated by the compiler.

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Gjaldbaek, J. C. (2) Hexadecafluoroheptane or Perfluoroheptane; C₇F₁₆; [335-57-9] VARIABLES: T/K: 297.88 - 321.90 P/kPa: 101.325 (1 atm) PRIGINAL MEASUREMENTS: Gjaldbaek, J. C. Acta. Chem. Scand. 1952, 6, 623-633. PREPARED BY: J. Chr. Gjaldbaek

# EXPERIMENTAL VALUES:

т/к	Mol Fraction $10^3 x_1$	Bunsen Coefficient 10 ² a	Ostwald Coefficient 10 L
297.88	14.2	14.1	15.4
297.95	14.1		15.3
321.45	17.4	16.6	19.5
321.90	17.4	16.6	19.6

The Ostwald and mole fraction solubility values were calculated by the compiler at 101.325 kPa ( 1 atm) hydrogen pressure assuming Henry's law is obeyed.

Smoothed Data:  $\ln x_1 = -3.8039 - 8.2063/(T/100K)$ 

Standard error about the regression line is  $5.85 \times 10^{-6}$ .

See the hydrogen + hexadecafluoroheptane evaluation for the recommended equation.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for calibration and as the confining liquid. The solvents were degassed in the apparatus. Details are in reference 1.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Freed from oxygen and dried. 99.5 per cent H₂, 0.5 per cent N₂.
- (2) Hexadecafluoroheptane. Sample described in earlier paper (2).

## ESTIMATED ERROR:

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

- Lannung, A.
   J. Am. Chem. Soc. <u>1930</u>, 52, 68.
- Gjaldbaek, J. C.; Hildebrand, J.H. J. Am. Chem. Soc. <u>1949</u>, 71, 3147.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Tetrachloromethane or carbon tetrachloride; CCl₄; [56-23-5]

# ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. pap. Inst. Phys. Chem. Res. (Jpn) 1931/32,17, 125-256.

# VARIABLES:

T/K: 273.15 - 332.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
273.15	2.73	6.50	6.50
294.05	3.18	7.38	7.94
311.95	3.58	8.13	9.28
332.15	4.128	9.243	11.24

The mole fraction and Bunsen coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -5.9012 -6.3128/(T/100K)$ 

Standard error about the regression line =  $4.10 \times 10^{-6}$ 

See the hydrogen + tetrachloromethane evaluation for the recommended equation.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret, a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption pipet.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by electrolysis.
- (2) Tetrachloromethane. Kahlbaum. Dried, and distilled. Boiling point 76.74 C (760 mmHg).

# ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
 $\delta x_1/x_1 = 0.01$ 

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Tetrachloromethane or carbon tetrachloride; CCl₄; [56-23-5]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

### VARIABLES:

T/K: 273.15 - 308.15 P/kPa: 101.325 (1 atm)

## PREPARED BY:

P. L. Long H. L. Clever

### EXPERIMENTAL VALUES:

т/к	Solubility ¹ mol g ⁻¹ x 10 ⁶	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
273.15	1.688	2.589	6.16	6.16
298.15	2.078	3.193	7.37	8.05
308.15	2.245	3.447	7.86	8.87

Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -5.7435 - 6.8721/(T/100K)$ 

Standard error about the regression line =  $4.16 \times 10^{-7}$ 

See the hydrogen + tetrachloromethane evaluation for the recommended equation.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N₂.
- (2) Tetrachloromethane. Baker and Adamson Reagent Grade. Distilled, center portion used, b.p. 349.95K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$  (authors)

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, <u>1954</u>.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Maxted, E.B., Moon, C.H. 2. Trichloromethane Trans. Faraday Soc. 1936,32,769-75. (Chloroform); CHCl₃; [67-66-3] VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: Mole fraction of T/K Bunsen hydrogen, $x_{\rm H_2}$ coefficient, 274.15 0.0563 0.000197 283.15 0.0576 0.000204 291.85 0.0584 0.000209 0.000222 298.45 0.0614 Partial pressure of hydrogen = 1 atm = 101.325 kPa. AUXILIARY INFORMATION METHOD:/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Volumetric apparatus with rocking absorption cell. Details in source. 1. Electrolytic grade. 2. Degassed, high purity sample, no other details given. ESTIMATED ERROR: $\delta T/K = \pm 0.2; \delta x_{H_2} = \pm 1%.$ (estimated by compiler). REFERENCES:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1,2-Dichloroethane; C2H4Cl2; [107-06-2]

# ORIGINAL MEASUREMENTS:

Waters, J. A.; Mortimer, G. A.; Clements, H. E.

J. Chem. Eng. Data 1970, 15, 174 -176 and 462 (correction).

### **VARIABLES:**

T/K; 263.15 - 298.15H₂ P/KPa: 101.325 (1 atm)

# PREPARED BY:

P. L. Long H. L. Clever

# EXPERIMENTAL VALUES:

Temper t/°C	T/K	$c_{\rm H2}/\text{mol dm}^{-3} \text{ atm}^{-1}$ $\times 10^3$	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
-10	263.15	1.557	1.18	0.0349	0.0336
0	273.15	1.739	1.34	0.0390	0.0390
10	283.15	1.890	1.48	0.0425	0.0441
25	298.15	2.239	1.78	0.0502	0.0548

The mole fraction and Ostwald coefficient values were calculated from the authors data by the compiler.

The authors also reported the vapor pressure of the solvent.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The authors reported two methods of solubility measurement. The hydrogen solubilities were measured by their method A.

The apparatus consisted of two glass bulbs connected by 1/4" stainless steel tubing fitted with Hoke valves and a strain gage. The strain gage signal was measured by a potentiometer. The bulbs were immersed in an oil bath. The temperature was measured with a Pt resistance thermometer and Mueller ESTIMATED ERROR: bridge.

The solvent was degassed three times at liquid  $N_2$  temperature. The solvent vapor pressure was measured in the apparatus. Gas in the second bulb at a known P and T was allowed into the bulb containing the solvent. The change in P was followed until equilibrium was reached. The gas uptake was calculated using Charles law A correction was made for H2 adsorption on the walls.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Minimum purity 99.50 per cent.
- (2) 1,2-Dichloroethane. Monsanto Co. Purity 99.95 per cent.

 $\delta P/mmHg = 0.1$  $\delta T/K = 0.01$ 

## 

### EXPERIMENTAL VALUES:

P/kPa: 101.325 (1 atm)

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
291.45	3.96	8.42	8.98
299.15	4.05	8.58	9.40
304.85	4.19	8.84	9.87

The mole fraction and Ostwald coefficient values were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -6.5798 - 3.6640/(T/100K)$ 

Standard error about the regression line =  $3.51 \times 10^{-6}$ 

T/K	Mol Fraction $x_1 \times 10^4$
288.15	3.89
293.15	3.98
298.15	4.06
303.15	4.15
308.15	4.23

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus is a modification of that used by Morrison and Billett (1) and others (2). The degassed solvent is saturated with gas as it flows down a glass helix containing the gas. The amount of solvent passed down the helix was such that 10 to 25 cm³ of gas was absorbed.

Degassing. The solvent is placed in a large continuously evacuated bulb until the solvent boils freely without further release of dissolved gases.

Saturation. The solvent is flowed in a thin film down the glass helix Containing the gas. The volume of gas absorbed is measured on an attached buret system.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given.
  Gas from commercial cylinders
  purified over activated charcoal at liquid air temperature.
  Impurities estimated to be less
  than 0.3 per cent.
- (2) 1,1,2,2-Tetrachloroethane. Source not given. Distilled immediately before use.

### ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

- Morrison, T. J.; Billett, F. J. Chem. Soc. <u>1948</u>, 2033; Ibid. <u>1952</u>, 3819.
- Clever, H. L.; Battino, R.;
   Saylor, J. H.; Gross, P. M.
   J. Phys. Chem. <u>1957</u>, 61, 1078.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1-Chlorohexane; C₆H₁₃Cl; [544-10-5]

ORIGINAL MEASUREMENTS:

Guerry, D. Jr.
Ph.D. thesis, 1944

Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

VARIABLES:

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
293.15	4.38	0.0715	0.0767
298.15	4.46	0.0724	0.0791

The Ostwald coefficients were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost complete recovery of the sample.

An improved temperature control system was used.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) 1-Chlorohexane. Eastman Kodak Co. Purified, distilled from P₂O₅ in a N₂ atm. B.p. (746.6 mmHg) t/°C 134.66 (corr.). Refractive index, density, and vapor pressure data are in the thesis.

# ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

- Van Slyke, D. D.
   J. Biol. Chem. 1939, 130, 545.
- 2. Ijams, C. C.
  Ph.D. thesis, <u>1941</u>
  Vanderbilt University

- (1) Hydrogen; H₂: [1333-40-7]

# ORIGINAL MEASUREMENTS:

Horiuti, J.

(2) Chlorobenzene; C₆H₅Cl; [108-90-7] Sci. pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, 17, 125 - 256.

VARIABLES:

T/K: 232.25 - 353.95 P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,			
T/K	Mol Fraction	Bunsen	Ostwald
	$x_1 \times 10^4$	Coefficient	Coefficient
	w1 ·· ***	$\alpha \times 10^2$	L x 10 ²
232.25	1.52	3.56	3.03
252.65	1.80	4.13	3.82
273.15	2.13	4.79	4.79
294.35	2.51	5.52	5.95
313.15	2.83	6.12	7.02
333.45	3.24	6.86	8.37
353.95	3.63	7.53	9.76

The mole fraction and Bunsen coefficient values were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -10.0240 - 0.7256/(T/100K) + 1.8288 \ln (T/100K)$ Standard error about the regression line =  $1.44 \times 10^{-6}$ 

T/K	Mol Fraction
	$x_1 \times 10^4$
233.15	1.53
243.15	1.67
253.15	1.82
263.15	1.97
273.15	2.13
283.15	2.30
293.15	2.47

J	
T/K	Mol Fraction
	$x_1 \times 10^4$
298.15	2.56
303.15	2.65
313.15	2.84
323.15	3.02
333.15	3.22
343.15	3.42
353.15	3.63

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a gas buret, (1) Hydrogen. Prepared by a solvent reservoir, and an absorption pipet. The volume of the pipet is determined at various meniscus heights by weighing a quantity of water. The meniscus height is read with a cathetometer.

The dry gas is introduced into the degassed solvent. The gas and solvent are mixed with a magnetic stirrer until saturation. Care is taken to prevent solvent vapor from mixing with the solute gas in the gas buret. The volume of gas is determined from the gas buret readings, the volume of solvent is determined from the meniscus height in the absorption pipet.

- SOURCE AND PURITY OF MATERIALS:
  - electrolysis.
- (2) Chlorobenzene. Kahlbaum. Dried, and distilled. Boiling point 131.96°C(760 mmHg).

ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
 $\delta x_1/x_1 = 0.01$ 

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon 113; C2Cl3F3; [76-13-1]

# ORIGINAL MEASUREMENTS:

Linford, R. G.; Hildebrand, J. H. Trans. Faraday Soc. 1970, 66, 577 - 581.

### VARIABLES:

T/K: 276.85 - 301.75 kPa: 101.325 (1 atm) P/kPa:

## PREPARED BY:

M. E. Ďerrick H. L. Clever

# EXPERIMENTAL VALUES:

$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$				
281.65     5.88     11.3     11.7       286.87     6.07     11.5     12.1       288.55     6.11     11.6     12.3       298.15     6.55     12.3     13.4       300.90     6.70     12.5     13.8	T/K		Coefficient	Coefficient
	281.65 286.87 288.55 298.15 300.90	5.88 6.07 6.11 6.55 6.70	11.3 11.5 11.6 12.3 12.5	11.7 12.1 12.3 13.4 13.8

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -5.3371 - 5.9346/(T/100K)$ 

Standard error about the regression line =  $2.88 \times 10^{-6}$ 

T/K	Mol Fraction
	$x_1 \times 10^4$
273.15	5.48
278.15	5.70
283.15	5.91
288.15	6.13
293.15	6.35
298.15	6.57
303.15	6.79

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

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

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Stuart Oxygen Co. Dried.
- (2) 1,1,2-Trichloro-1,2,2-trifluoroethane. Matheson, Coleman and Bell. Spectroquality.

### ESTIMATED ERROR:

# REFERENCES:

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Benzene; C₆H₆; [71-43-2]
- (3) 1,1,2-Trichloro-1,2,2-trifluoroethane or Freon 113; C₂Cl₃F₃; [76-13-1]

# ORIGINAL MEASUREMENTS:

Linford, R. G.; Hildebrand, J. H.

J. Phys. Chem. 1969, 73, 4410-4411.

# VARIABLES: T/K:

T/K: 298.15

P/kPa: 101.325 (1 atm)  $C_6H_6/x_2$ : 0.341, 0.695

PREPARED BY:

D. G. T. Thornhill

# EXPERIMENTAL VALUES:

T/K	Benzene Mol Fraction	Hydrogen Mol Fraction
	x ₂	10 ⁴ x x ₁
298.15	0.000 0.341 0.695 1.000	6.55 ^a 3.35 3.96 2.58 ^b

- a. Linford, R. G.; Hildebrand, J. H. Trans. Faraday Soc. 1970, 66, 577.
- b. Cook, H. W.; Hansen, D. N.; Alder, B. J. J. Chem. Phys. 1957, 26, 748.

The hydrogen solubility is almost a linear function of the benzene mole fraction. The equation  $x_1 = 6.63 \times 10^{-4} - 3.96 \times 10^{-4} x_2$  reproduces the hydrogen solubility with an average deviation of 2 per cent.

## AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Saturation of the liquid mixtures with dry gas. The gas solubilities were calculated from the initial and final Volumes and pressures of gas. The mole fraction solubilities of gas were corrected to 101.325 kPa (1 atm) partial pressure by Henry's law.

The Dymond-Hildebrand (1) apparatus was used. Each liquid mixture (total volume 250 cm³) was degassed by a freeze-thaw technique and loaded into the absorption vessel. Dry gas was then added to this vessel from a buret, and the liquid and gas were mixed together by means of a magnetically-operated all-glass pump. The pump allowed a thin film of liquid mixture to be repeatedly exposed to the gas, and thus speeded the attainment of equilibrium (c.a. 30 minutes).

# SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Stated to be highest purity commercially obtainable. Dried before use.
- (2) Benzene. Matheson, Coleman and Bell "Spectroquality". Used as received.
- (3) 1,1,2-Trichloro-1,2,2-trifluoroethane. Matheson, Coleman and Bell "Spectroquality". Used as received.

# ESTIMATED ERROR:

Temperature control was  $\pm$  0.05K (reference 1).  $\delta x_1/x_1 = \pm$  0.01 (evaluator).

# REFERENCES:

 Dymond, J. H.; Hildebrand, J. H. *Ind. Eng. Chem. Fundam.* <u>1967</u>, 6, 130.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1-Bromoheptane; C₇H₁₅Br; [629-04-9]

# ORIGINAL MEASUREMENTS:

Ijams, C. C.

Ph.D. thesis, <u>1941</u> Vanderbilt University Nashville, TN

### VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
298.15	3.99	0.0570	0.0622

The mole fraction and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co. was used.

The procedure of Van Slyke (1) for pure liquids was modified so that small solvent sample (2 cm³) could be used with almost 100 per cent recovery of the solvent.

An improved temperature control system was used.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) 1-Bromoheptane. Purified. Vapor pressure and boiling point also reported in the thesis.

### ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

# REFERENCES:

Van Slyke, D. D.
 J. Biol. Chem. 1939, 130, 545.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Carbon disulfide; CS2; [75-15-0]

### **EVALUATOR:**

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

1980, September

### CRITICAL EVALUATION:

Three laboratories have reported values of the solubility of hydrogen in carbon disulfide. Just (1) reported solubility measurements at 293.15 and 298.15 K which are 40 to 45 per cent smaller than more recent values. The Just data are rejected. Gjaldbaek (2) reported two solubility values near 298 K and Cook, Hanson and Alder (3) reported values at temperatures of 248.15, 273.15, and 298.15 K. The Gjaldbaek and the Cook et al. value agree within 2.5 per cent. Both sets of values are classed as tentative, however, the difference is greater than the accuracy claimed for the results of Cook et al. The tentative smoothed values are based entirely on a linear regression of the Cook et al. data.

The tentative equation for the mole fraction solubility over the 248.15 to 298.15 K temperature range is

$$\ln x_1 = -6.2421 - 7.4625/(T/100K)$$

with a standard error about the regression line of 1.19 x  $10^{-6}$ .

The values of the temperature independent changes in enthalpy and entropy for the transfer of one mole of hydrogen from the gas at 101.325 kPa to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 6.20 and  $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -51.9.

The smoothed values of the mole fraction solubility and partial molal Gibbs energy of solution are in Table 1.

Table 1. The solubility of hydrogen in carbon disulfide at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

т/к	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ \text{ mol}^{-1}$
248.15 258.15 268.15 278.15 288.15 298.15	0.962 1.081 1.204 1.330 1.460 1.593	19.083 19.602 20.121 20.640 21.159 21.678

# References:

- Just, G. Z. Phys. Chem. 1901, 37, 342.
- 2. Gjaldbaek, J. C. Acta Chem. Scand. 1952, 6, 623.
- 3. Cook, M. W.; Hanson, D. N.; Alder, B. J. J. Chem. Phys. 1957, 26, 748.

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Carbon disulfide; CS₂; [75-15-0] VARIABLES: T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha$ x $10^2$	Ostwald Coefficient L x 10 ²
293.15	0.842	3.128	3.358
298.15	0.931	3.438	3.753

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

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

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

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

# SOURCE AND PURITY OF MATERIALS:

- Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Carbon disulfide. No information.

# ESTIMATED ERROR:

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

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

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0]

ORIGINAL MEASUREMENTS: Gjaldbaek, J. C.

(2) Carbon disulfide; CS₂; [75-15-0]

Acta Chem. Scand. 1952, 6, 623-633.

VARTABLES:

297.97, 298.01 101.325 (1 atm) T/K: P/kPa:

PREPARED BY:

J. Chr. Gjaldbaek

EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
297.97	1.64	6.06	6.61
298.01		6.07	6.62

The Ostwald and mole fraction solubility values were calculated by the compiler. The solubilities are reported for an hydrogen partial pressure of 101.325 kPa (1 atm) assuming Henry's law is obeyed.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

A calibrated all-glass combined manometer and bulb was enclosed in an air thermostat and shaken until equilibrium. Mercury was used for Calibration and as the confining liquid. The solvents were degassed in the apparatus. Details are in reference 1.

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

# SOURCE AND FURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Freed from oxygen and dried. 99.5 per cent H2, 0.5 per cent N2.
- (2) Carbon disulfide. Merck. Analytical reagent grade. Distilled, boiling point 46.21 -46.26°C.

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

# REFERENCES:

1. Lannung, A. J. Am. Chem. Soc. 1930, 52, 68.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Carbon disulfide; CS₂; [75-15-0]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

### VARIABLES:

T/K: 248.15 - 298.15 P/kPa: 101.325 (1 atm)

### PREPARED BY:

P. L. Long H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Solubility ¹ mol g ⁻¹ x 10 ⁶	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient L
248.15	1.270	0.965	0.0378	0.0343
273.15	1.656	1.257	0.0478	0.0478
298.15	2.101	1.599	0.0591	0.0645

¹ Data from (1).

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -6.2421 - 7.4625/(T/100K)$ 

Standard error about the regression line =  $1.19 \times 10^{-6}$ 

See the evaluation of the hydrogen + carbon disulfide system for the recommended equation.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and (2) Carbon disulfide. Baker and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, after temperature equilibrium is reached, the gas is contacted with the degassed solvent. The system is shaken until solubility equilibrium is attained. Mercury is used as the displacement fluid.

The solubility is calculated from the REFERENCES: initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Co. Mass spectrographic analysis showed gas 99.75 per cent pure. Impurity mostly N2.
- Adamson Reagent Grade. Distilled, center portion used, b.p. 319.65K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$ 

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

²Recalculated by compiler from data in (1). Original paper gave 1.589.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Sulfinylbismethane or dimethylsulfoxide; C₂H₆OS; [67-68-5]

### **EVALUATOR:**

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

1980, September

### CRITICAL EVALUATION:

Two workers have reported solubility measurements on the hydrogen + dimethylsulfoxide system. Dymond (1) reports one solubility measurement at 298.15 K and Symons (2) reports six measurements over the 298.15 to 353.15 K temperature interval.

Both sets of data are classed as tentative. Dymond's experimental method is capable of better precision than Symons' method. The two agree well at the common temperature of measurement of 298.15 K. The temperature coefficient of solubility is determined by Symons data. The enthalpy of solution appears to be greater than expected when compared with the enthalpy of solution of similar solvents. Thus, there is reason to use the data with some caution.

A linear regression was applied to the seven mole fraction solubility values from the two papers to obtain the tentative equation for use between 298.15 and 353.15 K.

$$\ln x_1 = -6.0383 - 10.2726/(T/100K)$$

with a standard error of about the regression line of  $7.25 \times 10^{-6}$ .

The values of the temperature independent changes in enthalpy and entropy on transfer of one mole of hydrogen from the gas at  $101.325~\mathrm{kPa}$  to the infinitely dilute solution are

$$\Delta \overline{H}_{1}^{\circ}/kJ \text{ mol}^{-1}$$
 8.54 and  $\Delta \overline{S}_{1}^{\circ}/J \text{ K}^{-1} \text{ mol}^{-1}$  -50.2.

The smoothed values of mole fraction solubility and the partial molal Gibbs energy are in Table 1.

Table 1. The solubility of hydrogen in dimethylsulfoxide at a hydrogen partial pressure of 101.325 kPa.

Tentative values of the mole fraction solubility and partial molal Gibbs energy of solution as a function of temperature.

T/K	Mol Fraction $10^4 x_1$	$\Delta \overline{G}_1^{\circ}/kJ_{-mol}^{-1}$
298.15 308.15 318.15 328.15 338.15 348.15	0.76 0.85 0.945 1.04 1.14 1.25	23.51 24.01 24.51 25.02 25.52 26.02

# References:

- 1. Dymond, J. H. J. Phys. Chem. 1967, 71, 1829.
- Symons, E. A. Can. J. Chem. <u>1971</u>, 49, 3940.

# COMPONENTS: ORIGINAL MEASUREMENTS: Dymond, J. H. (1) Hydrogen; H₂; [1333-74-0] J. Phys. Chem. 1967, 71, 1829-1831. (2) Sulfinylbismethane or Dimethyl Sulfoxide; C2H6OS (CH3SOCH3); [67-68-5] VARIABLES: PREPARED BY: M. E. Derrick T/K: 298.15 P/kPa: 101.325 (1 atm) H. L. Clever EXPERIMENTAL VALUES: Bunsen Ostwald

T/K Mol Fraction Bunsen Coefficient  $x_1 \times 10^4$   $\alpha \times 10^2$  L x  $10^2$  298.15 0.761 2.39 2.61

The Bunsen and Ostwald coefficients were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The liquid is saturated with the gas at a gas partial pressure of 1 atm.

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Stuart Oxygen Co. Dried.
- (2) Dimethyl Sulfoxide. Matheson, Coleman, and Bell Co. Spectroquality reagent, dried, and a fraction frozen out. Melting pt.: 18.37°C.

ESTIMATED ERROR:

# REFERENCES:

1. Dymond, J.; Hildebrand, J. H.

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Sulfinylbismethane or dimethyl-sulfoxide; C₂H₆OS; [67-68-5]

## ORIGINAL MEASUREMENTS:

Symons, E. A.

Can. J. Chem. <u>1971</u>, 49, 3940 - 3947.

### VARIABLES:

T/K: 298.15 - 353.15 H₂ P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe t/°C	rature T/K	$C_{\rm H_2}/\text{mol dm}^{-3}$ $c \times 10^3$	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
25.0	298.15	1.05 ¹ 1.08 ¹	0.75 0.77	2.35 2.42	2.57 2.64
35.0	308.15	1.18	0.85	2.64	2.99
50.0	323.15	1.37	1.00	3.07	3.64
65.0	338.15	1.54	1.14	3.45	4.28
80.0	353.15	1.74	1.30	3.90	5.03

¹Values also quoted in Symons, E. A.; Buncel, E. Can. J. Chem. <u>1973</u>, 51, 1673. The mole fraction, Bunsen coefficient, Ostwald coefficient solubility values were calculated by the compiler.

SMOOTHED DATA:

 $\ln x_1 = -6.0375 - 10.2752/(T/100 K)$ 

Standard error about the regression line =  $8.10 \times 10^{-7}$ 

T/K	Mol Fraction $x_1 \times 10^4$
298.15	0.76
308.15	0.85
318.15	0.945
328.15	1.04
338.15	1.145
348.15	1.25

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Gas chromatographic method (1).

The gas-liquid equilibrium cell was a modified 100 cm³ round bottom flask equipped with magnetic stirrer, syringe sampling portal, and vacuum/gas line. The solvent was added, the flask evacuated several minutes to remove dissolved gases. The the gas was introduced to a partial pressure of one atm. The solution was stirred for five minutes, then sampled. Three to four successive samples were taken.

The 5.0 cm³ samples were taken by gas tight syringe. The sample was introduced to a stripping cell, stripped out over a period of 1-2 minutes by the nitrogen carrier gas and then passed into a Varian Aerograph (No. 1420) equipped with an injection portal, column (10' ½" stainless steel, packed with 40-60 mesh 13X molecular sieve) at ambient temperature, and a thermal conductivity cell at 65°C.

### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson Prepurified grade (99.5% min purity).
- (2) Sulfinybismethane. Fisher.
  Certified Reagent Grade. Dried
  48 h over 4A molecular sieves,
  vacuum distilled at ca. 1 mmHg.
  Fraction boiling 38-40°C was
  stored under nitrogen at ambient
  temperature for later use.

# ESTIMATED ERROR:

 $\delta T/K = 0.05$  $\delta c/c = 0.02$  (author's estimate)

# REFERENCES:

 Gubbins, K. E.; Carden, S. N.; Walker, R. D. Jr. J. Gas Chromatogr. 1965, 98.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclopentanamine or cyclopentylamine; C₅H₁₁N or C₅H₉NH₂; [1003-03-8]

# ORIGINAL MEASUREMENTS:

Symons, E. A.

private communication

### VARIABLES:

T/K: 203.15 - 298.15 P/MPa: 0.10 (1 atm)

### PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	erature	Mol Fraction 1	Bunsen	Ostwald
t/°C	<u>T/K</u>	x ₁ × 10 ⁴	Coefficient $\alpha \times 10^2$	Coefficient L x 10 ²
-70.0	203.15	1.04 ± 0.02 (2)	2.58	1.92
-50.0	223.15	$1.21 \pm 0.03 (4)$	2.95	2.41
-35.0	238.15	$1.48 \pm 0.01 (3)$	3.56	3.10
-20.1	253.05	$1.68 \pm 0.02 (5)$	3.98	3.69
-20.0	253.15	$1.73 \pm 0.09 (4)$	4.10	3.80
-16.7	256.45	$1.76 \pm 0.01 (4)$	4.15	3.90
-15.3	257.85	$1.77 \pm 0.03 (5)$	4.17	3.94
-10.0	263.15	$1.86 \pm 0.05 (4)$	4.37	4.21
- 5.0	268.15	$1.97 \pm 0.02 (3)$	4.59	4.51
+10.0	283.15	$2.22 \pm 0.03 (4)$	5.10	5.29
20.2	293.35	$2.50 \pm 0.03 (7)$	5.68	6.10
25.0	298.15	$2.44 \pm 0.04 (5)$	5.52	6.03

Mole fraction values are solubility ± range (number of samples). The data were provided by the author.

The Bunsen and Ostwald coefficients were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The gas-liquid equilibrium cell is a modified 100 cm³ r.b. flask equiped with a magnetic stirrer, and a sampling portal, and a vacuum/gas line. The solvent is added, and degassed by several evacuations. The gas is introduced to a one atm partial pressure. The solution is stirred for five minutes, then sampled. The stirring is continued while three to four successive samples are taken

The samples are taken in gas-tight syringes and weighed. The sample is introduced into a stripping cell, and stripped out over a 1-2 minute period. The sample then passes into a Varian Aerograph GLC by N2 carrier gas. The column is 10' ½" stainless steel, packed with 40-60 mesh 13X molecular sieve.aThe column is at ambient temperature, and the thermal conductivity cell is at 65 °C.

# SOURCE AND PURITY OF MATERIALS:

No information.

# ESTIMATED ERROR:

See ranges given with the data.

- Symons, E. A. Can. J. Chem. <u>1971</u>, 49, 3940.
- Symons, E. A.; Powell, M. E.;
   Schnittker, J. B.; Clermont, M. J.
   J. Am. Chem. Soc. <u>1979</u>, 101, 6704.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclohexanamine or cyclohexylamine; C₆H₁₃N or C₆H₁₁NH₂; [108-91-8]

# ORIGINAL MEASUREMENTS:

Symons, E. A.; Powell, M. E.; Schnittker, J. B.; Clermont, M. J.

J. Am. Chem. Soc. 1979, 101, 6704 - 6709.

### VARIABLES:

T/K: 258.15 - 288.15 H₂ P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

### EXPERIMENTAL VALUES:

Tempe	erature	Mol Fraction ¹	Bunsen Coefficient	Ostwald Coefficient
t/°C	<u>T/K</u>	x ₁ × 10 ⁴	$\frac{\alpha \times 10^2}{}$	L x 10 ²
-15.0	258.15	2.00 ± 0.09 (4)	4.06	3.84
-13.6	259.55	$1.90 \pm 0.09 (8)$	3.85	3.66
- 5.0	268.15	2.26 + 0.09 (4) - 0.07	4.54	4.46
+ 5.1	278.25	2.47 + 0.04 (4) - 0.09	4.91	5.00
15.0	288.15	$2.70 \pm 0.10 (5)$	5.32	5.61
15.2	288.35	$2.57 \pm 0.09 (10)$	5.06	5.34
25.0	298.15	$2.85^2 \pm 0.04$ (4)	5.55	6.06
25.0	298.15	2.91 ± 0.04 (4)	5.67	6.19

The mole fraction solubility values were provided by the author. Given is the mole fraction solubility ± range (number of samples).

The Bunsen and Ostwald coefficients were calculated by the compiler.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The gas-liquid equilibrium cell is a modified 100 cm³ round bottom flask equipped with a magnetic stirrer, syringe sampling portal, and vacuum/gas line. The solvent is added, the flask is evavuated several minutes to remove dissolved gases. The gas is introduced to a partial pressure of one atm. The solution is stirred for five minutes, then sampled. The stirring is continued while three to four successive samples are taken.

The samples are taken in a gas tight syringe and weighed. The sample is introduced into a stripping cell, stripped out over a period of 1-2 minutes, and then passed into a Varian Aerograph (No. 1420) by N2 carrier gas. The chromatograph is equiped with an injection portal, column (10' ½" stainless steel, packed with 40-60 mesh 13% molecular sieve) at ambient temperature, and a thermal conductivity cell at 65 °C.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Matheson of Canada, Ltd. Extra dry, 99.9 per cent.
- (2) Cyclohexanamine. Eastman Chemical Co. Original 97 per cent. Fractional distillation onto 4 A molecular sieves, dry over molten potassium. Impurity less than 0.02 weight % (gas chromatography), melting point/°C = -17.8 ± 0.1, ρ/g cm⁻³ = 0.868²/₄°.

# ESTIMATED ERROR:

$$\delta T/K = 0.05$$
  
 $\delta x_1/x_1 = 0.02$ 

# REFERENCES:

1. Symons, E. A. Can. J. Chem. 1971, 49, 3940.

 $^{^2}$  The solubility determined in the presence of cyclohexanamine, monocesium salt;  $\rm C_{6}H_{13}N.Cs;~4820-05-7$  , c/mol dm  3  0.0024.

COMPONENTS:	ORIGINAL MEASUREMENTS:	
(1) Hydrogen; H ₂ ; [1333-74-0]	Just, G.	
(2) Benzenamine or aniline; C ₆ H ₇ N; [62-53-3]	Z. Phys. Chem. <u>1901</u> , 37, 342 - 367.	
VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm)	PREPARED BY:  M. E. Derrick H. L. Clever	

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	1.15	2.826	3.033
298.15		2.610	2.849

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

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

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

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Benzenamine. No information.

# ESTIMATED ERROR:

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

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

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Cyclic amines; C4H9N, C5H5N, and C5H10N

# ORIGINAL MEASUREMENTS:

Guerry, D. Jr.

Ph. D. thesis, <u>1944</u> Vanderbilt University Nashville, TN

Thesis Director: L. J. Bircher

# VARIABLES:

T/K: 293.15, 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient a	Ostwald Coefficient L
Ру	rrolidine; C ₄ 1	H ₉ N; [123-75-1	]
293.15 298.15	2.17 2.39	0.0586 0.0642	0.0629 0.0701
Ру	ridine; C ₅ H ₅ N	; [110-86-1]	
293.15 298.15	1.48 1.62	0.0412 0.0449	0.0442 0.0490
Pi	peridine; C ₅ H.	11N; [110-89-1	]
293.15 298.15	2.49 2.58	0.0566 0.0582	0.0607 0.0635

The Ostwald coefficients were calculated by the compiler.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus was a modified Van Slyke-Neill Manometric Apparatus manufactured by the Eimer and Amend Co.

The procedure of Van Slyke (1) for pure liquids was modified (2) so that small solvent samples (2 cm³) could be used with almost 100 per cent recovery of the sample.

An improved temperature control system was used.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Air Reduction Co. Purity 99.5 per cent.
- (2) Cyclic amines. The pyridine and pyrrolidine were distilled from BaO under a N₂ atmosphere. The piperidine was distilled from KOH under a N₂ atmosphere. Experimental data on refractive index, density and vapor pressure are in the thesis.

# SOURCE AND PURITY OF MATERIALS:

Pyrrolidine. Pyrrole was prepared and catalytically reduced to pyrrolidine. B.p. (750 mmHg) t/°C 88.12 - 88.26 (corr.).

Pyridine. Mallincrodt Chemical Co. Purified and distilled. B.p. (743.9 mmHg) t/°C 114.96 - 115.06 (corr.).

Piperidine. Part was a commercial sample (Eastman Kodak Co.), part prepared by reduction of pyridine. B.p. (752.4 mmHg) t/°C 106.00-106.17. ESTIMATED ERROR:

 $\delta T/K = 0.05$ 

- Van Slyke, D. D.
   J. Biol. Chem. <u>1939</u>, 130, 545.
- 2. Ijams, C. C. Ph. D. thesis, 1941 Vanderbilt University

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Nitrobenzene; C₆H₅NO₂; [98-95-3] VARIABLES: T/K: 293.15 - 298.15 P/kPa: 101.325 (1 atm) ORIGINAL MEASUREMENTS: Just, G. Z. Phys. Chem. 1901, 37, 342 - 367. PREPARED BY: M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
293.15	1.51	3.292	3.533
298.15	1.56	3.397	3.708

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

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

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

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Prepared by the reaction of water with aluminum amalgam accelerated with mercury (II) chloride.
- (2) Nitrobenzene. No information.

# ESTIMATED ERROR:

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

- Timofejew, W.
   Physik. Chem. 1890, 6, 141.
- Steiner, Ann. Phys. (Leipzig) 1894, 52, 275.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 1,1,2,2,3,3,4,4,4-Nonafluoro-N,
  N-bis (nonafluorobutyl)-1butanamine or Perfluorotributylamine; C₁₂F₂₇N; [311-89-7]

# ORIGINAL MEASUREMENTS:

Powell, R. J.

J. Chem. Eng. Data 1972, 17, 302-304.

# VARIABLES:

T/K: 288.15 - 318.15 H₂ P/kPa: 101.325 (1 atm)

### PREPARED BY:

P. L. Long

# EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²	$\frac{\Delta \log X_1}{R \Delta \log T} = N$
298.15	15.52	9.76	10.7	3.28

The author states that solubility measurements were made between 288.15 and 313.15 K, but only the solubility at 298.15 was given in the paper. The slope R( $\Delta$ log X₁/ $\Delta$ log T) was given. The smoothed data below were calculated by the compiler from the slope in the form:

$$\log x_1 = \log(15.52 \times 10^{-4}) + (3.28/R)\log(T/298.15)$$

with R = 1.9872 cal  $K^{-1}$  mol⁻¹.

	_
T/K	Mol Fraction
÷	$x_1 \times 10^4$
288.15	14.67
293.15	15.10
298.15	15.52
303.15	15.95
308.15	16.39
313.15	16.83
318.15	17.28

The Bunsen and Ostwald coefficients were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Dymond and Hildebrand (1) apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressures. The solvent is degassed by freezing and pumping followed by boiling under reduced pressure.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Manufacturers research grade, dried over CaCl₂ before use.
- (2) Perfluorotributylamine.
   Minnesota Mining & Mfg. Co..
   Column distilled, used portion
   with b.p. = 447.85 448.64 K,
   & single peak GC.

# ESTIMATED ERROR:

$$\delta N/\text{cal } K^{-1} \text{ mol}^{-1} = 0.1$$
  
 $\delta X_1/X_1 = 0.002$ 

# REFERENCES:

 Dymond, J. H.; Hildebrand, J. H. *Ind. Eng. Chem. Fundam.* <u>1967</u>, 6, 130.

	:		ORIGINAL MEASUREMENTS:	
l. Hydro	ogen: Ho: [133	3-74-01	Chappelow, C.C.; Prausnitz, J.M.	
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Cyclotetrasiloxane,octamethyl-; C₆H₂ 4O₄Si₄; [556-67-2]</li> </ol>		,octamethyl-;	Am. Inst. Chem. Engnrs. J. 1974, 20, 1098-1104	
VARIABLES: Temperature			PREPARED BY: C.L. Young	
EXPERIMENT	AL VALUES:		L	
	T/K	Henry's Con /atm	stant ^a Mole fraction ^b of hydrogen at 1 atm partial pressure, ${}^x{ m H}_2$	
	300	706	0.00142	
	325	622	0.00161	
	350	555	0.00180	
	375	490	0.00204	
	400	420	0.00238	
	425	338	0.00296	
	h Calania	tod by sompiler	region.	
		mole fraction a	assuming linear relationship nd pressure.	
		mole fraction a	assuming linear relationship	
Volumetr: described (1). Pres	PARATUS/PROCEI ic apparatus s d by Dymond as ssure measured and precision	AUXILIARY DURE similar to that	assuming linear relationship nd pressure.	

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Petroleum VARIABLES: T/K: 283.15, 293.15 Pressure: "atmospheric" ORIGINAL MEASUREMENTS: Gniewosz, S.; Walfisz, A. Z. Physik. Chem. 1887, 1, 70 - 72. M. E. Derrick H. L. Clever

# EXPERIMENTAL VALUES:

т/к	Bunsen Coefficient a	Ostwald Coefficient L
283.15	0.0652	0.0676
293.15	0.0582	0.0625

The Ostwald coefficient was calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of an absorption flask connected to a gas buret by a flexible lead capillary. The system was thermostated in a large water bath.

The volume of gas absorbed in a volume of the degassed liquid was measured using the gas buret.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. No information.
- (2) Petroleum. Russian petroleum. Cleaned by boiling in a large copper flask.

# ESTIMATED ERROR:

 $\delta\alpha/\alpha = 0.10$  (compiler)

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] (2) Oils Daniel, S. G. J. Appl. Chem. 1952, 2, 161 - 165. J. Inst. Petrol., London, 1953, 39, 105 - 124. VARIABLES: T/K: 273.15 - 373.15 H₂ P/kPa: 101.325 (1 atm) PREPARED BY: P. L. Long H. L. Clever

# EXPERIMENTAL VALUES:

Runsen	Ostwald
	Coefficient
	L
A.2. viscosity 268	R centistokes at
r, mean mor we or	
0.0421	0.0421
0.0465	0.0499
0.0526	0.0642
0.0590	0.0806
0.0020	0.000
A.5. viscosity 34.	9 centistokes
oo i, mean mei we	. 400.
0.0452	0.0452
0.0483	0.0518
0.0549	0.0669
0.0658	0.0899
0.0000	0.0000
	0.0465 0.0526 0.0590 A.5, viscosity 34. 00 °F, mean mol wt 0.0452 0.0483

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

- 1. Degassing. The liquid was deaerated by passage through a continuously evacuated vessel. The liquid was saturated with the gas, then degassed again.
- 2. Saturation of liquid with gas. The gas was passed through a liquid air trap to remove water and carbon dioxide, then through a long coil thermostated at the temperature of the solubility measurement, and then bubbled through the liquid up to five hours.
- 3. Determination of the amount of gas liberated under vacuum from a known volume of the saturated liquid. The saturated liquid is placed in a vessel attached to a calibrated buret. The whole apparatus is intially evacuated. The gas released from the liquid was transferred to the calibrated buret by a Topler pump. Five operations and transfers recover all but a trace of the gas. The last trace (2 5 %) was removed by boiling.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Commercial cylinders, source not given. Gas analysis on a Bone and Wheeler apparatus shows gas to be at least 99.5 %.
- (2) Oils. The oils conform to DTD-472B specifications. Composition and physical properties of the oils are given in the appendix of the 1953 paper. The molecular weights were determined by freezing point depression in naphthalene (±5 %).

ESTIMATED ERROR:

 $\delta\alpha/\alpha = 0.01$  $\delta P/P = 0.01$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen; H ₂ ; [1333-74-0]	Nasini, A. G.; Corinaldi, G.
(2) Paraffin oil	Soc. Ital. Prog. Sci. Atti. Riun. 1932, 20, 264 - 266.
VARIABLES:	PREPARED BY:
T/K: 305.15 P/kPa: 101.325 (1 atm)	A. L. Cramer H. L. Clever
EXPERIMENTAL VALUES:	
T/K Bunsen* Coefficie α	Ostwald ent Coefficient L
305.15 0.0464	0.0518
*Original datum.	
AUXILIAR	Y INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus and procedure were based on those of Lannung (1).	(1) Hydrogen. Tank gas freed of oxygen by passage over red-hot metal.
	(2) Paraffin oil. Density, $\rho_{15}^{15} = 0.87$
	ESTIMATED ERROR:
	δT/K = 0.1
	REFERENCES:
	1. Lannung, A. J. Am. Chem. Soc. <u>1930</u> , 52, 68.

2/2 Trydiogen d	Join Miles up to 200Ki u
COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen; H ₂ ; [1333-74-0]	Vibrans, F. C.
(2) Vegetable oils	0il and Soap <u>1935</u> , 12, 14 - 15.
VARIABLES:	PREPARED BY:
T/K: 296.15 - 318.15	P. L. Long H. L. Clever
EXPERIMENTAL VALUES:	
T/K cm ³ (27	3.15 K,1 atm) H ₂ 100 cm ⁻³
Corn oil	

T/K	$cm^3$ (	273.15 1	K,1 atm	H ₂ 100 cm ⁻³	
					<u>av.</u>
Corn oi	l				
296.15-299.1					4.08
318.15	4.46	4.46	4.42	4.45	4.44
Cottons	eed oil				
296.15-299.1	5 4.12	4.32			4.22
318.15	4.28	4.22	4.28	4.38	4.29
Hydroge:	nated cot	tonseed	oil		
318.15	4.24	4.36			4.30

# AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: (1) Hydrogen. From commercial cylin-Van Slyke manometric method used (1). ders, source or purity not stated. (2) Corn oil. Commercial sample bought on the market. Represent - tive of its class. Cottonseed oil. Commercial sample bought on the market, representative of its class. ESTIMATED ERROR: $\delta T/K = 3$ at room T = 2 at 318 K $\delta c/c = 0.04$ REFERENCES: 1. Van Slyke, D. D.; et al. J. Biol. Chem. 1924, 61, 523 and 575.

Miscellaneous and Biological Fluids 273 COMPONENTS: ORIGINAL MEASUREMENTS: (1) Hydrogen; H₂; [1333-74-0] Vibrans, F. C. (2) Lard 0il and Soap 1935, 12, 14 - 15. VARIABLES: PREPARED BY: T/K: 318.15 P. L. Long P/kPa: 101.325 H. L. Clever EXPERIMENTAL VALUES: _  $cm^3$  (273.15 K, 1 atm)  $H_2$  100  $cm^{-3}$ T/K 318.15 4.16 4.24 4.26 4.43 4.27 av.

AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The manometric method of Van Slyke

(1) was used.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. From commercial cylinders, source and purity not given.
- (2) Lard. Made from a mixture of killing and cutting fats, steam rendered.

ESTIMATED ERROR:

$$\delta T/K = 2$$

$$\delta c/c = 0.04$$

#### REFERENCES:

Van Slyke, D. D.; et al.
 J. Biol. Chem. 1924, 61, 523
 and 575.

# COMPONENTS: (1) Hydrogen; H₂; [1333-74-0] Schaffer, P. S.; Haller, H. S. (2) Animal and vegetable oils Oil and Soap 1943, 20, 161 - 162. VARIABLES: T/K; 313.15, 333.15 P/kPa: 101.325 (1 atm) PRIGINAL MEASUREMENTS: Schaffer, P. S.; Haller, H. S. Oil and Soap 1943, 20, 161 - 162. PREPARED BY: P. L. Long H. L. Clever

T/K cm³ (273.15, 1 atm) H₂ 100 cm⁻³

Cottonseed oil

313.15 4.7

Butter oil

313.15 5.4

313.15 5.4 333.15 6.8 Lard

The authors solubility unit is the Bunsen coefficient x 100.

5.0

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus consists of a reaction flask connected to a water jacketed gas buret, a mercury leveling bulb, and a differential manometer. The reaction vessel is attached to a shaking mechanism in an air bath.

313.15

A 50 cm³ sample of oil is placed in the flask. Heat and vacuum are applied to remove dissolved gases. The sample is cooled to the temperature of the measurement. Hydrogen gas is admitted, a zero reading taken. Shaking is continued until the sample takes up no more gas at a pressure of l atm. Three determinations were made on each sample.

#### SOURCE AND PURITY OF MATERIALS:

- Hydrogen. From commercial cylinders, source and purity not given, used as received.
- (2) Cottonseed oil. Good grade commercial product.

Butter oil. Obtained from butter prepared in the lab from fresh cream.

Lard. Good grade commercial product.

#### ESTIMATED ERROR:

 $$\delta T/K = 0.5$$$ $\delta c/c = 0.003$ (Authors, error among three determinations)$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Power, G.G.; Stegall, H.  J. Appl. Physiology, 1970, 29,
2. Olive oil.	145-9.
VARIABLES:	PREPARED BY:
	C.L. Young.
EXPERIMENTAL VALUES:	
T/K Bunsen coefficient, α	S.D.* No. of measurements
310.15 0.0436	0.0003 5
* Standard deviation.	
	•
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Liquid saturated with gas in a	1. Matheson Co. sample, purity
stirred cell. 5.0 cm samples	better than 99.7 mole per cent.
Of liquid removed in a calibrated syringe and amount of gas extracted	
by two extraction in a van Slyke	2. No details given.
apparatus determined. Details in source and ref. (1).	
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1$
	, , , , , , , , , , , , , , , , , , , ,
	REFERENCES:
	1. Power, G.G. J. Appl. Physiology, 1968, 24, 468.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Longo, L. D.; Delivoria-
2. Sheep placental tissue	Papadopoulas, M.; Power, G. G.;
	Hill, E. P.; Forster, R. E.,
	Am. J. Physiology, <u>1970</u> , 219,
	561-569.
VARIABLES:	PREPARED BY:
	C. L. Young
EXPERIMENTAL VALUES:	
T/K Bunsen coeffi	cient, α S.D.*
310.15 0.0165	0.0004
* standard deviation	
AUXILIARY	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Liquid samples were equilibrated	
	No details siven
with gas and then the dissolved gas	No details given.
was stripped out under vacuum and	1
measured in a manometric Van Slyke	
apparatus. Some details in ref. 1.	
	1
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.03.$
	REFERENCES:
	1. Power, G. G.,
	J. Appl. Physiology, <u>1968</u> , 24, 468.
	100.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen; H ₂ ; [1333-74-0] (2) Rat abdominal muscle	Campos Carles, A.; Kawashiro, T.; Piiper, J.  Pflugers Arch. 1975, 359, 209 - 218.
VARIABLES: T/K: 310.15	PREPARED BY:  A. L. Cramer  H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Solubility Coefficient µmol dm ⁻³ torr ⁻¹	Corrected ² Solubility Coefficient µmol dm ⁻³ torr-1	Bunsen Coefficient $\alpha \times 10^2$
310.15	1.00 ± 0.05 ¹	1.13	1.92

¹ Mean value ± standard error of 11 measurements.

Another report from this laboratory gives Krogh's diffusion constant, K = (1.67  $\pm$  0.06) x 10-9 mmol m⁻¹cm⁻¹ torr⁻¹, and the diffusion coefficient, D = 24.7 x 10⁻⁶ cm² s⁻¹ for hydrogen in rat abdominal muscle at 310.15 K. The sample is a non-homogenised solid, not a liquid.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The hydrogen gas was presaturated with water vapor, then passed through an equilibration chamber containing the muscle sample resting on a screen to expose all sides. The gas was passed through the equilibration chamber for one hour at a rate of 8 cm³ m⁻¹.

The muscle was transfered to an extraction chamber filled with air for the same length of time as equilibration. The gas in the extraction chamber was then forced into a gas chromatograph by mercury entering the chamber.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Source not given. Stated to be 99.9 per cent pure.
- (2) Rat abdominal muscle. Flat abdominal wall muscle layer of about 1.6 g, 1.4 mm thick, and surface area of 10 cm² on one side. Sample taken from 250 430 g rat.

# ESTIMATED ERROR:

# REFERENCES:

 Kawashiro, T.; Campos Carles, A.; Perry, S. F.; Piiper, J. Pflugers Arch. 1975, 359, 219.

² Corrected for unextracted gas in the sample, and for gas lost during transfer of the sample.

# COMPONENTS: ORIGINAL MEASUREMENTS: (1) Deuterium; D₂; [7782-39-0] Symons, E. A.; Buncel, E. (2) Water; H₂O; [7732-18-5] Can. J. Chem. 1973, 51, 1673 - 1681. VARIABLES: PREPARED BY:

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

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	$c_{D_2}/mol dm^{-3}$ $c \times 10^4$	Mol Fraction  x1 × 10 ⁵	Ostwald Coefficient L x 10 ³
298.15	8.3	1.50	20.5

The mole fraction and Ostwald coefficient values were calculated by the compiler.

The value is 2.7 per cent higher than the value reported at 298.15 K by Muccitelli, J. and Wen, W.-Y. J. Solution Chem. 1978, 7, 257. The Muccitelli and Wen values are preferred.

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Gas chromatographic method (1, 2).

The gas-liquid equilibrium cell was a modified 100 cm³ round bottom flask equiped with magnetic stirrer, syringe sampling portal, and vacuum/gas line. The solvent was added, the flask evacuated several minutes to remove dissolved gases. Then the gas was introduced to a partial pressure of one atm. The solution was stirred for five minutes, then sampled. Three to four successive samples were taken.

The  $5.0 \text{ cm}^3$  samples were taken by gas tight syringe. The sample was introduced to a stripping cell, stripped out over a period of 1-2 minutes by the nitrogen carrier gas and then passed into a Varian Aerograph (No. 1420) equiped with an injection portal, column (10' %" stainless steel, packed with 40-60 mesh 13X molecular sieve) at ambient temperature, and a thermal conductivity cell at 65 °C.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Matheson Co., Inc. Technical grade. Traces of oxygen removed by treatment with uranium turnings.
- (2) Water. Deionized and distilled.

#### ESTIMATED ERROR:

 $\delta c/c = 0.02$  (author's estimate)

- 1. Symons, E. A. Can. J. Chem. 1971, 49, 3940.
- 2. Gubbins, K. E.: Carden, S. N.; Walker, R. D. Jr. J. Gas Chromatogr. 1965, 98.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Water; H₂O; [7732-18-5]

# ORIGINAL MEASUREMENTS:

Muccitelli, J.; Wen, W.-Y.

J. Solution Chem. 1978, 7, 257 - 267.

#### VARIABLES:

T/K: 278.15-303.15 P/kPa: 101.325 (1 atm)

#### PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

EXPERIMENTAL VALUES:				
	T/K	mol Fraction	Ostwald Coefficient	
		x ₁ x 10 ⁵	L x 10 ³	
	278.15	1.7829	22.795	
		1.7904	22.891	
		1.7891	22.875	
	000 75	1.7851	22.824	
	283.15	1.6825	21.970	
		1.6691	21.795	
		1.6757	21.882	
		1.6802 1.6714	21.940 21.825	
	288.15	1.6028	21.323	
	200.13	1.5936	21.265	
		1.5948	21.281	
		1.5892	21.207	
	293.15	1.5175	20.714	
		1.5118	20.636	
		1.5187	20.731	
		1.5016	20.559	
	298.15	1.4637	20.469	
		1.4555	20.354	
		1.4663	20.505	
		1.4569	20.374	
	303.15	1.3980	20.069	
		1.3901	19.956	
		1.3978	20.066	
		1.3952	20.029	

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure were similar to that described by Ben-Naim and Baer (1) as modified by Wen and Hung (2). It consisted of a mercury manometer, a gas-volume measuring buret, a dissolution cell of 450 cm³ capacity, and a mercury reservoir. The apparatus is immersed in a water bath. The degassing apparatus was similar to the one described by Battino et al. (3). The cell containing the solvent is degassed, the system is filled with solvent-saturated gas to a total pressure of 1 atm. The solvent is stirred, as gas dissolves the pressure is maintained at one atm until equilibrium is reached.

The measured Ostwald coefficient was converted to mole fraction taking in to account the second virial coefficient of  $D_2$ . The authors fitted the data to the equation

R ln (x/p) = -360.180 + 14525.6/(T/K)52.0206 ln (T/K) - 0.0234788 (T/K)

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Linde Speciality Gas. Minimum specified purity 99.5 per cent. Used as received.
- (2) Water. Distilled, then purified with the Millipore Corp. Milli-Q system.

#### ESTIMATED ERROR:

 $\begin{array}{lll} \delta T/K = & 0.005 \\ \delta P/torr = & 3 \\ \delta L/L = & 0.004 & (precision, \\ & & authors) \end{array}$ 

- Ben-Naim, A.; Baer, S. Trans. Faraday Soc. <u>1963</u>, 59, 2735.
- Wen, W.-Y.; Hung, J. H.
   J. Phys. Chem. 1970, 74, 170.
- 3. Battino, R.; Banzhof, M.; Bogan, M.; Wilhelm, E. Anal. Chem. 1971, 43, 806.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Organic solvents

**EVALUATOR:** 

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

1980, September

CRITICAL EVALUATION:

An Evaluation of the Deuterium Mole Fraction Solubility in Various Organic Solvents at a Deuterium Partial Pressure of 101.325 kPa (1 atm).

The solubility of deuterium in eleven organic solvents has been reported. There is only one set of measurements on each system, except for sulfinylbismethane for which two laboratories reported measurements at 298.15 K. Most of the solubility measurements were made by volumetric methods capable of better than average accuracy and precision (1, 2, 4). One laboratory (3, 5) used a gas chromatographic method, which may not be capable of as good an accuracy and precision. However, their work appears to have been carefully executed and all of the data are classed as tentative.

Tentative equations for the natural logarithm of the mole fraction solubility as a function of temperature, and a table of smoothed values of the mole fraction solubility appear on the individual data sheets, with the exception of the deuterium + cyclopentanamine system which did not have room on the sheet for the additional information. The smoothed data on the system is at the end of this section.

The changes in enthalpy, entropy and heat capacity for the transfer of one mole of deuterium from the gas phase at a deuterium partial pressure of  $101.325~\mathrm{kPa}$  to the infinitely dilute solution are summarized in Table 1 for the eleven systems.

The mole fraction solubilities of four of the systems studied by Cook, Hanson, and Alder (1) show a systematic curvature in  $\ln x_1$  as a function of 1/T. The measurements of Cook  $et\ al$ . were made with great care, and there is reason to believe the curvature is real. Thus the mole fraction solubilities of the four systems were fitted to a three constant equation, and values of the temperature dependent changes in enthalpy and entropy at 25 degree intervals are given in Table 1.

Both Dymond (2), and Symons and Buncel (3) measured the mole fraction solubility of deuterium in dimethylsulfoxide at  $298.15~\mathrm{K}$ . The two values agree within  $0.6~\mathrm{per}$  cent.

Table 1. Deuterium + organic solvent. Summary of the changes in enthalpy,  $\Delta \overline{H}_1^o$ , entropy,  $\Delta \overline{S}_1^o$ , and heat capacity,  $\Delta \overline{C}_{p_1}^o$ , on transfer of one mole of deuterium from the gas phase at a partial pressure of 101.325 kPa to the infinitely dilute solution.

T/K	$\Delta \overline{H}_1^{\circ}/kJ \text{ mol}^{-1} \Delta \overline{S}_1^{\circ}$	$\frac{1}{2}$ /J K ⁻¹ mol ⁻¹ $\Delta \overline{C}_p^o$	/J K ⁻¹ mol ⁻¹
Deuterium	+ Heptane [142-82	2-5] (1) 1	
248.15 273.15 298.15 323.15	3.42 3.79 4.17 4.54	-49.1 -47.7 -46.4 -45.2	14.8 14.8 14.8 14.8
Deuterium	+ Octane [111-65-	-9] (1)	
248.15 273.15 298.15	3.35 3.74 4.14	-49.4 -47.9 -46.5	15.7 15.7 15.7
Deuterium	+ 2,2,4-Trimethyl	pentane [540-84-1	1] (1)
248.15 273.15 298.15	3.14 3.50 3.87	-49.0 -47.6 -46.3	14.6 14.6 14.6
Deuterium	+ Benzene [71-43-	2] (1)	
283.15-308.15	6.18	-47.7	0
Deuterium	+ Methylbenzene [	108-88-3] (1)	
258.15-308.15	4.83	-50.5	0
Deuterium	+ Hexadecafluoroh	eptane [335-57-9]	(1)
248.15 273.15 298.15	3.39 3.89 4.39	-43.3 -41.4 -39.6	20.1 20.1 20.1
Deuterium	+ Tetrachlorometh	ane [56-23-5] (1)	
273.15-308.15	5.38	-48.6	0
Deuterium	+ Carbon disulfid	e [75-15-0] (1)	
248.15-298.15	5.80	-53.1	0
Deuterium	+ Sulfinylbismeth	ane ² [67-68-5] (2,	3)
Only two solubino temperature the calculation	ility values at 29 coefficient of sons.	8.15 K are reporte lubility on which	ed. There is to base
Deuterium	+ Perfluorotribut	ylamine [311-89-7]	(4)
288.15-318.15	3.85	-40.6	0
· Deuterium	+ Cyclopentenamin	e [1003-03-8] (5)	
213.15-298.15	4.93	-51.8	0

 $^{^{\}mathrm{l}}$  Numbers in ( ) are the reference numbers.

² Dimethylsulfoxide.

Deuterium + Cyclopentanamine [1003-03-8]

The smoothed data are presented here, because there were not room for them on the data sheet of Symons (5). The tentative equation for use over the 213.15 to 298.15 K temperature range is

$$\ln x_1 = -6.2335 - 5.9271/(T/100K)$$

with a standard error about the regression line of  $6.03 \times 10^{-6}$ . The smoothed values of the mole fraction solubility are in Table 2.

Table 2. Solubility of deuterium in cyclopentanamine at a partial pressure of deuterium of 101.325 kPa. Tentative values of the mole fraction solubility.

T/K	Mol Fraction $10^4 x_1$	т/к	Mol Fraction 10 ⁴ x ₁
213.15	1.22	273.15	2.24
223.15	1.38	278.15	2.33
233.15	1.54	283.15	2.42
243.15	1.71	288.15	2.51
253.15	1.89	293.15	2.60
263.15	2.06	298.15	2.69

#### References:

- Cook, M. W.; Hanson, D. N.; Alder, B. J. J. Chem. Phys. <u>1957</u>, 26, 748.
- 2. Dymond, J. H. J. Phys. Chem. 1967, 71, 1829.
- 3. Symons, E. A.; Buncel, E. Can. J. Chem. 1973, 51, 1673.
- 4. Powell, R. J. J. Chem. Eng. Data 1972, 17, 302.
- 5. Symons, E. A. In press.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Heptane; C₇H₁₆; [142-82-5]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N. Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

#### **EXPERIMENTAL VALUES:**

T/K	Solubility mol g ⁻¹ x 10 ⁶	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
238.15(s	ic)¹ 5.002	5.009	8.13	7.24
248.15	5.168 6.160	5.172	8.35	7.58
263.15	5.697	5.705	9.05	8.71
273.15	6.069 6.069	6.077	9.52	9.52
283.15	6.447	6.456	9.99	10.36
294.65	6.881	$6.891^{2}$	10.52	11.34
298.15	7.014 7.025 7.023 7.033 7.024 av.	7.033	10.69	11.67
308.15	7.406 7.410 7.430 7.424 7.429			
	7.420 av.	7.437	11.16	12.59
323.15	8.051	8.061 ²	11.87	14.04
338.15	8.741	8.752 ²	12.64	15.65

¹Context of paper indicates the temperature is 243.15 instead of 238.15.
²Calculated by the compiler.

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data: Solubility values at 323.15 and 338.15 K were omitted from the fit.

 $\ln x_1 = -9.3132 + 0.3106/(T/100K) + 1.7845 \ln (T/100K)$ 

Standard error about the regression line =  $4.72 \times 10^{-7}$ 

T/K	Mol Fraction X ₁ × 10 ⁴
243.15 253.15 263.15 273.15 283.15 293.15 298.15 303.15 313.15 323.15	5.005 5.351 5.707 6.074 6.450 6.837 7.034 7.233 7.640 8.056 8.481

COMPONENTS:

(1) Deuterium; D2; [7782-39-0]
(2) Heptane; C7H16; [142-82-5]

VARIABLES:

T/K: 243.15 - 338.15

P/kPa: 101.325 (1 atm)

ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.;
Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

EXPERIMENTAL VALUES:

See preceding page.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quanties of gas, the pressure measurments, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly  $N_2$  with a small amount of HD.
- (2) Heptane. Phillips Petroleum Co. 99 mole per cent grade distilled, used center cut, boiling point 371.45 K. Other solvent properties given in reference 1.

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$ 

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Octane; C₈H₁₈; [111-65-9]

#### ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

# VARIABLES:

248.15 - 308.15 T/K: P/kPa: 101.325 (1 atm)

#### PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

т/к	Mol Fraction  x 1 × 10 4	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
248.15	5.167	7.49	6.80
273.15	6.047	8.53	8.53
298.15	6.990	9.58	10.46
308.15	7.389	10.02	11.30

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -9.5382 + 0.6414/(T/100K) + 1.8834 \ln (T/100)$ 

Standard error about the regression line =  $1.98 \times 10^{-7}$ 

T/K	Mol Fraction
	$x_1 \times 10^4$
253.15	5.338
263.15	5.687
273.15	6.047
283.15	6.417
293.15	6.798
298.15	6.992
303.15	7.189
308.15	7.388

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath. (2) Octane. Eastman Kodak Co.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly N₂ with a small amount of HD.
- Distilled, center portion used, b.p. 398.65 K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.001 \text{ (authors)}$$

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. <u>1957</u>, 28, 370.

- (1) Deuterium; D₂; [7782-39-0]
- (2) 2,2,4-Trimethylpentane or isooctane;  $C_8H_{18}$ ; [540-84-1]

#### ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N. Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

#### VARTABLES:

T/K: 248.15 - 308.15 P/kPa: 101.325 (1 atm)

#### PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

Т/К	Mol Fraction  x ₁ x 10 ⁴	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
248.15	6.004	8.58	7.80
273.15	6.960	9.67	9.67
298.15	7.960	10.74	11.72
308.15	8.396	11.19	12.63

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -9.2434 + 0.5759/(T/100K) + 1.7534 \ln (T/100K)$ 

Standard error about the regression line =  $1.10 \times 10^{-6}$ 

T/K	Mol Fraction
	x_1 × 10 4
253.15	6.190
263.15	6.569
273.15	6.957
283.15	7.354
293.15	7.762
298.15	7.969
303.15	8.179
308.15	8.391
263.15 273.15 283.15 293.15 298.15 303.15	6.569 6.957 7.354 7.762 7.969 8.179

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath. (2) 2,2,4-Trimethylpentane. Phillips

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the REFERENCES: initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly  $\rm N_2$  with a small amount of HD.
- Petroleum Co. Pure grade, 99+ mol per cent. Distilled, center portion used, b.p. 372.35 K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$  (authors)

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Benzene; C₆H₆; [71-43-2]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N. Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

#### **VARIABLES:**

T/K: 283.15 - 308.15 P/kPa: 101.325 (1 atm)

#### PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient
	² 1 × 10	$\alpha \times 10^{2}$	<u>L x 10²</u>
283.15	2.328	5.94	6.16
298.15	2.655	6.66	7.26
308.15	2.881	7.13	8.05

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -5.7399 - 7.4344/(T/100K)$ 

Standard error about the regression line =  $1.59 \times 10^{-7}$ 

T/K	Mol Fraction
	x ₁ × 10 ⁴
283.15 288.15 293.15 298.15 303.15 308.15	2.328 2.436 2.546 2.656 2.768 2.880

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the Vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given.
  Mass spectrographic analysis
  showed gas 99.4 per cent pure.
  Impurity mostly N₂ with a small
  amount of HD.
- (2) Benzene. Baker and Adamson's Reagent Grade. Distilled, center portion used, b.p. 353.15K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$ 

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, <u>1954</u>.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. <u>1957</u>, 28, 370.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Methylbenzene or toluene; C₇H₈; [108-88-3]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

#### VARIABLES:

T/K: 258.15 - 308.15 P/kPa: 101.325 (1 atm)

#### PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient
258.15	2.424	$\frac{\alpha \times 10^2}{5.30}$	L x 10 ² 5.01
273.15 298.15	2.730 3.266	5.88 6.85	5.88 7.48
308.15	3.492	7.25	8.18

The Bunsen and Ostwald coefficients were calculated by compiler.

Smoothed Data:  $\ln x_1 = -6.0781 - 5.8052/(T/100K)$ 

Standard error about the regression line =  $8.87 \times 10^{-7}$ 

T/K	Mol Fraction
	x ₁ × 10 ⁴
263.15	2.525
273.15	2.737
283.15	2.951
293.15	3.164
298.15	3.271
303.15	3.378
308.15	3.485

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly N₂ with a small amount of HD.
- (2) Methylbenzene. Baker and Adamson Reagent Grade. Distilled, center portion used, b.p. 383.65K. Other solvent properties given in reference (1).

#### ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$ 

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. <u>1957</u>, 28, 370.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Hexadecafluoroheptane or perfluoroheptane; C₇F₁₆; [335-57-9]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

#### VARIABLES:

T/K: 248.15 - 308.15 P/kPa: 101.325 (1 atm)

#### PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

т/к	Mol Fraction  x ₁ × 10 ⁴	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
248.15	10.556	10.99	9.98
273.15	12.403	12.64	12.64
285.25	13.371	13.48	14.08
298.15	14.427	14.38	15.69
308.15	15.329	15.14	17.08

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -9.8296 + 1.9302/(T/100K) + 2.4186 \ln (T/100K)$ 

Standard error about the regression line =  $1.50 \times 10^{-6}$ 

T/K	Mol Fraction
	$x_1 \times 10^4$
253.15	10.91
263.15	11.64
273.15	12.40
283.15	13.19
293.15	14.02
298.15	14.44
303.15	14.88

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. All are attached to a mounting plate, and the assembly is shaken in an air bath.

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly N₂ with a small amount of HD.
- (2) Hexadecafluoroheptane. Source not given. Distilled, center portion used, b.p. 355.65K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

$$\delta x_1/x_1 = 0.001$$
 (authors)

- Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. <u>1957</u>, 28, 370.

- (1) Deuterium; D₂; [7782-39-0]
- (2) Tetrachloromethane or carbon tetrachloride; CCl,; [56-23-5]

# ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748 - 751.

#### VARIABLES:

T/K: 273.15 - 308.15 101.325 (1 atm) P/kPa:

#### PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient	Ostwald Coefficient
273.15	2.693	$\frac{\alpha \times 10^2}{6.41}$	$\frac{\text{L} \times 10^2}{6.41}$
298.15 308.15	3.280 2.527(sic)	7.57 8.04 ¹	8.26 9.07 ¹

¹ The compiler suspects the mole fraction value is 3.527. The Bunsen and Ostwald coefficients and the smoothed data equation were calculated with the 3.527 value.

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -5.8498 - 6.4741/(T/100K)$ 

Standard error about the regression line =  $5.23 \times 10^{-7}$ 

T/K	Mol Fraction
	$x_1 \times 10^4$
273.15	2.692
278.15	2.809
283.15	2.927
288.15	3.046
293.15	3.165
298.15	3.284
303.15	3.404
308.15	3.524

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. are attached to a mounting plate, and the assembly is shaken in an air bath (2) Tetrachloromethane. Baker and

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the displacement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly N2 with a small amount of HD.
- Adamson Reagent Grade. Distilled, center portion used, b.p. 349.95K. Other solvent properties given in reference (1).

ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001$  (authors)

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

- (1) Deuterium, D₂; [7782-39-0]
- (2) Carbon disulfide; CS₂; [75-15-0]

ORIGINAL MEASUREMENTS:

Cook, M. W.; Hanson, D. N.; Alder, B. J.

J. Chem. Phys. 1957, 26, 748-751.

#### VARIABLES:

T/K: 248.15 - 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

P. L. Long H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction	Bunsen	Ostwald
	$x_1 \times 10^4$	Coefficient	Coefficient
		$\alpha \times 10^2$	L x 10 ²
248.15	1.011	3.96	3.60
273.15	1.300	4.95	4.95
298.15	1.621	5.99	6.54

The Bunsen and Ostwald coefficients were calculated by the compiler.

Smoothed Data:  $\ln x_1 = -6.3884 - 6.9802/(T/100K)$ 

Standard error about the regression line =  $6.79 \times 10^{-7}$ 

T/K	Mol Fraction
	x ₁ × 10 ⁴
253.15	1.067
263.15	1.185
273.15	1.305
283.15	1.429
293.15	1.554
298.15	1.617

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus, designed especially for the determination of the solubility of hydrogen in liquids, consists of a gas bulb, a gas buret, a solvent bulb, and a manometer system. are attached to a mounting plate, and the assembly is shaken in an air bath (2) Carbon disulfide. Baker and

The solvent is degassed in the solvent bulb by heat and evacuation. The gas is placed in the gas bulb, and after temperature equilibrium is reached it is contacted with the degassed solvent. The system is shaken until solubility equilibrium is reached. Mercury is used as the dis-placement fluid.

The solubility is calculated from the initial and final quantities of gas, the pressure measurements, the vapor pressure of the solvent, and the solvent volume.

#### SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Mass spectrographic analysis showed gas 99.4 per cent pure. Impurity mostly N₂ with a small amount of HD.
- Adamson Reagent Grade. Distilled, center portion used, b.p. 319.65K. Other solvent properties given in reference (1).

# ESTIMATED ERROR:

 $\delta x_1/x_1 = 0.001 \text{ (authors)}$ 

- 1. Cook, M. W. University of California Radiation Lab, Report UCRL-2459, 1954.
- 2. Cook, M. W.; Hanson, D. N. Rev. Sci. Instr. 1957, 28, 370.

#### COMPONENTS: ORIGINAL MEASUREMENTS: (1) Deuterium; D₂; [7782-39-0] Dymond, J. H. J. Phys. Chem. 1967, 71, 1829-1831. (2) Sulfinylbismethane or Dimethyl Sulfoxide; C₂H₆OS (CH₃SOCH₃); [67-68-5] VARIABLES: PREPARED BY: T/K: 298.15 M. E. Derrick 101.325 (1 atm) H. L. Clever P/kPa:

#### EXPERIMENTAL VALUES:

T/K	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²	
298.15	0.799	2.51	2.74	

The Bunsen and Ostwald coefficients were calculated by the compiler.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

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

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

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Bio-Rad Labs. Dried.
- (2) Dimethyl Sulfoxide. Matheson, Coleman, and Bell Co. Spectroquality reagent, dried, and a fraction frozen out. Melting pt.: 18.37°C.

ESTIMATED ERROR:

# REFERENCES:

1. Dymond, J.; Hildebrand, J. H.

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

- (1) Deuterium; D₂; [7782-39-0]
- (2) Sulfinylbismethane or dimethylsulfoxide; C₂H₆OS; [67-68-5]

# ORIGINAL MEASUREMENTS:

Symons, E. A.; Buncel, E.

Can. J. Chem. 1973, 51, 1673 - 1681.

# VARIABLES:

298.15 T/K:

D₂ P/kPa: 101.325 (1 atm)

#### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

T/K	$C_{D_2}/\text{mol dm}^{-3}$ $c \times 10^3$	Mol Fraction $x_1 \times 10^4$	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²
298.15	1.13	0.805	2.53	2.76

The mole fraction, Bunsen coefficient, and Ostwald coefficient values were calculated by the compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Gas chromatographic method (1, 2).

The gas-liquid equilibrium cell was a modified  $100~{\rm cm}^3$  round bottom flask equipped with magnetic stirrer, syringe sampling portal, and vacuum/ gas line. The solvent was added, the flask evacuated several minutes to remove dissolved gases. Then the gas was introduced to a partial pressure of one atm. The solution was stirred for five minutes, then sampled. Three to four successive samples were taken.

The 5.0 cm³ samples were taken by gas tight syringe. The sample was introduced to a stripping cell, stripped Out over a period of 1-2 minutes by the nitrogen carrier gas and then passed into a Varian Aerograph (No. 1420) equipped with an injection Portal, column (10' 4" stainless steel, packed with 40-60 mesh 13X molecular sieve) at ambient temperature, and a thermal conductivity cell at 65°C.

# SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Matheson Co., Inc. Technical grade. Traces of oxygen removed by treatment with uranium turnings.
- (2) Sulfinylbismethane. Fisher Certified Reagent. Dried 48 h over 4A molecular sieves, vacuum distilled at ca. 1 mmHg. Fraction boiling 38-40°C was stored under N2 for use.

# ESTIMATED ERROR:

 $\delta T/K = 0.05$  $\delta c/c = 0.02$  (author's estimate)

- 1. Symons, E. A. Can. J. Chem. 1971, 49, 3940.
- Gubbins, K. E.; Carden, S. N.; Walker, R. D. Jr. J. Gas Chromatogr. 1965, 98.

(1) Deuterium; D₂; [7782-39-0]

#### ORIGINAL MEASUREMENTS:

Powell, R. J.

- (2) 1,1,2,2,3,3,4,4,4-Nonafluoro-N,N- J. Chem. Eng. Data 1972, 17, 302-304. bis (nonafluorobutyl) -1-butanamine or perfluorotributylamine;  $C_{12}F_{27}N; [311-89-7]$

#### VARIABLES:

T/K: 288.15 - 318.15 101.325 (1 atm) H₂ P/kPa:

PREPARED BY:

P. L. Long

EXPERIMENTAL VALUES:

T/K	Mol Fraction X1 × 10 ⁴	Bunsen Coefficient $\alpha \times 10^2$	Ostwald Coefficient L x 10 ²	$R_{\overline{\Delta \log T}}^{\Delta \log T} = N$
298.15	16.03	10.1	11.0	3.04

The author states that solubility measurements were made between 288.15 and 313.15 K, but only the solubility at 298.15 was given in the paper. slope  $R(\Delta \log X_1/\Delta \log T)$  was given. The smoothed data below were calculated by the compiler from the slope in the form:

$$\log X_1 = \log(16.03 \times 10^{-4}) - (3.04/R) \log(T/298.15)$$

with R = 1.9872 cal  $K^{-1}$  mol⁻¹.

T/K	Mol Fraction
	$x_1 \times 10^4$
288.15	15.22
293.15	15.62
298.15	16.03
303.15	16.44
308.15	16.86
313.15	17.28
318.15	17.71

The Bunsen and Ostwald coefficients were calculated by the compiler.

#### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Dymond and Hildebrand (1) apparatus which uses an all glass pumping system to spray slugs of degassed solvent into the gas. The amount of gas dissolved is calculated from the initial and final gas pressures. The solvent is degassed by freezing and pumping followed by boiling under reduced pressure.

### SOURCE AND PURITY OF MATERIALS:

- (1) Deuterium. Source not given. Manufacturers research grade, dried over CaCl, before use.
- (2) Perfluorotributylamine. Minnesota Mining & Mfg. Co.. Column distilled, used portion with b.p. = 447.85-448.64K, & single peak GC.

#### ESTIMATED ERROR:

$$\delta N/\text{cal } K^{-1} \text{ mol}^{-1} = 0.1$$
  
 $\delta X_1/X_1 = 0.002$ 

#### REFERENCES:

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

- (1) Deuterium; D₂ [7782-39-0]
- (2) Cyclopentanamine or cyclopentylamine; C₅H₁N or C₅H₉NH₂; [1003-03-8]

#### ORIGINAL MEASUREMENTS:

Symons, E. A.

private communication

#### VARIABLES:

T/K: 213.15 - 298.15 P/kPa: 101.325 (1 atm) PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:

Temperature		Mol Fraction 1	Bunsen	Ostwald
t/°C	T/K	$x_1 \times 10^4$	Coefficient $\alpha \times 10^2$	Coefficient L x 10 ²
-60.0	213.15	1.26 ± 0.03 (5)	3.10	2.42
-50.3	222.85	$1.39 \pm 0.02 (4)$	3.40	2.77
-40.0	233.15	$1.47 \pm 0.01$ (3)	3.55	3.03 3.62
-30.0 -21.0	243.15 252.15	1.70 ± 0.03 (4) 1.89 ± 0.11 (8)	4.07 4.48	3.62 4.14
-20.0	253.15	$1.89 \pm 0.04 (4)$	4.48	4.15
-15.0	258.15	$1.87 \pm 0.04 (12)$	4.41	4.17
-10.0	263.15	2.07 ± 0.05 (4)	4.86	4.68
0.0	273.15	$2.31 \pm 0.03 (3)$	5.36	5.36
+10.0	283.15	$2.48 \pm 0.01 (3)$	5.70	5.91
20.1	293.25	2.53 ± 0.03 (7)	5.76	6.18
25.0	298.15	$2.75 \pm 0.03$ (6)	6.23	6.80

The mole fraction solubility values were provided by the author. Given is the mole fraction solubility ± range (number of samples).

The Bunsen and Ostwald coefficients were calculated by the compiler.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Gas chromatography method described by author (1).

The author studied the solubility of hydrogen in the same system. The results are:

T/K	Mol Fraction $x_1 \times 10^4$
223.15	1.45
263.15 298.15	2.19 2.97

The expected isotope effect of 5 - 10 per cent was not found. The system is being studied further.

# SOURCE AND PURITY OF MATERIALS:

No information on the source and purity of materials.

# ESTIMATED ERROR:

Results show a range of 5 - 8 %.

#### REFERENCES:

Symons, E. A.
 Can. J. Chem. 1971, 49, 3940.

# COMPONENTS: (1) Deuterium; D₂; [7782-39-0] Bar-Eli, K.; Klein, F. S. (2) Ammonia; NH₃; [7664-41-7] J. Chem. Phys. 1961, 35, 1915. (3) Potassium amide; KNH₂; [17242-52-3] VARIABLES: T/K: 209.15, 231.55 PREPARED BY: H. L. Clever

# EXPERIMENTAL VALUES:

T/K	Bunsen Coefficient α/cm³(STP) cm-³atm-1		
209.15	$0.0117 \pm 0.0005$		
231.55	0.025 ± 0.0013		

The concentration of potassium amide was not given, it was stated to be dilute. The authors appear to assume that the salt does not affect the solubility of deuterium in liquid ammonia.

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A kinetic method in which the rate of reaction between a gas and its solvent is utilized to estimate the amount of gas dissolved. The principle of the method is to measure the apparent rate of reaction, while shaking the reaction mixture intermittently for varying time intervals.

The chemical reaction has to be slow enough to be easily measured, and the mixing need to be efficient, so that the partition equilibrium is established rapidly, compared to the time for the chemical reaction.

#### SOURCE AND PURITY OF MATERIALS:

No information.

ESTIMATED ERROR:

 $\delta \alpha / \alpha = 0.10$ 

HYDROGEN AND DEUTERIUM SOLUBILITIES ABOVE 200 kPa
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# HYDROGEN SOLUBILITIES ABOVE 200 kPa

General Remarks for High Pressure Solubilities Studies on Mixtures Containing Hydrogen

C. L. Young

Up until the last two decades there was comparatively little data available on the solubility of hydrogen in liquids above 200 kPa. However, this position has now completely changed and there is currently much interest in the solubility of hydrogen in liquids, particularly at high pressures. The major reasons for this interest arise from design considerations for processes concerned with the liquefaction of coal and from the "unusual" phase behaviour of some hydrogen mixtures. Some hydrogen mixtures exhibit the barotropic or phase inversion phenomenon and some exhibit the phenomenon of gas-gas immiscibility (1,2).

Unfortunately it has not been possible to give many detailed critical evaluations for hydrogen solubilities at high pressures because there are surprisingly few systems which have been studied over the same pressure and temperature range by more than two workers. In no case has it been possible to classify data as recommended because even when several workers have studied the same system usually the overlap of temperature and pressure ranges are fairly small.

#### Work of Chao and collaborators

Chao and coworkers have made fairly extensive measurements on hydrogen and coal-related organic compounds. The results are thought to be reliable but since, in general, there are no other measurements with which to compare their data at the higher temperatures, any evaluation is In several cases at the highest temperanecessarily rather speculative. tures, Chao and coworkers noticed some decomposition or reaction and it would be surprising if the effects of such were not significant and the dominant factor in determining the overall accuracy of some of the measurements under these conditions. The effect of decomposition or reaction cannot be simply allowed for as hydrogen appears to reduce the For example, Sebastian et al. thermal decomposition of some hydrocarbons. (3) found that hydrogen appeared to reduce the decomposition of thianaphthalene.

#### Work of Frolich, Trauch, Hogan and Peer

Frolich et al. (4) studied the solubility of hydrogen, nitrogen and methane in a range of organic substances. Unfortunately the data were presented in small graphical form. The data have been compiled but in view of the lack of any estimate of probable error the compiled data should be regarded with some caution and are generally classified as doubtful. They have been included principally because they are widely

quoted in the literature. In some instances the data were not even presented in graphical form but the solubility data of hydrogen in one liquid quoted as being equivalent to that of hydrogen in another liquid.

# Isotopic effects on solubility

Augood (5) made a study of the solubility of isotopic hydrogen, HD and  $H_2$ , in a number of solvents in order to obtain information for the production of heavy water. The table below gives values of  $\beta_{2/1}$  i.e., the ratio of Henry's law constant for the solubility of HD to  $H_2$ .

Solvent	T/K	P/MPa	β2/1	Solvent	T/K	P/MPa	β2/1
H ₂ O	293.2	18.72	1.029	H ₂ S	213.6	18.72	1.058
1777			1.024			10.44	1.025
NH ₃	293.2	19.06	1.028			10.44	1.025
		19.06	1.018			10.30	1.042
		15.61	1.026	NO	119.5	17.61	1.154
		15.61	1.022			15.54	1.155
		8.86	1.015			11.41	1.152
	239.7	19.13	1.040			11.27	1.172
		18.23	1.038	CO ₂	239.7	19.27	1.048
		15.61	1.030			18.85	1.036
		15.61	1.049			18.58	1.018
_		14.51	1.036			10.44	1.043
SO ₂	293.2	19.23	1.025			10.44	1.053
		19.13	1.021			10.44	1.040
		10.44	1.061	CO	81.4	18.16	1.090
		10.44	1.039			9.96	1.121
	263.2	19.20	1.038			9.61	1.199
		19.06	1.030	Ar	87.4	18.37	1.090
		12.92	1.040			18.37	1.084
		10.44	1.036			11.61	1.100
CH ₄	111.7	18.03	1.055			11.61	1.130
	,	10.44	1.085	N ₂	.77.7	17.89	1.033
		6.58	1.065	2		16.85	1.038
		2.38	1.079			15.61	1.043
C4H10	273.2	18.99	1.013			15.44	1.056
• •	-/3.2	9.06	1.005			11.55	1.061
		9.06	1.018			9.75	1.075
	213.6	18.82	1.040			8.79	1.075
	217.0	18.82	1.034			5.27	1.130
		18.30	1.034			2.86	1.147
		17.47	1.032			2.72	1.147
		9.06	1.043			1.82	1.165
					67.0		
H ₂ S	212 6	9.06	1.060		67.0	8.86	1.200
-20	213.6	18.72	1.053			8.72	1.217

The ratio  $\beta_{2/1}$  was determined by dissolving a HD + H₂ mixture containing 0.09 mole per cent of HD in the solvent and analysing the dissolved gas by mass spectrometry. Lachowicz *et al*. (6) carried out solubility experiments using H₂ and D₂ separately in n-heptane and octane to pressures of 30 MPa in the temperature range 298 to 323 K but found no differences in the solubility of the two isotopic gases.

# Gas-gas immiscibility

Many hydrogen + organic substance mixtures probably exhibit the phenomenon referred to as gas-gas immiscibility although the occurrence of this phenomenon in hydrogen mixtures has not been extensively investigated or documented. The phenomenon was predicted by the author to occur in several hydrogen + alkane mixtures on theoretical grounds and has subsequently been observed experimentally. This phenomenon is relevant to the determination and interpretation of "solubilities" at high temperatures and pressures and is therefore briefly discussed here.

The phenomenon is conveniently considered in terms of the pressure-temperature projection of the pressure-temperature composition diagram of a binary mixture. Figure 1 shows the pressure, temperature projection of a simple system such as propane + hexane. In this case there is a continuous gas-liquid critical locus between the critical points of the two pure components. In many cases there is also a liquid-liquid gas line at lower temperatures which meets a liquid-liquid critical line at an upper critical end point as is illustrated in figure 2. There are several other possible types of phase behaviour. Two of these involve gas-gas immiscibility and are illustrated in figures 3 and 4.

In many cases some part of the p, T projection as illustrated in figures 1, 2, 3 and 4 are obscured by solidification of the mixture. In the case of most hydrogen + organic compound mixtures there is a solid phase present for temperatures considerably above the critical temperature of hydrogen (33 K). Therefore, for the present purpose it is only necessary to consider the right hand side of the pressure-temperature projection. The left hand side of projections modified for the existence of solid phases has not been studied for mixtures of hydrogen + organic compounds.

The phase behaviour exhibited in figure 3 is referred to as gas-gas immiscibility of the second kind whereas that exhibited in figure 4 is referred to as gas-gas immiscibility of the first kind. gas immiscibility of the first kind the critical locus starting at the critical point of the less volatile component moves to higher pressures and higher temperatures as the concentration of the more volatile component is increased from zero. It is possible to have two immiscible Phases present at pressures and temperatures denoted by all points to the left of the critical locus. Since some of these temperatures are above the critical temperature of both components the phenomenon is referred to as gas-gas immiscibility. In gas-gas immiscibility of the second kind, which has a phase diagram as in figure 3, the critical locus starting at the critical point of the less volatile compound moves initially to lower temperatures and higher pressures but eventually moves back to higher temperatures and still higher pressures. it is possible at high pressures to have two phases present above the critical temperature of either component.

Probably hydrogen + most hydrocarbons with a carbon number of 8 or more will exhibit gas-gas immiscibility of the first kind. During the last two years several "gas" solubilities for hydrogen + hydrocarbons have been studied 30-50 °C below the critical temperature of the hydrocarbon. No detailed studies have been reported near the critical temperature of the hydrocarbon for systems which exhibit gas-gas immiscibility but it is to be expected that such studies may well soon be extended to such a region in view of the importance of hydrogen "solubilities" to coal liquefaction processes. It should also be pointed out that extrapolation of existing high temperature solubilities to tempera-

tures near the critical region will lead to grossly inaccurate values.

#### References:

- 1. Rowlinson, J. S. Liquids and Liquid Mixtures 2nd edn. Butterworths, London, 1969.
- Schneider, G. M. in Spec. Period. Reports No. 22. Chemical Thermodynamics Vol. 2, ed. McGlashan, M. L. Chem. Soc. London, 1978.
- 3. Sebastian, N. M.; Simnick, J. J.; Lin, H. M.; Chao, K.-C. Can. J. Chem. Engng. 1978, 56, 743.
- Frolich, P. K.; Trauch, E. J.; Hogan, J. J.; Peer, A. A.
   Ind. Eng. Chem. 1931, 23, 548.
- 5. Augood, D. R. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 6. Lachowicz, S. K.; Newitt, D. M.; Weale, K. E. *Trans. Faraday Soc.* 1955, *51*, 1198.

COMPONENTS:	EVALUATOR:
1. Hydrogen; H ₂ ; [1333-74-0] 2. Water; H ₂ O; [7732-18-5]	Colin L. Young, Department of Physical Chemistry, University of Melbourne, Parkville , Victoria 3052, Australia.
	October 1980.

# CRITICAL EVALUATION:

HAD - U

This system has been fairly extensively investigated but the evaluator is unable to recommend any particular set of data. Wiebe and COWORKERS'(1), (2) data cover the temperature range 273.15 to 373.15 K and pressures up to 100 MPa and are almost certainly the most reliable in this range. The data of Ipat'ev et al. (3), which are mostly at 298 K are significantly lower than those of Wiebe and because of their limited scope the former work is not considered further. The data of Ipat'ev and Theodorovich (4) covered the temperature range 373 to 498 K and are in general lower than the data of Wiebe and coworkers and the more recent data of Suciu (5). The data of Frolich et al. (6) were presented in a small graphical form and are rejected.

The data of Pray  $et\ al.$  (7), Stephan  $et\ al.$  (8), Wiebe and coworkers (1) and (2) and Suciu, Zoss and Sibbitt (9) are all classified as tentative although the latter work is considerably more doubtful. The data of Stephan  $et\ al.$  (8) cover the temperature range 373.15 to 435.93 K and the pressure range up to 10 MPa. However there is significant disagreement between the Stephan  $et\ al.$  (8) data and that of Wiebe (1), (2). The data of Pray  $et\ al.$  (7) are limited to pressures below 2.5 MPa but are included in the compilation since they cover the temperature range 297.0 to 616.5 K. The data of Suciu  $et\ al.$  (9) were presented in graphical form, the details given in the compiled tables being taken from theses by Suciu and Zoss. As can be seen from the compilation these data have very significant scatter for each isobar.

The table below gives smoothed values of Kuenen coefficient for the solubility taken from Wiebe and Gaddy.

	Kuenen coefficients						
T/K	25 atm	50 atm	75 atm	100 atm	150 atm	200 atm	300 atm
273.15 283.15 293.15 303.15 313.15 323.15 333.15 343.15 353.15 363.15 373.15	0.5363 0.4870 0.4498 0.4263 0.4133 0.4067 0.4053 0.4093 0.4203 0.4385 0.4615	1.068 0.9690 0.8945 0.8215 0.8215 0.8090 0.8095 0.8171 0.8385 0.8720 0.9120	1.601 1.453 1.341 1.271 1.232 1.212 1.211 1.224 1.254 1.298 1.355	2.130 1.932 1.785 1.689 1.638 1.612 1.610 1.628 1.667 1.727 1.805	3.168 2.872 2.649 2.508 2.432 2.395 2.393 2.422 2.485 2.576 2.681	4.187 3.796 3.499 3.311 3.210 3.165 3.168 3.208 3.286 3.402 3.544	6.139 5.579 5.158 4.897 4.747 4.695 4.692 4.746 4.866 5.042 5.220
273.15 283.15 293.15 303.15 313.15 323.15 333.15 343.15 353.15 363.15 373.15	400 atm 8.009 7.300 6.766 6.430 6.245 6.166 6.173 6.249 6.392 6.600 6.841	500 atm 9.838 8.980 8.328 7.922 7.705 7.613 7.625 7.717 7.885 8.129 8.429	600 atm 11.626 10.610 9.856 9.390 9.135 9.017 9.016 9.131 9.324 9.665 9.994	700 atm 13.370 12.214 11.362 10.818 10.524 10.389 10.405 10.527 10.757 11.093 11.512	800 atm 15.013 13.746 12.808 12.218 11.889 11.735 11.746 11.893 12.169 12.555 12.980	900 atm 16.548 15.215 14.217 13.583 13.230 13.072 13.084 13.233 13.533 13.533 13.946 14.394	1000 atm  18.001  16.623  15.592  14.928  14.569  14.404  14.407  14.557  14.867  15.303  15.775

These smoothed data are presented as tentative values and are expected to be accurate to  $\pm$  1 or 2%.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Water; H₂O; [7732-18-5]

#### **EVALUATOR:**

Colin L. Young,
Department of Physical Chemistry,
University of Melbourne,
Parkville, Victoria 3052,
Australia.
October 1980.

#### CRITICAL EVALUATION:

#### References:

- 1. Wiebe, R.; Gaddy, V. L.; Heins, C. Ind. Eng. Chem. 1932, 24, 823.
- 2. Wiebe, R.; Gaddy, V. L. J. Am. Chem. Soc. 1934, 56, 76.
- 3. Ipat'ev, V. V.; Druzhina-Artemovich, S. I.; Tikhovirov, V. I. Zh. Obshchei. Khim. 1931, 1, 594.
- 4. Ipat'ev, V. V.; Theodorovich, V. P. Zh. Obshchei. Khim. 1934, 4, 395.
- 5. Suciu, S. Ph.D. Thesis, Purdue University 1951.
- 6. Frolich, K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A. Ind. Eng. Chem. 1931, 23, 548.
- 7. Pray, H. A.; Schweichert, C. E.; Minnich, B. H. Ind. Eng. Chem. 1952, 44, 1147.
- 8. Stephan, E. L.; Hatfield, N. S.; Peoples, R. S.; Pray, H. A.

  Battelle Memorial Institute Rep. BMI-1067, 1956.
- 9. Suciu, S.; Zoss, L. M.; Sibbitt, W. L. Paper no. 53-A64 Am. Soc.

  Mech. Engnrs. Nov/Dec 1953 New York.

COMPONENTS:	ORIGINAL MEASUREMENTS:					
1. Hydrogen; H ₂ ; [1333-	74-0]	J	Gaddy, V ₉ HL.; Chem. <u>1932</u> , 24,			
2. Water; H ₂ O; [7732-18	-5]					
VARIABLES:		PREPARED BY:		<del>-</del>		
Pressure		C. L. Young				
EXPERIMENTAL VALUES:		<del></del>	<u> </u>			
T/K P/bar	fraction o in water 10 ³ x _{H2}					
			_			
298.15 25.33 50.66 101.3 202.6 405.3 607.9 810.6 1013.3	0.311 0.619 1.233 2.417 4.673 6.799 8.825 10.745					

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Simple steel cylinder containing water through which hydrogen was passed. Pressure measured using dead weight gauge. Water saturated with hydrogen and liquid phase analysed using a volumetric technique. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- Purity 99.8 mole per cent, major impurity being nitrogen.
- 2. No details given.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \quad \delta P/\text{bar} = \pm 0.2;$   $\delta x_{\text{H}_2} = \pm 0.5 \text{% (estimated by compiler)}.$ 

# 306 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Wiebe, R.; Gaddy, V. L. 2. Water; H₂O; [7732-18-5] J. Am. Chem. Soc. 1934, 56, 76-79. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

NTAL VALUES:	Mole fraction			Mole fraction	
P/bar	of hydrogen in liquid, ^x H ₂	T/K	P/bar	of hydrogen in liquid, $^{x}{ m H}_{2}$	
25.33 50.66 101.33 202.65	0.000383 0.000768 0.001520 0.002983	323.15	405.30 607.95 810.60	0.004387 0.006402 0.008316 0.010188	
405.30 607.95 810.60 1013.25	0.005690 0.008239 0.010619	348.15	25.33 50.66 101.32	0.000295 0.000590 0.001173 0.002310	
25.33 50.66 101.33 202.65	0.000311 0.000619 0.001233 0.002417		405.30 607.95 810.60 1013.25	0.004487 0.006545 0.008504 0.010385	
405.30 607.95 810.60 1013.25	0.004673 0.006799 0.008825 0.010745	373.15	25.33 50.66 101.32 202.65	0.000330 0.000651 0.001288 0.002526	
25.33 50.66 101.33 202.65	0.000290 0.000578 0.001151 0.002256		405.30 607.95 810.60 1013.25	0.004865 0.007091 0.009190 0.011147	
	25.33 50.66 101.33 202.65 405.30 607.95 810.60 1013.25 25.33 50.66 101.33 202.65 405.30 607.95 810.60 1013.25 25.33 50.66	## P/bar of hydrogen in liquid,  ##2  25.33	Of hydrogen in liquid, T/K  25.33	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	

# AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

Single pass flow method with two vessel adsorption train. Second vessel used as source of sample for analysis. Pressure measured with dead weight gauges. Measurements taken both for a high pressure and low pressure approach to equilibrium. Details in source and ref. 1.

#### SOURCE AND PURITY OF MATERIALS:

- Purity 99.9 mole per cent; major impurity nitrogen.
- 2. No details given.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ ;  $\delta P/bar = \pm 0.5$ ;  $\delta x_{\rm H_2} = \pm 1\%.$ 

# REFERENCES:

1. Wiebe, R.; Gaddy, V. L.; Heins, C. Ind. Eng. Chem. 1931, 23, 401.

Water

#### COMPONENTS:

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

# ORIGINAL MEASUREMENTS:

Suciu, S. Ph. D. thesis, 1951 Purdue University

Zoss, L. M. Ph. D. thesis, 1952 Purdue University

VARIABLES: T/K: 273.15 -

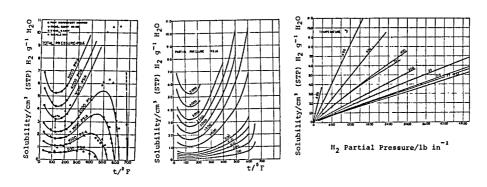
(32- 637 °F)

Total P/kPa: 6895 - 20,680 (1000 - 3000 lb in⁻²)

#### PREPARED BY:

H. L. Clever

#### EXPERIMENTAL VALUES:



The figures above which show (a) hydrogen solubility vs temperature total pressure isobars (left), (b) hydrogen solubility vs temperature hydrogen partial pressure isobars (middle), and (c) hydrogen solubility vs hydrogen partial pressure isotherms were constructed by Suciu, Zoss, and Sibbitt (2).

In addition to the data from the Ph. D. theses of Suciu and of Zoss, they used data from:

Pray, H. A. H.; Schweichert, C. E.; Minnick, B. H. Battelle Memorial Inst. Report BMI-T-25; Ind. Eng. Chem. 1952, 44, 1146 - 1151. Wiebe, R.; Gaddy, V. L.; Heins, C. Ind. Eng. Chem. 1932, 24, 823 - 825.

Wiebe, R.; Gaddy, V. L. J. Am. Chem. Soc. 1934, 56, 76 - 79.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

The apparatus was described by Zoss, Suciu, and Sibbitt (1). The apparatus consisted of a high pressure vessel With integral vapor and liquid sample chambers, heaters, temperature controls, auxillary pumps, and analytical equipment.

The sequence of operations was: (a) The pressure vessel was evacuated, (b) charged with a known volume of water (about 175 cm⁻³), (c) brought to a selected temperature level, (d) charged with gas (under conditions of Constant total pressure, constant temperature, and continual agitation) until phase equilibrium was reached, (e) fastened in a vertical position until the vapor and liquid phases separated.

The gas and liquid phases were separatly analyzed.

The results were summarized in graphs (2).

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. Water-pumped. 99.9+ per cent pure.
- (2) Water. Distilled water, boiled three hours and cooled. Tested for pH and for oxygen content (polarography).

#### ESTIMATED ERROR:

 $\delta t/{}^{0}F = 0.5$  $\delta P/1b in^{-2} = 3$  $\delta S/S = 0.03$ 

- Zoss, L. M.; Suciu, S.; Sibbitt, W. L.
- Trans. ASME 1954, 76, 69 71. 2. Suciu, S.; Zoss, L.M.; Sibbitt, W.L.
- Paper No. 53-A64 American Society of Mechanical Engineers Meeting, Nov/Dec 1953,Ni

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hydrogen; H ₂ ; [1333-74-0] (2) Water; H ₂ O; [7732-18-5]	Suciu, S. Ph. D. thesis, 1951 Purdue University
	Zoss, L. M. Ph. D. thesis, 1952 Purdue University

			Purdue	University	
EXPERIMENTAL V	ALUES:				
Temperatu t/ºF T	re P/K	Pressure _lb_in^2	Hydrogen Solubility S/cm ³ (STP) q ⁻¹	Vapor Composit: cH2O/mol dm-3	ion mol fraction ^x H ₂ O
124 200 300 4350 400	299.8 324.3 366.5 122.0 149.8 177.6	500 (34.0 atm, 3450 kPa)	0.55 ¹ 0.70 ¹ 0.57 ¹ 0.59 ¹ 0.58 ¹ 0.50 ¹ 0.27 ¹		
76 2 77 2 78 2 103 3 112 3	273.15 297.6 298.15 298.7 312.6 317.6	1000 (68.0 atm, 6895 kPa)	0.847 1.197 1.170 1.095	0.050 ² 0.009 ² 0.018	0.0067
145 155 192 245 246	334.8 335.9 341.5 362.0 391.5 392.0		0.951 1.11 ² 1.30 ²	0.037 0.037 0.087 ²	0.0145 ² 0.0134 0.022 ² 0.031 ²
297 298 302 4 355 4 359 4	120.4 120.9 123.15 152.6 154.8		1.64 ² 1.90 ²	0.170 ² 0.309 ²	0.067 ² 0.150 ² 0.263 ² 0.489 ²
497 5 500 5 517 5 520 5	508.15 531.5 533.15 542.6 544.3	1500	1.94 ² 1.64 ² 1.20 ²	1.787 ²	0.661 ² 0.750 ²
125 155 245 410 508	324.8 341.5 391.5 483.15 537.6 563.7	(102.1 atm, 10,340 kPa)	, 1.70		
85 125 200	273.15 302.6 324.8 366.5 367.0	2000 (136.1 atm, 13,790 kPa)		0.0492	
252 3 254 3 300 4	367.6 395.4 396.5 122.0 123.15		2.942	0.170²	0.0065 ² 0.0189 ² 0.040 ²
305 4 400 4 401 4 402 4	124.8 177.6 178.15 178.7		3.342	0.5102	0.131 ² 0.144 ²
483 5 487 5	179.3 523.7 525.9 526.5		4.69 ² 5.86 ²	1.0492	0.295²
			Co	ontinued on next	page.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Suciu, S. Ph. D. thesis, 1951 Purdue University

Zoss, L. M. Ph. D. thesis, 1952 Purdue University

### **EXPERIMENTAL VALUES:**

Temper	rature	Pressure	Hydrogen	Vapor Com	
t/ºF	T/K	p/lb in ⁻²	Solubility S/cm ⁻³ (STP) g ⁻¹	$c_{\rm H_2O}/{\rm mol~dm^{-3}}$	mol fraction #H20
500	533.15	2000	6.112	1.200 ²	0.3452
545 567	558.15		6.302	1.8252	0.535 ²
575	570.4 574.8		6.07 ²	2.612 ²	0.333
577	575.9		0.07	2.012	0.6952
620	599.8				$0.782^{2}$
622	600.9		2.50 ²	2.750 ²	
637	609.3			4.725 ²	
32	273.15	3000	1.215		
89	304.8	(204.1 atm	, 3.40		
115	319.3	20,680 kPa			
128	326.5		3.38		
142	334.3		3.45		
151	339.3		3.42		
201	367.0		3.86		
238	387.6		4.28		
305	424.8		5.18		
340	444.3			0.257	0.035
405	480.4		7.18	0.407	0.101
510	538.7			1.341	0.175
523	545.9		10.03		
575	574.8		10.45	1.655	0.218
632	606.5		10.50	2.400	0.266

All of the values in the table above appeared in the Ph. D. thesis of L. M. Zoss.

Both Ph. D. thesis were directed by W. L. Sibbitt of the Department of Mechanical Engineering.

The hydrogen solubility values were reported as Kuenen coefficients, S/cm 3  H $_2$  at 1 atm and 273.15 K g $^{-1}$  water.

¹Values calculated from the data of Pray, H. A.; Schweickert, C. E.; Minnick, B. H. Battelle Memorial Institute; BMI-T-25, May 1950.

²Values from the Ph. D. thesis of Suciu, S.

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Pray, H. A.; Schweichert, C. E.; Minnich, B. H.; Ind. Eng. Chem. 2. Water; H₂O; [7732-18-5] 1952, 44, 1147-1151. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

T/K	P/bar	$0^3$ Mole fraction of hydrogen in water, $10^3x_{ m H_{2}}$
297.0	13.79	0.24
	20.68 24.13	0.29 0.32
533.1	6.89	0.32
333,1	13.79	0.65
	20.68	0.89
588.7	6.89	0.46
	13.79	0.94
	20.68	1.43
616.5	6.89	1.00
	7.93	1.16
	8.27	1.20
	8.62	1.24

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Rocking equilibrium cell of 3 1 capacity. Pressure measured with dead weight gauge and temperature measured using chromel-alumel thermocouple. Cell contents equilibrated and liquid sample removed. The amount of dissolved gas estimated volumetrically.

# SOURCE AND PURITY OF MATERIALS:

No details given.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1$ ;  $\delta P/\text{bar} = \pm 1$ ;  $\delta x_{\text{H}_2} = 1-5\%$  (estimated by compiler).

COMPONENTS	IONY OT VALVE
COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Stephan, E. L.; Hatfield, N. S.;
	Peoples, R. S.; Pray, H. A. H.
2. Water; H ₂ O; [7732-18-5]	Battelle Memorial Institute Report
	BMI-1067, 1956.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young
EXPERIMENTAL VALUES: Mole fraction of hydrogen	Mole fraction of hydrogen
T/K $P/bar$ in liquid,	T/K P/bar in liquid,
<i>x</i> _{H 2}	$x_{ m H_{2}}$
373.15 15.5 0.000257	408.15 61.7 0.00111
15.5 0.000265 16.2 0.000281	63.1 0.00111 64.5 0.00114
16.9 0.000281	94.8 0.00173
16.9 0.000246 36.2 0.000539	95.5 0.00174 96.9 0.00165
37.6 0.000571	97.2 0.00169
39.0 0.000595 39.0 0.000595	435.93 15.5 0.000386 17.6 0.000400
70.7 0.00111	17.6 0.000410
71.4 0.00108 72.1 0.00108	36.2 0.000836
72.1 0.00108 72.7 0.00108	39.2 0.000868 40.3 0.000868
97.6 0.00145	40.7 0.000882
98.9 0.00151 100.3 0.00155	41.7 0.000940 45.2 0.001032
408.15 14.1 0.000291	54.9 0.00132
14.8 0.000292 15.5 0.000289	68.3 0.00152 69.3 0.00155
16.2 0.000333	75.2 0.00170
35.5 0.000643 36.2 0.000675	77.6 0.00181 84.4 0.00197
36.9 0.000699	88.9 0.00194
† 61.0 0.00114 partial pressure of hydrogen	91.0 0.00202
	INFORMATION
METHOD /APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Static equilibrium cell. Gas and	TOTAL TOTAL OF THE LAND.
liquid equilibrated for 18 hours.	
Pressure measured with Bourdon gauge and temperature measured with thermo-	No details given.
Couple. Composition of liquid	, , , , , , , , , , , , , , , , , , , ,
estimated by volumetric method. Details in source. Partial pressure	
estimated by subtracting vapor pres-	
sure from total pressure.	
Į.	ESTIMATED EDDOR
	ESTIMATED ERROR: $\delta T/K = \pm 0.6$ ; $\delta P/bar = \pm 0.3$ ;
	$\delta x_{\rm H_2} = \pm 0.00002 \text{ (estimated by}$
	compiler).
	REFERENCES:
i e	i i

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Nitrogen; N₂; [7727-37-9]</li> <li>Water; H₂O; [7732-18-5]</li> </ol>	Wiebe, R.; Gaddy, V. L.  J. Am. Chem. Soc.  1935, 57, 1487-8.
VARIABLES:	PREPARED BY:
Pressure	C. L. Young

EXPERIMENTAL VALUES:

p/atm	p*/MPa	${\tt Solubility}^{\#}$	Mole perc of hydr in liquid	ogen	Mole [*] frac hydrogen ^x H ₂	tion of nitrogen ^x N ₂
50	5.07	0.8344	80.27	76.57	0.000538	0.000132
		0.8359	80.08	76.41 76.40	0.000538 0.00106	0.000134 0.000254
100	10.13	1.638 1.643	80.73 80.96	76.40	0.00100	0.000254
		1.645	80.88	76.60	0.00107	0.000253
200	20.27	3.215	82.22	-	0.00212	0.000459
		3.205	83.13	-	0.00214	0.000434
400	40.53	6.063	84.20	76.31	0.00409	0.000769
		6.072	84.46	76.32	0.00411	0.000758
600	60.80	8.805	85.05	76.36	0.00598	0.001057
		8.813	84.80	76 20	0.00597	0.001076 0.00131
800	81.06	11.312	85.60 85.04	76.39 76.41	0.00772 0.00769	0.00131
1000	101.33	11.342 13.748 13.701	85.96 85.66	76.41 76.28	0.00941 0.00934	0.00155 0.00158

^{*} Calculated by compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

One pass flow method with two vessel absorption train. Second vessel used as source of sample for analysis. Pressure measured with dead weight gauges.

### SOURCE AND PURITY OF MATERIALS:

- 1 and 2. Mixture prepared by
   burning hydrogen in air.
   Major impurity was
   argon.
  - 3. No details.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.05; \quad \delta p/MPa = \pm 0.05;$  $\delta x_{H_2}, \quad \delta x_{N_2} = \pm 2$ .

Wolume of gas, measured at 273.15 K and 101.3 kPa, dissolved by 1 g of water at the specified temperature and pressure.

		•	Water	313
	_	[7782-39-0] [7789-20-0]	ORIGINAL MEASUREMENTS:  Stephan, E. L.; Hatfield, N. S.; Peoples, R. S.; Pray, H. A. H.  battelle Memorial Institute Report  bMI-1067, 1956.	t
VARIABLES: Temperat	ure, press	ure	PREPARED BY: C. L. Young	
EXPERIMENTAI	P*/bar	Mole fraction of in liqui ^x D ₂		
435.93	16.7 17.4	0.00037	3	

T/K	P*/bar	in liquid,  *D2
435.93	16.7	0.000375
	17.4	0.000433
	18.5	0.000464
	26.5	0.000660
	27.2	0.000625
	27.9	0.000696
533.15	20.6	0.001088
	21.4	0.001115
	22.3	0.001124
	25.0	0.001293
	26.4	0.001257
	28.5	0.001444
574.82	4.1	0.000312
374.02	5.1	0.000419
	6.5	0.000553
	21.6	0.001729
	22.3	0.001907

p* partial pressure of deuterium

0.001845

# METHOD/APPARATUS/PROCEDURE:

23.4

Gas and liquid equilibrated for 18 hours. Pressure measured with Bourdon gauge and temperature measured with thermocouple; composition of liquid estimated by volumetric method. Details in source. Partial pressure estimated by subtracting vapor pressure from total pressure.

# SOURCE AND PURITY OF MATERIALS:

No details given.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.6; \quad \delta P/\text{bar} = \pm 0.3;$   $\delta x_{D_2} = \pm 3 \text{ (estimated by compiler).}$ 

### 314 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Wisniak, J.; Hershkowitz, M.; 1. Leibowitz, R.; Stein, S. Water; H₂O; [7732-18-5] 2. J. Chem. Engng. Data, 1974, 19, 247-249. 3. D-mannitol (cordycepic acid); $C_6H_{14}O_6$ ; [69-65-8] VARIABLES: PREPARED BY: C.L. Young Temperature, pressure, concentration EXPERIMENTAL VALUES: 104 Mole fraction of hydrogen in liquid, Conc. /mol 1-1 P/bar T/K (soln) 10 4 x H2 1.13 353.15 6.895 0.5 2.12 13.79 0.5 3.03 20.68 0.5 3.99 27.58 0.5 5.00 0.5 34.47 5.96 41.37 0.5 0.5 48.26 7.75 55.16 0.5 7.87 0.5 1.29 373.15 6.895 2.35 13.79 0.5 3.45 20.68 0.5 4.48 0.5 27.58 34.47 0.5 5.66 6.75 0.5 41.37 48.26 0.5 7.84 0.5 8.84 55.16 0.5 1.36 393.15 6.895 2.55 13.79 0.5 0.5 3.72 20.68 0.5 4.92 27.58 0.5 6.19 34.47

### AUXILIARY INFORMATION

0.5

0.5

0.5

# METHOD /APPARATUS/PROCEDURE:

Large high pressure autoclave fitted with liquid sampling port. Analysis carried at by stripping solution in gas buret apparatus. Cell charged with components pressurized with hydrogen and equilibrated for at least 15 minutes. Liquid sample transferred to a two buret stripping apparatus.

41.37

48.26

55.16

### SOURCE AND PURITY OF MATERIALS:

- No details given.
- 2. Distilled.
- Sigma sample purity 99.9 mole per cent.

7.33

8.47

9.69

### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0$ ;  $\delta P/bar = \pm 0.7$ ;

 $\delta x_{\rm H_2} = \pm 3 - 5\%.$ 

### **Aqueous Solutions** COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Wisniak, J.; Hershkowitz, M.; Leibowitz, R.; Stein, S. 2. Water; H₂O; [7732-18-5] J. Chem. Engng. Data, 1974, 19, 3. $Xylose; C_5H_{10}O_5; [25990-60-7]$ 247-249 VARIABLES: PREPARED BY: C.L. Young Temperature, pressure, concentration EXPERIMENTAL VALUES: 104 Mole fraction of Conc. $/mol 1^{-1}$ T/K *P/*bar (soln) hydrogen in liquid, 10" x_{H2} 353.15 6.895 0.5 1.20 13.79 2.16 0.5 20.68 0.5 3.13 0.5 4.06 27.58 34.47 0.5 5.12 0.5 6.10 41.37 0.5 7.05 48.26 55.16 0.5 8.15 373.15 6.895 0.5 1.18 2.21 13.79 0.5 3.36 20.68 0.5 27.58 0.5 4.33 0.5 5.47 34.47 41.37 0.5 6.57 0.5 7.53

### AUXILIARY INFORMATION,

0.5

0.5

0.5

0.5

0.5

0.5

0.5

# METHOD /APPARATUS/PROCEDURE:

393.15

Large high pressure autoclave fitted With liquid sampling port. Analysis carried at by stripping solution in gas buret apparatus. Cell charged With components pressurized with hydrogen and equilibrated for at least 15 minutes. Liquid sample transferred to a two buret stripping apparatus.

48.26 55.16

20.68

27.58

34.47

41.37

6.895 13.79

### SOURCE AND PURITY OF MATERIALS:

8.66

1.52

2.76

4.07

5.21

6.43

7.77

cont.

- No details given.
- 2. Distilled.
- 3. Sigma sample purity 99.9 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0$ ;  $\delta P/bar = \pm 0.7$ ;

 $\delta x_{\rm H}$ = ±3-5%.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Water; H₂O; [7732-18-5]
- 3.  $Xylose; C_5H_{10}O_5; [25990-60-7]$

# ORIGINAL MEASUREMENTS :

Wisniak, J.; Hershkowitz, M.; Leibowitz, R.; Stein, S.

J. Chem. Engng. Data, <u>1974</u>, 19, 247-249.

TVDI	יסדאדסי	. דילידיני	VALUES	

т/к	P/bar	Conc./mol l ⁻¹ (soln)	10 4 Mole fraction of hydrogen in liquid, $10^4x_{ m H_2}$
393.15	48.26 55.16	0.5 0.5	8.97 10.29
353.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.37 2.73 3.86 4.97 6.35 7.56 8.65 9.88
373.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.20 2.28 3.25 4.31 5.58 6.36 7.41 8.47
393.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.33 2.56 3.78 4.99 6.20 7.37 8.49 9.76
373.15	6.895 13.79 20.68 27.58 34.47 41.37 42.26 55.16	3.0 3.0 3.0 3.0 3.0 3.0 3.0	1.41 2.88 3.99 5.44 6.65 7.86 8.51 10.41
393.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	3.0 3.0 3.0 3.0 3.0 3.0 3.0	1.51 2.66 4.02 5.38 6.72 7.69 9.01 10.33

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Wisniak, J.; Hershkowitz, M.; Leibowitz, R.; Stein, S. 2. Water; H₂0; [7732-18-5] J. Chem. Engng. Data. 1974, 19, 247-249. 3. $Xylitol; C_5H_{12}O_5; [87-99-0]$ VARIABLES: PREPARED BY: C.L. Young Temperature, pressure, concentration EXPERIMENTAL VALUES: 104 Mole fraction of T/K Conc. $/mol 1^{-1}$ P/bar hydrogen in liquid, (soln) 104x_{H2} 353.15 6.895 0.5 1.13 0.5 2.03 13.79 20.68 0.5 2.92 27.58 0.5 3.98 34.47 0.5 4.91 41.37 0.5 5.74 0.5 48.26 6.67 55.16 0.5 7.75 373.15 6.895 0.5 1.23 13.79 0.5 2.20 0.5 3.22 20.68 27.58 0.5 4.35 5.37 34.47 0.5 0.5 41.37 6.22 48.26 0.5 7.37 8.34 55.16 0.5 0.5 393.15 6.895 1.60 13.79 0.5 2.89 20.68 0.5 4.18 27.58 0.5 5.47 34.47 41.37 0.5 6.77 0.5 7.95 48.26 AUXILIARY INFORMATION METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Large high pressure autoclave fitted No details given. With liquid sampling port. Analysis 2. Distilled carried at by stripping solution in gas buret apparatus. Cell charged 3. Sigma sample purity 99.9 mole with components pressurized with per cent. hydrogen and equilibrated for at least 15 minutes. Liquid sample transferred to a two buret stripping apparatus. ESTIMATED ERROR: $\delta T/K = \pm 1.0$ ; $\delta P/bar = \pm 0.7$ ;

 $\delta x_{\rm H_2} = \pm 3 - 5\%.$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Water; H₂O; [7732-18-5
- 3. Xylitol;  $C_5H_{12}O_5$ ; [87-99-0]

# ORIGINAL MEASUREMENTS:

Wisniak, J.; Hershkowitz, M.; Leibowitz, R.; Stein, S.

J. Chem. Engng. Data. <u>1974</u>, 19, 247-249.

### EXPERIMENTAL VALUES :

т/к	P/bar	Conc. /mol 1 ⁻¹ (soln)	10 ⁴ Mole fraction of hydrogen in liquid,
			10 ⁴ x _{H2}
393.15	55.16	0.5	10.73
353.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	0.5 2.0 2.0 2.0 2.0 2.0 2.0	1.35 2.61 3.88 5.03 6.22 7.45 8.91 9.87
373.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.50 2.92 4.11 5.44 6.84 8.04 9.43
393.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.60 2.96 4.41 5.94 7.33 8.73 9.92
353.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	3.0 3.0 3.0 3.0 3.0 3.0 3.0	1.41 2.54 3.58 4.69 5.83 7.07 8.17 9.27
373.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	3.0 3.0 3.0 3.0 3.0 3.0 3.0	1.34 2.42 3.50 4.56 5.92 6.92 8.30 9.44
393.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	3.0 3.0 3.0 3.0 3.0 3.0 3.0	1.40 2.73 3.84 5.00 6.34 7.42 8.71 10.05

		71440040				
COMPONENTS:			ORIGINAL MEASUREMENTS:			
l. Hydrogen; H	H ₂ ; [1333-74-0	]	Wisniak, J.; Hershkowitz, M.;			
2. Water; H ₂ O;	[7732-18-5]		Leibowitz, R.; Stein S.			
3. D-Glucitol, [50-70-4]	, (Sorbitol);	C ₆ H ₁ 4O ₆ ;	J. Chem. Engng. Data, <u>1974</u> ,19, 247-9			
/ARIABLES:			PREPARED BY:			
Temperature, p	ressure, conc	entration	C.L. Young			
EXPERIMENTAL VALUE						
T/K	P/bar	Conc. /mol (soln)				
353.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	0.5 0.5 0.5 0.5 0.5 0.5	1.08 2.08 2.97 3.94 5.01 5.86 6.81 7.75			
373.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	0.5 0.5 0.5 0.5 0.5 0.5	1.29 2.38 3.58 4.72 5.86 6.85 8.02 9.29			
393.15	6.895 13.79 20.68 27.58 34.47 41.37	0.5 0.5 0.5 0.5 0.5	1.25 2.54 3.64 4.68 5.85 7.21 8.28			
		AUXILIARY	INFORMATION -			
METHOD /APPARATU Large high pre With liquid sa carried at by gas buret appa With component hydrogen and e least 15 minut transferred to apparatus.	ssure autoclav mpling port. stripping solu ratus. Cell of s pressurized quilibrated for es. Liquid sa	ve fitted Analysis Ition in Charged With Or at	SOURCE AND PURITY OF MATERIALS:  1. No details given.  2. Distilled.  3. Sigma sample purity 99.9 mole per cent.  ESTIMATED ERROR:			
			ESTIMATED ERROR: $\delta T/K = \pm 1.0; \ \delta P/\text{bar} = \pm 0.7;$ $\delta x_{\text{H}_2} = \pm 3.5 \text{\%}.$ REFERENCES:			

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Water; H₂O; [7732-18-5]
- D-Glucitol, (Sorbitol); C₆H₁,O₆;
   [50-70-4]

# ORIGINAL MEASUREMENTS:

Wisniak, J.; Hershkowitz, M.; Leibowitz, R.; Stein, S.

J. Chem. Engng. Data, <u>1974</u>, 19, 247-9.

# EXPERIMENTAL VALUES :

T/K	P/bar	Conc./mol l ⁻¹ (soln)	$10^4$ Mole fraction of hydrogen in liquid, $10^4x_{ m H_2}$
393.15	55.16	0.5	9.43
353.15	6.859 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.22 2.29 3.25 4.54 5.44 6.47 7.61 8.53
373.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.23 2.22 3.21 4.37 5.28 6.32 7.47 8.50
393.15	6.895 13.79 20.68 27.58 34.47 41.37 48.26 55.16	2.0 2.0 2.0 2.0 2.0 2.0 2.0 2.0	1.45 2.52 3.83 5.30 6.46 7.89 8.98 10.24

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH₄; [74-82-8]

### **EVALUATOR:**

Colin L. Young,

Department of Physical Chemistry, University of Melbourne, Parkville, Victoria 3052,

Australia.

October 1980.

# CRITICAL EVALUATION:

The most extensive data on this system are those of Tsang  $et \ al.$ (1) who made measurements up to 138 MPa at temperatures between 92.3 K and 180.0 K. The mixture critical line and the pressure-temperature locus of solid-liquid-vapor equilibrium were also determined. Their measurements Were carried out using proven apparatus and experimental technique and are classified as recommended.

The limited results of Augood (2) at 111.7 K are broadly consistent With those of Tsang et al. but the scatter is very great and therefore Augood's data are classified as doubtful. The results of Freeth and Verschoyle (3) at 90.6 K show considerable scatter and are somewhat smaller than would be expected from an extrapolation of the data of Tsang  $et\ al$ . (1) and are therefore classified as doubtful. The data of Steckel and Tsin (4) were presented in small graphical form and are not considered further.

The data of Fastovskii and Gonikberg (5) appear to be in reasonable agreement with those of Tsang  $et\ al.$  (1) although they are considerably less precise. Similarly the measurements of Kirk and Ziegler (6) are in reasonable agreement with those of Tsang et  $\alpha l$ . (1) but show more scatter and are restricted to pressures below 13 MPa. The limited dof Benham and Katz (7) at 116.5 K, 144.3 K and 172 K are also in fair The limited data beindam and katz (7) at 110.5 k, 144.3 k and 1/2 k are also in large agreement with those of Tsang et al. (1) but are limited to pressure below 16 MPa. The data of Sagara et al. (8) give mole fraction solubilities which are slightly greater than those of Tsang et al. (1). The data of Fastovskii and Gonikberg (5), Kirk and Ziegler (6), Benham and Katz (7) and Sagara et al. (8) are all classified as tentative but all thought to be considerably less reliable than the measurements of Tsang et  $\alpha l$ . (1).

The data of Yorizane et al. (9) deviate considerably from the data of Tsang et al. (1) at pressure below 10 MPa but are in fair agreement at the second se ment at the pressures above 10 MPa. The former data are therefore classified as doubtful.

# References:

- 1. Tsang, C. Y.; Clancy, P.; Calado, J. C. G.; Streett, W. B. Chem. Eng. Comm. 1980, 6, 365-383.
- 2. Augood, D. R. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 3. Freeth, F. A.; Verschoyle, T. T. H. Proc. Roy. Soc. A 1931, 130, 453.
- 4. Steckel, F. A.; Tsin, N. M. Zh. Khim. Prom. 1939, 16, 24.
- 5. Fastovskii, V. G.; Gonikberg, M. G. Acta Physicochim. U.S.S.R. 1940, 12, 485.
- 6. Kirk, B. S.; Ziegler, W. T. Adv. Cryogenic Engng. 1965, 10, 160.
- 7, Benham, A. L.; Katz, D. L. Am. Inst. Chem. Engnrs. J. 1957, 3, 33.
- 8. Sagara, H.; Arai, Y.; Saito, S. J. Chem. Eng. Japan 1972, 5, 339.
- ٩. Yorizane, M.; Yoshimura, S.; Mazouka, H.; Toyama, A. Proc. ICECI 1968, p.59. Heywood Temple, London.

COMPONENTS:		ORIGINAL MEASU	REMENTS:			
l. Hydrogen; H2;	[1333-74-0]	Freeth, F.	A.; Verschoyle, T. T. H.;			
2. Methane; CH ₄	; [74-82-8]	Proc. Roy. Soc. A 1931, 130, 453-463.				
VARIABLES:		PREPARED BY:				
Pre	ssure	(	C. L. Young			
EXPERIMENTAL VALUES:	Mole fraction		Mole fraction			
T/K P/bar	of hydrogen in liquid, in var $x_{\rm H_2}$		of hydrogen ar in liquid, in vapor, $egin{array}{cccc} x_{\mathrm{H}}, & y_{\mathrm{H}}, \end{array}$			

EXPERIMENTA	L VALUES:						
T/K	P/bar	Mole fra of hydr in liquid, ^x H ₂	rogen	T/K	P/bar	Mole fra of hydr in liquid, $x_{\rm H_2}$	
90.66 90.68 90.64 90.67 90.63 90.65 90.65 90.63 90.66 90.68	17.11 17.18 21.90 26.97 30.13 36.89 44.47 46.71 46.81 56.35 56.56 80.61	0.0038 	0.9835 0.9790 0.9854 0.9873 0.9857 0.9799 0.9895 0.9863 0.9895 0.9875 0.9885 0.9905	90.63 90.67 90.62 90.61 90.65 90.64 90.67 90.63 90.62	100.64 129.89 129.92 166.97 168.99 188.55 198.34 208.14	0.0559 0.0819 0.0760 0.0784 0.0890 0.1016 0.1020 - 0.0958	0.9882 0.9846 0.9683 0.9789 0.9783 - 0.9789 0.9769 0.9787

# METHOD /APPARATUS/PROCEDURE:

Static equilibrium cell fitted with liquid and vapor sampling parts and magnetically operated stirrer. Pressure measured on pressure balance (dead weight gauge). Temperature measured with platinum resistance thermometer. Gas analysed by combustion and absorption. See ref. 1 and source, few details given.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Crude sample passed through fuming sulfuric acid, ordinary sulfuric acid and potassium hydroxide solution fractionally distilled six times.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$ ;  $\delta P/bar = \pm 0.1$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 0.005$ .

### REFERENCES:

1. Verschoyle, T. T. H.;

Phil. Trans. A 1931, 230, 189.

COMPONENT	rs:			ORIGINAL	MEASUREME	NTS:		
1. Hyd	rogen; H	-74-0]	Fasto	vskii, V.	G.; G	Gonikberg, M. G.		
-	•		Acta Physicochim. U.S.S.R.					
2. Met	hane; CH	2-8]	1940,	12, 485-	-488 and	l		
	•			$\overline{Zh}$ . $F$	iz. Khim.			
				1940,	14, 426.	,		
VARIABLES	٠.		-	PREPARED		<del></del>		
				FREPARED				
	Tempera	ture, pres	ssure	Ī	C	C. L. Yo	oung	
EXPERIMEN	NTAL VALUES	:		L	<del></del>			
		Ma	ole fraction				Mole fraction	
			of hydrogen				of hydrogen	
T/K	P/atm	P/MPa	in liquid,	T/K	P/atm	P/MPa	-	
			$x_{ m H_2}$				$x_{ m H_{2}}$	
90.5	40		0.024	110.2	78	7.9	0.064	
90.5	49 76	5.0 7.7	0.024	110.2	90	9.1	0.077	
90.5	102	10.3	0.050	110.2	97	9.8	0.085	
90.5 90.5	139 164	14.1 16.6	0.064 0.081	110.2 110.2	103 138	10.4 14.0	0.087 0.111	
90.5	171	17.3	0.082	110.2	141	14.3	0.119	
90.5	221	22.4	0.097	110.2	187	18.9	0.156	
103.3	39 77	4.0 7.8	0.022 0.063	122.2 122.2	36 77	3.6 7.8	0.032 0.063	
103.3	104	10.5	0.003	122.2	96	9.7	0.092	
103.3	111	11.2	0.099	122.2	112	11.3	0.099	
103.3 103.3	146	14.8	0.075	122.2	140	14.2	0.116	
103.3	175 234	17.7 23.7	0.105 0.138	122.2 127.2	187 37	18.9 3.7	0.162 0.038	
110.2	32	3.2	0.033	127.2	62	6.3	0.067	
110.2 110.2	49 66	5.0 6.7	0.042 0.058	127.2 127.2	85 131	8.6 13.3	0.093 0.143	
			AUXILIARY	INFORMAT	ION			
METHOD/A	PPARATUS/PR	OCEDURE:		SOURCE A	ND PURITY	OF MATER	IALS:	
<b>h</b>						-		
Kecirc	ulating v	apor flow	method					
descri	bed in re	ef. (1) wh	ich could			7		
not be	obtained	by compil	ler.		No	aetails	given.	
				}				
				ECTIVATO	ED ERROR		· · · · · · · · · · · · · · · · · · ·	
				1	ED ERROR: = ±0.5;	δ <i>P</i> /MPa	$= \pm 0.1;$	
				H ₂	= ±0.002			
				REFERENC	~FQ.	comp	oiler).	
				i	kolov, A.	Δ		
				1			+ + + + + + + + + + + + + + + + + + + +	
				, "Me	etnoas fo	or inves	stigating native	

gases", 1932 (Russian).

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Benham, A. L.; Katz, D. L. Am. Inst. Chem. Engnrs. J. 2. Methane; CH₄; [74-82-8] VARIABLES: Temperature, pressure PREPARED BY: C. L. Young

# EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction in liquid, $x_{\rm H_2}$	of hydrogen in vapor, yH2
172	34.5	0.0170	0.1583
	68.95	0.0877	0.4060
144.3	88.25	0.1255	0.4631
	103.4	0.1622	0.4678
	34.5	0.0343	0.6392
	68.95	0.0781	0.7618
116.5	102.7	0.1310	0.7931
	137.2	0.1805	0.7823
	33.8	0.0318	0.9279
	102.7	0.0950	0.9466
	158.6	0.1394	0.9383

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Recirculating vapor flow system described in ref. 1. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Vapor recirculated by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room temperature and pressure; analysed by gas density measurements. Details in ref. 1.

### SOURCE AND PURITY OF MATERIALS:

- Purity better than 99.5 mole per cent; further purified to remove water vapour.
- Purity better than 99.0 mole per cent; further purified to remove water and higher hydrocarbons.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.6$ ;  $\delta P/bar = \pm 0.5\%$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 0.5\%$ .

### REFERENCES:

Aroyan, H. J.; Katz, D. L.
 Ind. Eng. Chem. <u>1951</u>, 43, 185.

	325				
COMPONENTS:			ORIGINAL MEASUREMENTS:		
1. Hydro	ogen; H ₂ ; [	1333-74-0]	Augood, D. R.		
2. Metha	ane; CH4; [	74-82-8]	Trans. Instn. Chem. E	ngnrs.,	
			<u>1957</u> , <i>35</i> , 394-408.		
VARIABLES:			PREPARED BY:		
	Pressure		C. L. Young		
EXPERIMENTA	AL VALUES:				
T/K	P/psig ⁺	P/MPa	Mole fraction of hydin liquid, $x_{ m H_2}$ in g	rogen ras, y _{H2}	
111.7	2600 1500 330	18.03 10.44 2.38		942 940 -	
	[‡] psig ·	- pounds per	square inch gauge pressure		

ETHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
tatic equilibrium cell fitted with agnetically operated stirrer. fter equilibrium had been stablished samples of gas and liquid hases taken. The methane was ondensed out and both	1. Electrolytic sample containing 0.09 mole per cent HD.
omponents estimated volumetrically. atio of H ₂ /HD in liquid estimated Y mass spectrometry.	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1;  \delta P/MPa = \pm 0.1;$
	$\delta x_{\rm H_2}$ , $\delta y_{\rm H_2} = \pm 4\%$ (estimated by compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:				
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Methane; CH₄; [74-82-8]</li> </ol>	Kirk, B. S.; Ziegler, W. T.  Int. Adv. Cryog. Eng.  1965, 10, 160-170.				
VARIABLES: Temperature, pressure	PREPARED BY: C. L. Young				

EXPERIMEN'	TAL VALUES:	Mole fra of hydr					raction drogen
T/K	P/bar	in liquid, ^x H ₂	in vapor,	T/K	P/bar	in liquid x _{H2}	in vapor
90.74	20.32	0.0143	0.99028	116.57	126.32	0.1188	0.9432
	40.73 61.07	0.0275 0.0394	0.99193 0.99183	116.49 116.52	101.32 81.0	0.0967 0.0771	0.9466 0.9469
90.70	126.9	0.0748	0.98794	116.49	40.67	0.0382	0.9360
90.69	101.3 80.99	0.0612 0.0497	0.98997 0.99128	116.48	40.67 20.44	0.0383 0.0192	0.9357 0.9018
90.74	50.87 30.52	0.0336 0.0212	0.99242 0.99201	110.03 109.92	126.5 101.47	0.108 0.0880	0.9599 0.9629
	10.25	0.00761	0.98523	109.96	81.13	0.0711	0.9641
103.06	101.60	0.0789	0.9760	110.02	60.94	0.0532	0.9637
103.07	81.19	0.0634	0.9776	110.00	45.94	0.0407	0.9608
103.06	60.79	0.0480	0.9778	109.99	30.48	0.0275	0.9531
103.08 103.07	30.43 15.30	0.0252 0.0126	0.9735 0.9598	110.01	15.17	0.0134	0.9249

# METHOD /APPARATUS/PROCEDURE:

Single flow apparatus with two-compartment equilibrium cell. Pressure measured with Bourdon gauge. Temperature measured with a platinum resistance thermometer. Pure hydrogen bubbled through liquid methane. Samples analysed by gas chromatography. Details in source ref. and ref. 1.

### SOURCE AND PURITY OF MATERIALS:

- Purified gas, traces of nitrogen and oxygen.
- 2. Phillips research grade; purity 99.57 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.03; \quad \delta P/bar = \pm 0.03; \\ \delta x_{H_2}, \quad \delta y_{H_2} = \pm 2 \text{%}.$ 

### REFERENCES:

Kirk, B. S. Ph.D. Thesis,
 Georgia Institute of Technology,
 1964.

### COMPONENTS: ORIGINAL MEASUREMENTS: Yorizane, M.; Yoshimura, S.; l. Hydrogen; H₂; [1333-74-0] Masuoko, H.; Toyama, A. Methane; CH4; [74-82-8] Proc. ICECI, 1968, p.59, Heywood Temple, London. VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen P/atm T/K P/MPa in liquid, in vapor, $y_{\rm H_2}$ $x_{\rm H_2}$ 163.15 20 2.03 _ 0.136 20 0.132 2.03 30 3.04 0.011 0.341 0.030 0.456 40 4.05 50 0.028 0.521 5.07 0.521 60 0.047 6.08 0.081 0.569 80 8.11 0.140 0.608 100 10.13 120 12.16 0.178 0.599 0.576 140 14.19 0.286 150 15.20 0.286 0.550 143.15 10 1.01 0.003 0.152 20 2.03 0.008 0.510 30 3.04 0.035 0.682 40 4.05 0.055 0.693 50 5.07 0.064 0.745 2.03 123.15 20 0.020 0.886 30 3.04 0.038 0.931 40 0.909 4.05 0.038 50 5.07 0.056 0.902 0.004 103.15 0.930 10 1.01 15 1.52 0.010 0.953 20 2.03 0.013 0.962 30 3.04 0.030 0.968 50 5.07 0.050 0.963 AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Vapor recycle equilibrium cell with Purity 99.99 mole per cent or magnetic pump. Temperature measured better. with platinum resistance thermometer and pressure measured with Bourdon 2. Purity 99.93 mole per cent oxygen gauge. Vapor and liquid sampled and nitrogen being principle simultaneously and expanded to 200 impurities. cm³ at room temperature, analysed using GC. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.2$ ; $\delta P/MPa = \pm 0.03$ up to 7.5 MPa; $\delta x_{\text{H}_2}$ , $\delta y_{\text{H}_2} = \pm 2\%$ . (estimated by compiler.) REFERENCES:

COMPONENTS:				ORIGINAL MEASUREMENTS:						
1. Hydrogen; H ₂ ; [1333-74-0]					Sagara, H.; Arai, Y.; Saito, S.  J. Chem. Eng. Japan 1972, 5, 339-					
2.	Met	hane;	СН4; [74-82	-8]	348.					
VAR	IABLES	3:			PREPARED	BY:	<u> </u>			
Ter	mpera	ture, p	ressure		С. L. Y	oung				
EXP	ERIMEN	ITAL VALU	ES: Mole fra of hydr		•		Mole fra of hydr			
T/1	K	P/bar		in vapor,	T/K	P/bar			,	
10	3.05	20.0 41.3 61.2	0.0142 0.0337 0.0569	0.953 0.967 0.969	143.05	59.9 79.7 101.5	0.0684 0.0992 0.127	0.779 0.802 0.810		
12	3.15	82.0 91.2 10.2 20.3 40.3 60.6	0.0303 0.0708 0.0819 0.00730 0.0192 0.0385 0.0616	0.970 0.969 0.683 0.818 0.886	172.05 173.65	87.5 103.6 35.7 40.6 60.7 71.0	0.136	0.435 0.429 0.148 0.206 0.362 0.406		
14	3.05	81.8 101.8 10.7 20.2 40.7	0.0816 0.101 0.00310 0.0168 0.0477	0.911 0.908 0.214 0.541 0.721		81.7 83.8 100.5 103.4 108.3	0.124 0.131 0.190 0.205 0.225	0.424 0.424 0.420 0.411 0.401		

# METHOD/APPARATUS/PROCEDURE:

Static stainless steel cell of capacity  $5 \times 10^5 \text{ mm}^3$  fitted with magnetic stirrer and sampling valves. ture measured with thermocouple. Pressure measured using Bourdon Gases added to cell and gauge. equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. Nippon Sanso Co. Ltd. sample; purity 99.99 mole per cent.
- 2. Takachiho Chemical Industry Co. Ltd. sample; purity 99.9 mole per cent.

$$\delta T/K = \pm 0.1$$
;  $\delta P/bar = \pm 0.1$ ;

$$\delta x_{\rm H_2} = \delta y_{\rm H_2} = \pm 1\%.$$

_			Jaluraleu i	- Tyurocarbons	,		UZ.
COMPONEN	TS:			ORIGINAL M	EASUREMENTS	:	
1. Hydrogen; H ₂ ; [1333-74-0]				Tsang,	C. Y .;	Clancy, P.	;
			-	-	, J. C. G	_	, W. B.
2. Met	hane; Cl	H ₄ ; [74-82-	8]	1	•	. 1980, 6,	
				Chem.	eng. comm	. 1500, 0,	303-303.
				Ì			
VARIABLE	S:			PREPARED B	Υ:		
	Tempe	erature, pre	ssure		c.	L. Young	
	-0	oradaro, pro					
EXPERIME	NTAL VALUE	S:		L			
		Mole fra				Mole fra	
T/K	P/MPa	of hydr	ogen in vapor,	T/K	P/MPa	of hydr in liquid,	
-/1	1 / FIF a		•	1/1	1/HFa	m riquid,	y _H ,
		$x_{ m H_2}$	$y_{\rm H_2}$			H ₂	H ₂
92.3	0.22	0.0018	0.9084	92.3	55.26	0.2393	0.9386
	0.31	0.0023	0.9257		69.07	0.2836	0.9233
	0.38	0.0031	0.9509		82.96	0.3300	0.8998
	0.45 0.52	0.0035 0.0040	0.9561 0.9625		97.01 110.77	0.3780 0.4324	0.8808 0.8571
	0.52	0.0040	0.9672		125.08	0.4967	0.8264
	0.65	0.0050	0.9722		131.38	0.5361	0.7983
	0.79	0.0060	0.9770		134.58	0.5591	0.7918
	1.14	0.0085	0.9821		137.98	0.5875	0.7563
	1.48 1.83	0.0113 0.0140	0.9857 0.9875	100.0	0.51 0.60	0.0041 0.0050	0.9175 0.9285
	2.18	0.0140	0.9888		0.60	0.0055	0.9358
	2.87	0.0209	0.9904		0.77	0.0063	0.9420
	3.56	0.0251	0.9917		1.12	0.0094	
	4.22	0.0293			1.40	0.0116	0.9607
	5.63	0.0382	0.9914		1.67	0.0140	0.9667
	7.02	0.0461	0.9904		1.96	0.0163	0.9717
	10.42 13.91	0.0647 0.0826	0.9893 0.9860		2.86 3.56	0.0230 0.0283	0.9758 0.9786
	17.47	0.0826	0.9821		4.23	0.0283	0.9788
	20.83	0.1134	0.9791		4.92	0.0388	0.9819
	27.87	0.1416	0.9707		5.63	0.0436	0.9819
	41.56	0.1926	0.9546			(0	ont.)
	<u>"-</u>	<del></del>	AUVITIARY	INFORMATION	T		·

# METHOD/APPARATUS/PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetically operated pump. Pressure measured with manganin pressure gauge.
Temperature measured with platinum

Temperature measured with platinum resistance thermometer. Samples of liquid gas analysed using a thermal conductivity gas analyser.

# SOURCE AND PURITY OF MATERIALS:

- Matheson ultra high purity sample, purity 99.999 mole per cent or better.
- 2. Matheson sample, purity 99.99 mole per cent or better.

### ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.02; \quad \delta P/\text{MPa} = \pm 0.5\$; \\ \delta x_{\text{H}_2}, \ \delta y_{\text{H}_2} = \pm 0.005 \ \text{(but may be as large as } \pm 0.02 \ \text{near critical point)}.$ 

# REFERENCES:

Streett, W. B.; Calado, J. C. G.
 J. Chem. Thermodyn. <u>1978</u>, 10,
 1089.

1. Hydrogen; H ₂ ; [1333-74-0] 2. Methane; CH ₄ ; [74-82-8]  EXPERIMENTAL VALUES:    Mole fraction of hydrogen of hydrogen in liquid, in vapor	COMPON	ENTS:			ORIGINA	L MEASURI	EMENTS:	
EXPERIMENTAL VALUES:  **Mole fraction of hydrogen in liquid, in vapor, T/K	l. Hyd	rogen; H	2; [1333-74	1-0]	Tsang, (	C. Y.; (	Clancy, P.;	
EXPERIMENTAL VALUES:  **Mole fraction of hydrogen in liquid, in vapor, #H2	2. Met	hane; CH	4; [74-82-8	3]	Calado,	J. C. G.	.; Streett,	W. B.
EXPERIMENTAL VALUES:  **Mole fraction of hydrogen in liquid, in vapor, #H2	!				Chem. E	na. Comm	. 1980, <i>6</i> , 30	65-383.
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$								
T/K P/MPa in liquid, in vapor, T/K P/MPa in liquid, in vapor	EXPERI	MENTAL VA	LUES:		<u>.l</u>			
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$								
100.0	T/K	P/MPa	in liquid,	in vapor,	T/K	P/MPa	in liquid,	in vapor
10.42 0.0753 0.9796 12.22 0.1204 0.9351 13.94 0.0965 0.9742 13.95 0.1362 0.2929 17.32 0.1162 0.9705 17.53 0.1710 0.9292 17.32 0.1162 0.9705 17.53 0.1710 0.9182 20.91 0.1396 0.9660 20.94 0.2027 0.9104 24.35 0.1579 0.9507 24.21 0.2332 0.8982 27.71 0.1755 0.9553 27.82 0.2693 0.8878 41.74 0.2449 0.9280 31.29 0.3031 0.8685 55.37 0.3080 0.9016 34.58 0.3384 0.8437 68.95 0.3813 0.8733 38.17 0.3819 0.8325 89.78 0.5324 0.8037 43.51 0.4651 0.7839 93.17 0.5777 0.7574 44.87 0.4963 0.7560 95.61 - 0.7096 130.0 0.81 0.0053 0.6245 110.0 0.34 0.0021 0.7252 1.48 0.0139 0.7572 0.45 0.0032 0.8355 2.17 0.0212 0.8128 0.56 0.78 0.0068 0.8867 5.66 0.0602 0.8478 1.11 0.0096 0.8958 6.99 0.0744 0.8656 0.78 0.0068 0.8867 5.66 0.0602 0.8478 1.11 0.0096 0.8958 6.99 0.7748 0.8850 1.49 0.0136 0.9228 9.75 0.1070 0.8957 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0136 0.9228 9.75 0.1070 0.8954 1.49 0.0058 0.0442 0.9607 27.63 0.3295 0.0044 0.9605 0.9632 33.20 0.4320 0.7617 9.07 0.0780 0.9632 33.20 0.4320 0.7617 9.07 0.0780 0.9632 33.00 0.4320 0.7617 9.07 0.0780 0.9632 33.00 0.4320 0.7617 9.07 0.0780 0.9632 33.00 0.4320 0.07617 9.07 0.0780 0.9632 33.00 0.4320 0.07617 9.07 0.0780 0.9632 33.00 0.4320 0.07617 9.07 0.0780 0.9632 33.00 0.4320 0.07617 9.07 0.0780 0.9632 33.00 0.998 0.0255 5.39 0.0255 0.7000 48.86 0.3755 0.8509 4.26 0.0646 0.7628 4.88 0.0755 0.8509 4.26 0.0646 0.7628 5.89 0.0255 0.7000 0.9632 3.0000 0.0665 0.6902 2.593 0.3923 0.7288 5.500 0.04145 0.8229 8.33 0.0998 0.0243 5.500			<i>x</i> _{H₂}	^у н ₂			^ж н ₂	^y _{H₂}
13.94	100.0				120.0			
17,32								
24,35	1					17.53		0.9182
10.0								
1.74								
68.95         0.3813         0.8733         38.17         0.3293         0.8325           89.78         0.5324         0.8037         43.51         0.4651         0.7839           93.17         0.5777         0.7574         44.87         0.4963         0.7560           94.58         0.6103         0.7396         46.73         0.5746         0.6941           110.0         0.34         0.0021         0.7252         1.48         0.0139         0.7572           0.45         0.0032         0.8355         2.17         0.0212         0.8128           0.56          0.6649         2.87         0.0289         0.8478           0.58         0.046          4.20         0.0444         0.8656           0.78         0.0068         0.8958         6.99         0.0748         0.8850           1.49         0.0136         0.9228         9.75         0.1070         0.8927           1.83         0.0165         0.9308         12.49         0.1394         0.8850           1.49         0.0136         0.9228         9.75         0.1070         0.8867           2.82         0.252         0.9485         2.097						31.29		
10.0								
10.0								
10.0						43,51		0.7839
10.0								
110.0		94.58 95.61			130.0			
0.56	110.0	0.34	0.0021		10010	1.48	0.0139	0.7572
0.58         0.0046          4,20         0.0444         0.8656           0.78         0.0068         0.8867         5.66         0.0602         0.8774           1.11         0.0096         0.8958         6.99         0.0748         0.8850           1.49         0.0136         0.9228         9.75         0.1070         0.8927           1.83         0.0165         0.9308         12.49         0.1394         0.8894           2.18         0.0198         0.9391         15.26         0.1719         0.8867           2.82         0.0252         0.9485         20.97         0.2386         0.8649           3.56         0.0318         0.9541         24.41         0.2834         0.8447           4.98         0.0442         0.9607         27.63         0.3295         0.8254           6.37         0.0556          31.07         0.3874         0.7935           7.78         0.0672         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9632         34.01         0.4521         0.7456           13.97         0.1153         0.953         35.60          0.								
0.78         0.0668         0.8867         5.66         0.0602         0.8774           1.11         0.0096         0.8958         6.99         0.0748         0.8850           1.49         0.0136         0.9228         9.75         0.1070         0.8827           1.83         0.0165         0.9308         12.49         0.1394         0.8867           2.82         0.0252         0.9485         20.97         0.2386         0.8649           3.56         0.0318         0.9541         24.41         0.2834         0.8447           4.98         0.0442         0.9607         27.63         0.3295         0.8254           6.37         0.0556          31.07         0.3874         0.7935           7.78         0.0672         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9632         34.01         0.4521								
1.49 0.0136 0.9228 9.75 0.1070 0.8927 1.83 0.0165 0.9308 12.49 0.1394 0.8894 2.18 0.0198 0.9391 15.26 0.1719 0.8867 2.82 0.0252 0.9485 20.97 0.2386 0.8649 3.56 0.0318 0.9541 24.41 0.2834 0.8447 4.98 0.0442 0.9607 27.63 0.3295 0.8254 6.37 0.0556 31.07 0.3874 0.7935 7.78 0.6672 0.9632 33.20 0.4320 0.7617 9.07 0.0780 0.9632 33.20 0.4320 0.7617 9.07 0.0780 0.9632 33.20 0.4320 0.7617 1.34 0.1417 0.9497 36.27 0.6363 20.86 0.1684 0.9422 140.0 1.59 0.0124 0.6363 20.86 0.1684 0.9422 140.0 1.59 0.0124 0.6558 41.54 0.3152 0.8837 2.89 0.0285 0.6558 41.54 0.3152 0.8837 2.89 0.0285 0.6558 41.89 0.3413 0.8690 3.18 0.7291 48.81 0.3703 0.8505 2.89 0.0285 0.7200 48.86 0.3755 0.8509 4.26 0.0464 0.7628 51.86 0.4012 0.8325 5.66 0.0635 0.7971 53.20 0.4145 0.8229 8.33 0.0998 0.8243 55.29 0.4361 0.8181 11.15 0.1386 0.8305 55.39 0.4372 0.8108 13.90 0.1780 0.8276 57.32 0.4592 0.8017 17.28 0.2278 0.8138 58.85 0.4768 0.7973 20.24 0.2746 0.7929 62.28 0.5402 0.7634 21.17 0.2912 0.7856 63.58 0.5830 0.7053 22.95 0.3242 0.7654 63.90 0.6065 0.6902 2.583 0.3923 0.7288 1.51 0.0138 0.8300 3.22 0.0325 0.6511 2.18 0.0206 0.8741 4.26 0.0468 0.6910 3.58 0.0345 0.9104 5.58 0.0657 0.7193 5.65 0.0549 0.9280 7.01 0.0871 0.7329 7.20 0.0702 0.9325 8.47 0.1102 0.7449		0.78	0.0068			5.66	0.0602	0.8774
1.83       0.0165       0.9308       12.49       0.1394       0.8894         2.18       0.0198       0.9391       15.26       0.1719       0.8867         2.82       0.0252       0.9485       20.97       0.2386       0.8649         3.56       0.0318       0.9541       24.41       0.2834       0.8447         4.98       0.0442       0.9607       27.63       0.3295       0.8254         6.37       0.0556        31.07       0.3874       0.7935         7.78       0.0672       0.9632       33.20       0.4320       0.7617         9.07       0.0780       0.9632       34.01       0.4521       0.7456         13.97       0.1153       0.9593       35.60        0.7305         17.34       0.1417       0.9497       36.27        0.6363         20.86       0.1684       0.9264       1.85       0.0152       0.5782         34.70       0.2674       0.9050       2.49        0.6558         41.54       0.3152       0.8837       2.89       0.0285          44.89       0.3413       0.8690       3.18        0.7291								
2.18         0.0198         0.9391         15.26         0.1719         0.8867           2.82         0.0252         0.9485         20.97         0.2386         0.8649           3.56         0.0318         0.9541         24.41         0.2834         0.8447           4.98         0.0442         0.9607         27.63         0.3295         0.8254           6.37         0.0556          31.07         0.3874         0.7935           7.78         0.0672         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9632         34.01         0.4521         0.7456           13.97         0.1153         0.9593         35.60          0.6363           20.86         0.1684         0.9422         140.0         1.59         0.0124            27.64         0.2164         0.9264         1.85         0.0152         0.5782           34.70         0.2674         0.9050         2.49          0.6558           41.54         0.3152         0.8837         2.89         0.0285            44.89         0.3413         0.8690         3.18 <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>								
3.56		2.18	0.0198	0.9391				
4.98       0.0442       0.9607       27.63       0.3295       0.8254         6.37       0.0556        31.07       0.3874       0.7935         7.78       0.0672       0.9632       33.20       0.4320       0.7617         9.07       0.0780       0.9632       34.01       0.4521       0.7456         13.97       0.1153       0.9593       35.60        0.7305         17.34       0.1417       0.9497       36.27        0.6363         20.86       0.1684       0.9422       140.0       1.59       0.0124          27.64       0.2164       0.9264       1.85       0.0152       0.5782         34.70       0.2674       0.9050       2.49        0.6558         41.54       0.3152       0.8837       2.89       0.0285          44.89       0.3413       0.8690       3.18        0.7291         48.31       0.3703       0.8505       2.89       0.0285       0.7200         48.86       0.3755       0.8509       4.26       0.0464       0.7628         51.86       0.4012       0.8325       5.66       0.0635								
6.37         0.0556          31.07         0.3874         0.7935           7.78         0.0672         0.9632         33.20         0.4320         0.7617           9.07         0.0780         0.9593         35.60          0.7305           17.34         0.1417         0.9497         36.27          0.6363           20.86         0.1684         0.9422         140.0         1.59         0.0124            27.64         0.2164         0.9264         1.85         0.0152         0.5782           34.70         0.2674         0.9050         2.49          0.6558           41.54         0.3152         0.8837         2.89         0.0285            44.89         0.3413         0.8690         3.18          0.7291           48.81         0.3703         0.8505         2.89         0.0285         0.7200           48.86         0.3755         0.8509         4.26         0.0464         0.7628           51.86         0.4012         0.8325         5.66         0.0635         0.7971           53.20         0.4145         0.8229         8.33         0.0998								
9.07       0.0780       0.9632       34.01       0.4521       0.7456         13.97       0.1153       0.9593       35.60        0.7305         17.34       0.1417       0.9497       36.27        0.6363         20.86       0.1684       0.9422       140.0       1.59       0.0124          27.64       0.2164       0.9264       1.85       0.0152       0.5782         34.70       0.2674       0.9050       2.49        0.6558         41.54       0.3152       0.8837       2.89       0.0285          44.89       0.3413       0.8690       3.18        0.7291         48.31       0.3703       0.8505       2.89       0.0285       0.7200         48.86       0.3755       0.8509       4.26       0.0464       0.7628         51.86       0.4012       0.8325       5.66       0.0635       0.7971         53.20       0.4145       0.8229       8.33       0.0998       0.8243         55.39       0.4372       0.8108       13.90       0.1780       0.8276         57.32       0.4592       0.8017       17.28       0.227						31.07	0.3874	
13.97								
17.34							0.4521	
27.64		17.34	0.1417	0.9497		36.27		
34.70					140.0			
41.54								
48.31		41.54	0.3152	0.8837		2.89		
48.86								
51.86         0.4012         0.8325         5.66         0.0635         0.7971           53.20         0.4145         0.8229         8.33         0.0998         0.8243           55.29         0.4361         0.8181         11.15         0.1386         0.8305           55.39         0.4372         0.8108         13.90         0.1780         0.8276           57.32         0.4592         0.8017         17.28         0.2278         0.8138           58.85         0.4768         0.7973         20.24         0.2746         0.7929           62.28         0.5402         0.7634         21.17         0.2912         0.7856           63.58         0.5830         0.7053         22.95         0.3242         0.7674           63.90         0.6065         0.6902         25.83         0.3923         0.7288           120.0         0.79         0.0062         0.7178         27.85         0.4751         0.6652           1.13         0.0101         0.7893         150.0         1.55         0.0089         0.4428           1.51         0.0138         0.8300         3.22         0.0325         0.6511           2.18         0.0206         0.8741								
11.15		51.86		0.8325		5.66		
55.39								
57.32         0.4592         0.8017         17.28         0.2278         0.8138           58.85         0.4768         0.7973         20.24         0.2746         0.7929           62.28         0.5402         0.7634         21.17         0.2912         0.7856           63.58         0.5830         0.7053         22.95         0.3242         0.7674           63.90         0.6065         0.6902         25.83         0.3923         0.7288           120.0         0.79         0.0062         0.7178         27.85         0.4751         0.6652           1.13         0.0101         0.7893         150.0         1.55         0.0089         0.4428           1.51         0.0138         0.8300         3.22         0.0325         0.6511           2.18         0.0206         0.8741         4.26         0.0468         0.6910           3.58         0.0345         0.9104         5.58         0.0657         0.7193           5.65         0.0549         0.9280         7.01         0.0871         0.7329           7.20         0.0702         0.9325         8.47         0.1102         0.7449								
62.28						17.28	0.2278	
63.58								
120.0 0.6065 0.6902 25.83 0.3923 0.7288 120.0 0.79 0.0062 0.7178 27.85 0.4751 0.6652 1.13 0.0101 0.7893 150.0 1.55 0.0089 0.4428 1.51 0.0138 0.8300 3.22 0.0325 0.6511 2.18 0.0206 0.8741 4.26 0.0468 0.6910 3.58 0.0345 0.9104 5.58 0.0657 0.7193 5.65 0.0549 0.9280 7.01 0.0871 0.7329 7.20 0.0702 0.9325 8.47 0.1102 0.7449								
1.13 0.0101 0.7893 150.0 1.55 0.0089 0.4428 1.51 0.0138 0.8300 3.22 0.0325 0.6511 2.18 0.0206 0.8741 4.26 0.0468 0.6910 3.58 0.0345 0.9104 5.58 0.0657 0.7193 5.65 0.0549 0.9280 7.01 0.0871 0.7329 7.20 0.0702 0.9325 8.47 0.1102 0.7449		63.90	0.6065	0.6902		25.83	0.3923	
1.51     0.0138     0.8300     3.22     0.0325     0.6511       2.18     0.0206     0.8741     4.26     0.0468     0.6910       3.58     0.0345     0.9104     5.58     0.0657     0.7193       5.65     0.0549     0.9280     7.01     0.0871     0.7329       7.20     0.0702     0.9325     8.47     0.1102     0.7449	120.0				150 0			
2.18 0.0206 0.8741 4.26 0.0468 0.6910 3.58 0.0345 0.9104 5.58 0.0657 0.7193 5.65 0.0549 0.9280 7.01 0.0871 0.7329 7.20 0.0702 0.9325 8.47 0.1102 0.7449					120.0			
5.65 0.0549 0.9280 7.01 0.0871 0.7329 7.20 0.0702 0.9325 8.47 0.1102 0.7449		2.18	0.0206	0.8741		4.26	0.0468	0.6910
7.20 0.0702 0.9325 8.47 0.1102 0.7449		3.58						
		1.40	0.0.02	0.0000		J		

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]

# ORIGINAL MEASUREMENTS:

Tsang, C. Y.; Clancy, P.;

Calado, J. C. G.; Streett, W. B.

Chem. Eng. Comm. 1980, 6, 365-383.

# EXPERIMENTAL VALUES:

T/K	P/MPa	Mole frac of hydro in liquid, x H ₂	ogen	T/K	P/MPa	Mole fra of hydr in liquid, $x_{\rm H_2}$	
150.0	9.70 12.52 15.38 17.77 20.21 20.90 21.59 22.41 2.43 2.84 3.68 5.07 6.26 8.71 10.43 11.75 12.79 14.03 15.27 16.06 16.64 17.32	0.1311 0.1784 0.2305 0.2782 0.3449 0.3695 0.3985 0.4708 0.0146 0.0204 0.0355 0.0582 0.0793 0.1231 0.1569 0.1838 0.2059 0.2364 0.2725 0.3006 0.3238 0.3629	0.7492 0.7468 0.7366 0.7115 0.6605 0.6605 0.6392 0.5860 0.2661 0.3363 0.4505 0.5457 0.5950 0.6491 0.6491 0.6491 0.6466 0.6357 0.6181 0.6030 0.5842 0.5527	170.0	3.74 4.44 5.76 7.10 8.56 9.78 11.14 11.79 12.58 12.82 4.76 5.30 5.80 6.19 6.73 7.21 7.77 8.33 8.67	0.0271 0.0405 0.0662 0.0949 0.1307 0.1617 0.2066 0.2275 0.2702 0.2933 0.0332 0.0460 0.0589 0.0700 0.0873 0.1023 0.1023 0.1241 0.1517 0.1810	0.2436 0.3137 0.3995 0.4481 0.44750 0.4816 0.4754 0.4647 0.4384 0.4147 0.1608 0.1953 0.2242 0.2399 0.2581 0.5159 0.2726 0.2667 0.2528

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ethane;  $C_2H_6$ ; [74-84-0]

### **EVALUATOR:**

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

August 1980

### CRITICAL EVALUATION:

This system has been investigated by five groups. The data of Levitskaya (1) and Levitskaya and Pryannikov, (2) are rejected since they are of low precision and deviate considerably from more recently published The data of Hiza et al. (3), which cover the temperature range data. 107 to 190 K and pressures between 2 and 15 MPa, and those of Cohen  $et \ al.$ (4), which cover the range 144 to 200 K and pressures between 0.7 and 140 MPa, are in good agreement. Both sets of data give K-values which are in good agreement with those quoted by Williams and Katz (5). fraction solubility data of Sagara et al. (6) are somewhat smaller than those of Hiza  $et \ al.$  (3) and Cohen  $et \ al.$  (4). Sagara et al. (6) data are more limited than those of refs. (3) and (4) and cover the temperature range 148 to 223 K and pressure between 2 and 8 MPa, and are classified Williams and Katz (5) data are only presented in graphical as doubtful. form and in the form of K-values (K = mole fraction in gas phase/mole fraction in liquid phase). The data of Hiza et al. (3) and Cohen et al. (4) are classified as tentative.

### References:

- 1. Levitskaya, E. P. Zh. Tekh. Fiz. 1941, 11, 197.
- Levitskaya, E. P.; Pryannikov, K. Zh. Tekh. Fiz. 1939, 9, 1849.
- 3. Hiza, M. J.; Heck, C. K.; Kidnay, A. J. Adv. Cryogenic Engng. 1968, 13, 343.
- 4. Cohen, A. E.; Hipkin, H. G.; Koppany, C. R. Chem. Engng. Progr. Symp. Ser. 1967, no. 81, 63, 10.
- 5. Williams, R. B.; Katz, D. L. Ind. Eng. Chem. 1954, 46, 2512.
- Sagara, H.; Arai, Y.; Saito, S. J. Chem. Eng. Japan <u>1972</u>, 5, 339.

### COMPONENTS: ORIGINAL MEASUREMENTS: Williams, R.B.; Katz, D.L. Hydrogen: H2: [1334-74-0] Ind. Eng. Chem. 1954, 46,2512-20. 2. Ethane: CoHe: [74-84-0] VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: K-value of ethane T/K P/bar K-value of hydrogen 0.922 283.15 34.5 12.1 0.657 69.0 6.45 3.21 0.567 137.9 172.4 2.135 0.632 17.2 48.8 0.896 255.37 34.5 24.4 0.534 0.347 12.2 69.0 6.12 137.9 0.264 275.8 2.82 0.296 413.7 1.853 0.616 227.59 17.2 75.4 0.424 34.5 36.8 0.246 0.148 18.1 69.0 137.9 9.05 0.113 275.8 0.116 4.49 551.6 2.17 0.219 101.2 199.82 17.2 0.150 34.5 49.0 0.0850 69.0 24.3 0.0545 137.9 12.4 0.0432 6.35 0.0463 275.8 AUXILIARY INFORMATION METHOD: /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. Purity 99.9 mole %. Dried. Flow system described in ref. (1). Temperature measured with thermo-2. Phillips Petroleum Co. pure grade, couple. Pressure measured with Bourdon gauge. Vapor recirculated purity 99.7 mole %, dried. by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room temperature and pressure analysed by gas density measurements. Details ref. (1). ESTIMATED ERROR: $\delta T/K = \pm 0.6$ ; $\delta P/bar = \pm 0.5$ %;

 $\delta T/K = \pm 0.6$ ;  $\delta P/bar = \pm 0.5$ %;  $\delta K/K < 0.01$ .

### REFERENCES:

Aroyan, H.J.; Katz, D.L.
 Ind. Eng. Chem. <u>1951</u>, 43,185.

- 1. Hydrogen; H₂; [1334-74-0]
- 2. Ethane;  $C_2H_6$ ; [74-84-0]

# ORIGINAL MEASUREMENTS

Williams, R.B.; Katz, D.L.

Ind. Eng. Chem. 1954, 46,2512-20

# EXPERIMENTAL VALUES:

т/к	P/bar	K-value of hydrogen	K-value of ethane
199.92	551.6	3.38	0.0750
172.04	17.2	124.4	0.0362
	34.5	62.2	0.0206
	69.0	31.3	0.0143
	137.9	16.3	0.0127
	275.8	8.75	0.0157
144.26	551.6	4.86	0.0277
	17.2	160	0.00462
	34.5	83.0	0.00314
	69.0	43.2	0.00266
	137.9	23.6	0.00272
	275.8	13.1	0.00432
	551.6	7.45	0.00934
152.04	17.2 34.5 69.0 137.9 275.8 551.6	238 129 70.8 40.0 22.7 13.5	- - - - -
138.15	17.2	320	-
	34.5	179	-
	69.0	100	-
	137.9	57.4	-
	275.8	33.3	-
	551.6	19.8	-

### Saturated Hydrocarbons 335 COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen, H₂; [1333-74-0] Cohen, A.E.; Hipkin, H.G.; Ethane, C₂H₆; [74-84-0] Koppany, C.R. Chem. Eng. Prog. Symp. Ser. No. 81, 1967, 63, 10-17. VARIABLES: PREPARED BY: Temperature, pressure. C.L. Young EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/bar in liquid, in vapor, $x_{\rm H_2}$ $y_{\rm H_2}$ 144.21 9.20 0.0036 0.9933 144.21 21.00 0.0062 0.9967 144.21 34.40 0.0118 0.9975 144.21 51.04 0.0185 0.9979 144.15 68.32 0.0258 0.9975 143.48 104.66 0.0378 0.9951 143.42 137.21 0.0454 0.9979 158.15 7.38 0.0033 0.9728 21.11 158.15 0.0103 0.9884

0.0175

0.0266

0.0345

0.0470

0.0545

0.0036

0.0078

0.0169

0.0256

0.0355

0.0510

0.0674

0.0043

0.0135

0.0235

0.0341

0.0470

0.0700

199.65 137.9 0.0897 METHOD /APPARATUS/PROCEDURE : Equilibrium established in cell by re- 1. Air Reduction Corp. sample "bone-Circulating vapor through external flow line at room temperature. Pressure measured with dead weight gauge. Temperature measured with platinum resistance thermometer. Liquid and vapor samples analysed by gas chromatography using thermal conductivity and flame ionisation detectors. Details in source and ref. 1.

158.21

158.21

158.21

158.21

158.15

171.93

171.93

171.93

171.87

171.87

171.87

171.98

199.32

199.32

199.32

199.32

199.32

199.54

34.83

51.59

68.80

103.77

137.21

7.08

21.02

34.69

51.36

69.53

7.66

20.68

34.84

51.90

67.91

103.4

103.6

137.2

SOURCE AND PURITY OF MATERIALS:

dry" grade minimum purity 99.8 mole per cent. Dried over molecular sieve.

0.9928

0.9939

0.9956

0.9953

0.9944

0.9398 0.9769

0.9815

0.9852

0.9878

0.9887 0.9890

0.7290 0.8870

0.9284

0.9453

0.9528

0.9600

0.9618

2. CP grade from Matheson, purity 99 mole per cent. Dried over molecular sieve.

ESTIMATED ERROR:  $\delta T/K = \pm 0.05$ ;  $\delta P/bar = \pm 0.07$  or 1% whichever greater;  $\delta x_{\rm H_2} \simeq \delta y_{\rm H_2} \simeq 3\%$ at high concentration varying to ±0.001 at 0.01 and 0.0003 at 0.0005. REFERENCES:

1. H.G. Hipkin, Am. Inst. Chem. Eng. J. 1966, 12,484.

336	Hydrogen and Deuterium	Solubilities above	200kPa
COMPONENTS:		ORIGINAL MEASUR	EMENTS:
1. Hydrogen; H ₂ ;	[1333-74-0]	Hiza, M.J.;	Heck, C.K. Kidnay, A.J.
1			
2. Ethane; C ₂ H ₆ ;	[/4-84-0]	343-355.	nic Eng. <u>1968</u> , 13,
VARIABLES:		PREPARED BY:	
Temperatu	are, pressure		C.L. Young
EXPERIMENTAL VALUES:			
T/K	<i>p/</i> 10 ⁵ Pa	Mole fraction	<b>-</b> . •
		in liquid, $x_{\rm H_2}$	in gas, ^y H ₂
189.55	25.2		0.9327
189.55	25.5	0.0145	_
189.57	41.4	0.0239	0.9538
189.59	60.9	0.0354	0.9640
189.73	91.9	-	0.9706
189.59	102.7	0.0570	0.9718
189.73	121.8	<b>-</b>	0.9730
189.55	145.4	0.0775	0.9739
189.58	153.5	-	0.9741
169.40	24.6	0.0121	0.9779
169.40	40.7	0.0193	0.9846
169.39	61.0	0.0286	0.9876
169.43	89.9	0.0409	0.9890
169.43	121.6	-	0.9895 0.9892
169.46 169.41	146.2 149.9	0.0651	0.9894
149.43	19.0	0.00745	-
149.44	20.3	0.00787	-
149.69	22.0	_	0.99424
149.62	39.3	-	0.99611
149.41	40.0	0.0150	_
149.09	60.2	0.0226	-
149.52	60.8	-	0.99670
149.68	89.2	_	0.99690
149.31	91.2	0.0332	cont.
	AUXILIARY	INFORMATION	
METHOD/APPARATUS/PRO	CEDURE:	SOURCE AND PURI	TY OF MATERIALS:
Flow cell descri	bed in detail in	1	ls given.
	erature measured		
	sistance thermometer	2. Purity 9	9.96 mole per cent.
	sured with Bourdon		
	rged with components,	·	
	ed and vapor and	,	

liquid samples withdrawn and analysed by gas chromatography. Details of apparatus in source and ref. (1).

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.02$$
;  $\delta P/10^5 Pa = \pm 0.1$ ;  $\delta x_{\rm H_2}$ ,  $\delta (1-y_{\rm H_2}) = \pm 2-3$ %

# REFERENCES:

1. Herring, R.N.; Barrick, P.L. Int. Adv. Cryogenic Engng, 1965, 10, 151.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ethane; C₂H₆; [74-84-0]

### ORIGINAL MEASUREMENTS:

Hiza, M.J. Heck, C.K.; Kidnay, A.J.

Adv. Cryogenic Eng. 1968, 13, 343-355.

		343-355.	•	
EXPERIMENTAL VALUES:				
	/* a 5-	Mole fraction o		
T/K	p/10⁵Pa	in liquid,	in gas,	
		x _{H2}	у _{Н2}	
149.54	120.5	0.0414	-	
149.78	148.6	0.0507	-	
130.00	5.02	-	0.99742	
130.00	6.35	-	0.99786	
130.00	10.13	-	0.99855	
130.00	10.59	-	0.99863	
129.74	25.6	0.00769	-	
130.00	26.73	-	0.999254	
130.00	40.53	-	0.999377	
129.58	51.3	0.0154	_	
130.00	60.79	-	0.999422	
129.49	80.9	0.0223	_	
130.00	91.8	-	0.999395	
129.59	113.3	0.0299	-	
130.00	121.9	-	0.999328	
129.78	148.2	0.0368	-	
130.00	151.7	-	0.999207	
122.00	5.83	-	0.999106	
122.00	10.45	-	0.999444	
122.00	10.51	-	0.999446	
121.91	25.7	0.00670	-	
122.00	26.41	-	0.999697	
122.00	40.92	<del>-</del>	0.999731	
121.91	51.5	0.0126	<del>-</del>	
122.00	59.6	_	0.999738	
121.86	80.6	0.0191	<del>-</del>	
122.00	81.7	-	0.999724	
121.71	109.8	0.0249	<u>-</u>	
122.00	113.4	-	0.999675	
122.00	137.2	-	0.999619	
122.00	143.3	_	0.999605	
121.84	156.0	0.0326	-	
108.00	10.4	-	0.9999349	
108.00	25.9	-	0.9999571	
108.00	42.4	-	0.9999608	
107.83	61.3	0.0114	0 0000574	
108.00	61.6	-	0.9999574	
108.00	84.7	0.0160	0.9999467	
107.76 108.00	91.0	0.0160	- 0000300	
107.85	111.5	0.0201	0.9999300	
108.00	122.8 146.1	U.UZUI	0 000000	
107.85		0 0237	0.999889	
107.05	152.9	0.0237	<b>-</b>	

Additional vapor-liquid equilibrium data in source. Vapor composition at 130.00 K and below were determined in a single-pass flow apparatus.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Sagara, H.; Arai, Y.; Saito, S J. Chem. Eng. Japan <u>1972</u> , 5, 339-
2. Ethane; C ₂ H ₆ ; [74-84-0]	348.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young

EXPERIMENT	AL VALUES:		
T/K	P/bar	Mole fraction in liquid,	
1/1	1/Dal		in gas,
		$x_{ m H_{2}}$	y _{H2}
148.15	20.3	0.00618	0.986
	40.5	0.0122	0.991
	60.8	0.0156	0.994
	81.1	0.0221	0.995
173.15	20.3	0.00888	0.964
	40.5	0.0168	0.977
	60.8	0.0240	0.983
1	81.1	0.0336	0.985
198.15	20.3	0.0108	0.881
	40.5	0.0210	0.930
1	60.8	0.0319	0.947
	81.1	0.0448	0.951
223.15	20.3	0.0118	0.688
	40.5	0.0257	0.812
	60.8	0.0412	0.862
	81.1	0.0557	0.884

# METHOD /APPARATUS/PROCEDURE:

Static stainless steel cell of capacity 5 × 10⁵ mm³ fitted with magnetic stirrer and sampling valves. ture measured with thermocouple. Pressure measured using Bourdon gauge. Gases added to cell and equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- Nippon Sanso Co. Ltd. sample; purity 99.99 mole per cent.
- 2. Takochiho Chemical Industry Co. Ltd. sample; purity 99.7 mole per cent.

### ESTIMATED ERROR:

$$\begin{split} &\delta \text{T/K} = \pm 0.1; \quad \delta P/\text{bar} = \pm 0.1; \\ &\delta x_{\text{H}_2} = \delta y_{\text{H}_2} = \pm 1\text{s}. \end{split}$$

- 1. Hydrogen; H₂; [1334-74-0]
- 2. Propane; C₃H₈; [74-98-6]

### **EVALUATOR:**

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

# CRITICAL EVALUATION:

This system has been investigated by five groups of workers. Benham and Katz (1) presented a limited amount of data as part of a more general study of ternary and multicomponent systems containing hydrogen and propane. Their binary data are not considered further here. Frolich et al. (2) studied the hydrogen + propane system but there is some uncertainty as to the interpretation of their data when both components are gases at 298.15 K. Their data give mole fraction solubilities which are considerably greater than those derived by interpolation from the data of Williams and Katz (3), Trust and Kurata (4) and Buriss et al. (5). The data of Frolich  $et \ al.$  (2) are therefore classified as doubtful. Williams and Katz (3) studied this system between 88.7 K and 297 K at pressures up to 55 MPa but presented their results in terms of K-values (i.e., mole fraction in the liquid phase divided by mole fraction in the gas phase). Trust and Kurata (4) studied the system between 98 K and 348 K at pressures up to 20 MPa. Buriss et al. (5) studied the system between 273 K and 348 K up to pressures of 55 MPa. There is good agreement between the data of Trust and Kurata (4) and Williams and Katz (3). The mole fraction solubility data of Buriss etal. (5) are slightly smaller than those of the other two groups of workers at pressures above 7 MPa when the data are interpolated. In view of the need to convert Williams and Katz K-values into mole fractions and the interpolation needed because of the different temperatures employed, it is difficult to make a more precise evaluation.

The data of the three groups, (3), (4)—and (5) are classified as tentative.

# References:

- Benham, A. L.; Katz, D. L. Am. Inst. Chem. Engnrs. J. 1957, 3, 33.
- Frolich, P. K.; Trauch, E. J.; Hogan, J. J.; Peer, A. A.
   Ind. Eng. Chem. 1931, 23, 548.
- 3. Williams, R. B.; Katz, D. L. Ind. Eng. Chem. 1954, 46, 2512.
- 4. Trust, D. B.; Kurata, F. Am. Inst. Chem. Engnrs. J. 1971, 17, 86.
- Buriss, W. L.; Hsu, N. T.; Reamer, H. H.; Sage, B. H.
   Ind. Eng. Chem. 1953, 45, 210.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Frolich, P. K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A.
2. Propane; C ₃ H ₈ ; [74-98-6]	Ind. Eng. Chem. <u>1931</u> , 23, 548-550.
VARIABLES:	PREPARED BY:
Pressure	C. L. Young
EXPERIMENTAL VALUES:	

T/K	P/MPa	Solubility*, S	Mole fraction of hydrogen in liquid,† $x_{\rm H_2}$
298.15	1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 18.04	4.25 8.5 12.7 17.0 21.2 25.45 29.7 33.95 38.2 42.45 91.5	0.0152 0.0300 0.0442 0.0583 0.0717 0.0848 0.0976 0.110 0.122 0.134

- * Data taken from graph in original article. Volume of gas measured at 101.325 kPa pressure and 298.15K dissolved by unit volume of liquid measured under the same conditions.
- + calculated by compiler.

### METHOD 'APPARATUS / PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for vapor pressure of liquid and the solubility of the gas at atmospheric pressure. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Highest purity available.
- 2. Purity 98 to 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta x_{H_2} = \pm 5\%.$ 

COMPON	FNTS.			ORIGINAL N	Æ ASHREMEN	ITC •	
Join Oil	ENIO.			OKIGINAL	TERO UNEFEE	113.	
1. H	Hydrogen;	H ₂ ; [1333-	74-0]	Buriss,	W. L.;	Hsu, N. T.	;
				Reamer.	н. н.:	Sage, B. H	
2. F	Propano. C	3H8; [74-9	9_61	1		1953, 45,	-
	Topane, C	3118, [74-3	001	Ina. Ing	j. Onem.	1933, 40,	210-213.
<b>\</b>							
VARIA	BLES:			PREPARED	BY:		
l_							
Tempe	erature, pr	essure		C. L. Yo	oung		
EXPERI	MENTAL VALUE						
			raction				raction drogen
T/K	P/bar	in liquid	drogen in vapor,	T/K	P/bar		
•	- / 2.2	<i>x</i> _{H₂}	y _{H2}	-,	,	x _{H₂}	y _{H2}
		11 2	112			112	11 2
277.5		0.025	0.810	310.93	241.3		0.841
	69.0	0.052	0.882		275.8	0.275	0.842
	103.4	0.079	0.909		310.3	0.310	0.841
	137.9 172.4	0.10 0.131	0.921 0.929		344.7 413.7	0.346 0.415	0.840 0.822
ŀ	206.8	0.156	0.932		482.6	0.413	0.822
<b>.</b>	241.3	0.136	0.932		543.3	0.493	0.793
	275.8	0.206	0.935	344.26	34.5	0.012	0.142
	310.3	0.231	0.936	344.20	69.0	0.071	0.437
	344.7	0.255	0.934		103.4	0.128	0.534
]	413.7	0.303	0.931		138.0	0.186	0.581
	482.6	0.350	0.925		172.4	0.245	0.593
l	551.6	0.399	0.922		206.8	0.319	0.591
310.9	34.5	0.024	0.534		236.5	0.477	0.477
	69.0	0.062	0.717	360.93	69.0	0.075	0.235
	103.4	0.099	0.780		86.2		0.277
l	137.9	0.136	0.814		103.4		0.278
l	172.4	0.171	0.829		108.9	0.244	0.244
_	206.8	0.206	0.835				

# METHOD/APPARATUS/PROCEDURE:

Static cell. Pressure measured with pressure balance. Temperature measured using platinum resistance thermometer. Details of apparatus in refs. 1 and 2. Coexisting liquid and gas phase properties determined using vapor density at atmospheric pressure.

# SOURCE AND PURITY OF MATERIALS:

- Matheson Chemical Co. electrolytic sample; purity 99.8 mole per cent; oxygen main impurity.
- Phillips Petroleum sample. Stated purity 99.9 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$ ;  $\delta P/bar = \pm 0.015$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 0.001$ .

- Sage, B. H.; Lacey, W. N. Trans. Am. Inst. Mining Met. Engrs. 1940, 136, 136.
- Sage, B. H.; Lacey, W. N. Trans. Am. Inst. Mining Met. Engrs. 1948, 174, 102.

342	,	ım Solubilities above 200kPa		
COMPONENTS:		ORIGINAL MEASUREMENTS:		
<ol> <li>Hydrogen; H₂;</li> </ol>	[1334-74-0]	Williams, R.B.; Katz, D.L.		
2. Propane; C ₃ H ₈ ;	[74-98-6]	Ind. Eng. Chem. <u>1954</u> , 46, 2512-		
VARIABLES:	····	PREPARED BY:		
Temperature	e, pressure	C.L. Young		
EXPERIMENTAL VALUES:				
T/K	p/10 ⁵ Pa	K-values of hydrogen		
297.04	17.24 34.47 68.95 137.90 275.79 551.58	52.0 26.0 13.2 6.85 3.62 1.825		
283.15	17.24 34.47 68.95 137.90 275.79 551.58	60.8 30.4 15.3 7.85 4.15 2.27		
255.37	17.24 34.47 68.95 137.90 275.79 551.58	78.4 39.4 19.8 10.1 5.40 3.00		
277.59	17.24 34.47 68.95 137.90	100 51.0 26.0 13.3	cont.	
	AUXILIA	RY INFORMATION		
METHOD/APPARATUS/PROCEI	DURE:	SOURCE AND PURITY OF MATERIALS:		

Flow system described in ref. (1). Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Vapor recirculated by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room temperature and pressure; analysed by gas density measurements. K-values of propane given in source.

2. Phillips Petroleum Co. purity 99.8 mole %.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.6$ ;  $\delta p/Pa = \pm 0.5$ %;  $\delta K < 1$ %.

### REFERENCES:

Aroyan, H.J.; Katz, D.L.;
 Ind. Eng. Chem., 1951, 43, 185.

### Saturated Hydrocarbons 343 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1334-74-0] Williams, R.B.; Katz, D.L. Propane; C₃H₈; [74-98-6] Ind. Eng. Chem. 1954, 46,2512-20. EXPERIMENTAL VALUES: $p/10^5$ Pa T/K K-values of hydrogen 277.59 275.79 6.95 3.95 551.58 17.24 123 199.82 34.47 63.8 68.95 32.9 137.90 16.9 9.08 275.79 551.58 172.04 17.24 158 34.47 82 68.95 43.6 137.90 22.5 275.79 12.1 551.58 7.0 214 144.26 17.24 34.47 114

68.95

137.90

275.79

551.58

17.24

34.47

68.95

137.90

275.79

551.58

17.24

34.47

68.95

137.90

275.79

551.58

116.48

88.71

61.3

33.3

18.6

10.8

96.1

55.5

32.3

19.5

330

177

664

366

204

120

71.9 45.7

COMPONENTS:			ORIGINAL MEASUREMENTS:	
1. Hydroge	n; H ₂ ; [1333	-74-0]	Trust, D. B.; Kur	ata, F.
2. Propane	; C ₃ H ₈ ; [74-	98-6]	Am. Inst. Chem. En	gnrs. J.
			<u>1971</u> , <i>17</i> , 86-91.	
VARIABLES:	***************************************		PREPARED BY:	
Те	emperature, pre	ssure	C. L. Yo	ung
EXPERIMENTAL	VALUES:			
T/K	p/psia	p/MPa	Mole fraction in liquid,	in vapor,
			^ж н ₂	^у н ₂
98.15	250	1.72	0.0021	_
	1000	6.89	0.0056	-
	1500	10.34	0.0074	-
	2250	15.51 20.68	0.0108 0.0134	<del>-</del>
113.15	3000 300	2.07	0.0027	_
113.13	1000	6.89	0.0093	-
	1700	11.72	0.0147	-
	2600	17.93	0.0214	-
123.15	250	1.72	0.0031 0.0110	_
	1000 2000	6.89 13.79	0.0207	-
	2500	17.24	0.0242	-
	3000	20.68	0.0281	-
148.15	150	1.03	0.0025	-
	30 <b>0</b>	2.07 4.14	0.0052 0.0106	_
	600 900	6.21	0.0154	_
	1300	8.96	0.0218	-
	1700	11.72	0.0274	-
	2100	14.48	0.0329	-
	2800 3000	19.31 20.68	0.0443 0.0473	_
	3000	20.00		cont.)
	***************************************	AUXTLIAR	Y INFORMATION	
METHOD/APPARA	ATUS/PROCEDURE:		SOURCE AND PURITY OF MATE	ERIALS:
	ıılibrium cell	(0 1 dm ³		•
_	fitted with ma		1. Purity 99.93 mol	e per cent.
stirrer.	Temperature m			-
with platinum resistance thermo-			2. Purity 99.91 mol	e per cent.

Static equilibrium cell (0.1 dm³ capacity) fitted with magnetic stirrer. Temperature measured with platinum resistance thermometer. Pressure measured with Bourdon gauge. Contents charged into cell, equilibrated, samples withdrawn and analysed by gas chromatography. Details in source and ref. (1).

ESTIMATED ERROR:  $\delta T/K = \pm 0.05$ ;  $\delta p/MPa = \pm 0.02$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 1$  to 2%.

### REFERENCES:

Sinor, J. E.; Schindler, D. L.;
 Kurata, F.
 Am. Inst. Chem. Engnrs. J.
 1966, 12, 353.

COMPONENTS:		ORIGINAL MEASUREMENTS:  Trust, D. B.; Kurata, F.		
1. Hydrogen; H ₂ ;	[1333-74-0]			
2. Propane; C3H8;	[74-98-6]	Am. Inst. Chem. En	gnrs. J.	
		<u>1971</u> , <i>17</i> , 86-91.		
EXPERIMENTAL VALUES:				
		Mole fraction of hydrogen in liquid, in vapor,		
T/K p/psi	.a <i>p/</i> MPa	m liquid,  wH ₂	y _{H2}	
173.15 250	1.72	0.0061	0.99783	
300 500	2.07 3.45	0.0077 0.0121	0.99812 0.99865	
1000	6.89	0.0241	0.99899	
2000 2500	13.79 17.24	0.0441 0.0545	0.99901	
2600	17.93	-	0.99888	
2900	19.99	0.0618 0.0645	0.99884 0.99880	
198.15 3000 250	20.68 1.72	-	0.98712	
270	1.86	0.00908 0.01659	0.99300	
500 1000	3.45 6.89	0.03159	0.99530	
1500	10.34	-	0.99581 0.99602	
2000 2500	13.79 17.24	0.07220	0.99592	
3000	20.68	0.08468	0.99570 .	
223.15 200 500	1.38 3.45	0.00777 0.02047	0.95620 0.97422	
750	5.17	0.02952	0.98127	
1000 1500	6.89 10.34	0.03960 0.05761	0.98585	
2000	13.79	0.07418	0.98892	
2500	17.24 20.68	0.08869 0.10750	0.99069 0.98964	
248.15 3000 250	1.72	0.01065	0.8333	
500	3.45	0.02427	0.91859 0.96270	
1000 1500	6.89 10.34	0.04751 -	0.97140	
2000	13.79	0.09034	0.97500 0.98720	
2500 3000	17.24 20.68	0.13400	0.97860	
²⁷³ .15 300	2.07	0.01342	0.7245	
500 1000	3.45 6.89	0.02373 0.05220	0.8063 0.8970	
1500	10.34	0.07724	0.91912	
2000 2500	13.79 17.24	0.10920 0.13400	0.92840 0.93192	
3000	20.68	0.15860	0.93344	
^{298.15} ²⁵⁰ 400	1.72 2.76	0.00884	0.5760	
500	3.45	0.02486	-	
1000	6.89	0.06020 0.09712	0.8002 0.8455	
1500 2000	10.34 13.79	0.1239	0.8573	
2500	17.24	0.1649 0.1945	0.8793 0.8868	
323.15 3000 500	20.68 3.45	0.02284	0.3884	
1000	6.89	0.06794	0.6013 0.6976	
1500 2000	10.34 13.79	0.11140 0.15470	0.7341	
2500	17.24	0.20100	0.7602 0.7750	
348.15 3000 750	20.68 5.17	0.24460 0.03819	0.2587	
1000	6.89	0.06804	0.3840 0.4300	
1250 1500	8.62 10.34	0.09755 0.13050	0.4892	
2250	15.51	0.23650	0.5223 0.5231	
2700 3000	18.62 20.68	0.35260		

COMPONENTS:	EVALUATOR:
1. Hydrogen; H ₂ ; [1333-74-0]	Colin L. Young, School of Chemistry, University of Melbourne,
2. Butane; C4H10; [106-97-8]	Parkville, Victoria 3052, Australia.
	August 1980

### CRITICAL EVALUATION:

This system has been investigated by five groups. The data of Aroyan and Katz (1), which cover the temperature range 144 K to 297 K and pressures up to 54 MPa, the data of Klink et al. (2), which cover the temperature range 328 K to 394 K and pressures up to 17 MPa and the data of Nelson and Bonnell (3), which cover the temperature range 297 K to 389 K and pressure up to 10 MPa are in satisfactory agreement. An exact comparison of the three sets of data is impossible because the work was not carried out at one common temperature.

The data of Augood (4) agree within experimental error with that of Aroyan and Katz (1). However, in view of the poor precision of Augood data for this system, his data are classified as doubtful. Frolich  $et\ al.$  (5) studied this system at 298 K at pressures up to 10 MPa. Their results, which are classified as doubtful, yield mole fraction solubilities which are significantly larger than those of Aroyan and Katz (1) and Nelson and Bonnell (3).

The data of Aroyan and Katz (1), Nelson and Bonnell (3) and Klink  $et\ al.$  (2) are classified as tentative.

### References:

- 1. Aroyan, H. J.; Katz, D. L. Ind. Eng. Chem. 1951, 43, 185.
- Klink, A. E.; Chen, H. Y.; Amick, A. H. Jr. Am. Inst. Chem. Engnrs. J. 1975, 21, 1142.
- 3. Nelson, E. E.; Bonnell, W. S. Ind. Eng. Chem. 1943, 35, 204.
- 4. Augood, D. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- Frolich, P. K.; Trauch, E. J.; Hogan, J. J.; Peer, A. A.
   Ind. Eng. Chem. <u>1931</u>, 23, 548.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Frolich, P. K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A.
2. Butane; C ₄ H ₁₀ ; [106-97-8]	Ind. Eng. Chem. <u>1931</u> , 23, 548-550.
VARIABLES:	PREPARED BY:
Pressure	C. L. Young

L VALUES:			
P/MPa	Solubility*, S	Mole fraction of hydrogen in liquid,† $^x\mathrm{H}_2$	
1.0	2.7	0.0115	
2.0		0.0227	
3.0	8.15	0.0338	
4.0	10.85	0.0445	
5.0	13.6	0.0552	
6.0	16.3	0.0654	
	19.0	0.0755	
		0.0853	
		0.0949	
10.0	27.15	0.104	
	P/MPa  1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0	P/MPa Solubility*, S  1.0 2.7 2.0 5.4 3.0 8.15 4.0 10.85 5.0 13.6 6.0 16.3 7.0 19.0 8.0 21.7 9.0 24.4	

^{*} Data taken from graph in original article. Volume of gas measured at 101.325 kPa pressure and 298.15K dissolved by unit volume of liquid measured under the same conditions.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for vapor pressure of liquid and the solubility of the gas at atmospheric pressure. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Highest purity available.
- 2. Purity 98 to 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta x_{H_2} = \pm 5\%.$ 

[†] Calculated by compiler.

### 

### EXPERIMENTAL VALUES:

т/к	P/bar	Mole fraction of in liquid, $^{x}\mathrm{H}_{2}$	of hydrogen in gas, ^y H ₂
297.05	22.5	0.020	0.832
	79.6	0.062	_
	104.4	0.074	-
355.35	43.2	0.040	0.627
	61.6	0.063	-
	69.9	0.070	-
	94.8	0.099	0.833
	107.2	0.111	-
388.75	39.1	0.032	-
	49.5	0.051	0.420
	66.8	0.075	-
	71.9	0.083	_
	93.0	0.111	0.624

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Rocking stainless steel bomb fitted with sampling tube. Pressure measured by Bourdon gauge. Temperatures measured by iron-constantan thermocouple. Bomb charged with hydrocarbon, heated to desired temperature. Charged with hydrogen, equilibrated. Composition of liquid and gas samples estimated from change in volume on removal of hydrogen by oxidation. Source reference contains details.

### SOURCE AND PURITY OF MATERIALS:

- 1. Commercially pure. Purity
   estimated as > 99.5 mole per
   cent.
- Purity estimated as > 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/bar = \pm 0.2$ ;  $\delta x_{H_2} = \pm 5\%$ ;  $\delta y_{H_2} = \pm 7\%$ .

•		348		
COMPONENTS:		ORIGINAL MĘ	ASUREMENTS:	
1. Hydrogen; H2;	1. Hydrogen; H2; [1333-74-0]		Aroyan, H.J.; Katz, D.L.	
2. Butane; C ₄ H ₁₀ ;	2. Butane; C ₄ H _{1 0} ; [106-97-8]		. Chem. <u>1951</u> ,43, 185-9	
VARIABLES:		PREPARED BY	:	
Temperature	, pressure		C.L. Young	
EXPERIMENTAL VALUES:				
T/K	P/bar	in liquid	n of hydrogen in vapor	
		<i>x</i> _{H₂}	$y_{ m H_2}$	
297.04	22.41 77.91 104.46 233.39 275.86	0.019 0.062 0.080 0.216 0.341	0.869 0.954 0.964 0.975	
277.59	21.37 54.68 164.79 286.13 541.2	0.016 0.036 0.111 0.182 0.302	0.974 0.931 0.967 0.983 0.984	
260.93	21.10 56.68 166.16 274.41 289.58 501.94 524.00 534.34	0.0165 0.040 0.105 0.163 0.162 0.260 0.268	0.958 0.979 0.989 0.989 0.989 0.990 0.988	•
244.26	21.72	0.015	0.979	

## 0.036 AUXILIARY INFORMATION

## METHOD /APPARATUS/PROCEDURE:

Recirculating vapor flow system based on that described in ref. (1). Details of present apparatus in source. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. High pressure magnetic circulating pump employed.

58.47

Cell charged under pressure. Samples of each phase expanded to room temperature and pressure; analysed by gas density measurements.

### SOURCE AND PURITY OF MATERIALS:

1. Purity 99.9%, dried over anhydrous CaSO4

0.990

 Phillips Petroleum Co., pure grade purity > 99.0 mole %, major impurity 2-methylpropane.

cont.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3-0.5$ ;  $\delta P/bar = \pm 1.3$ ;  $\delta x_{H_2} = \pm 0.0025$ ;  $\delta y_{H_2} = \pm 0.001$ .

### REFERENCES:

Dodge, B.F.; Dunbar, A.K.;
 J. Am. Chem. Soc. <u>1927</u>, 49,591.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Butane; C₄H₁₀; [106-97-8]

### ORIGINAL MEASUREMENTS:

Aroyan, H.J.; Katz, D.L.

Ind. Eng. Chem. 1951, 43, 185-9.

### EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction in liquid $^{x}{ m H}_{2}$	of hydrogen in vapor ^y H ₂	
244.26	136.52 288.20 513.66	0.074 0.1445 0.229	0.993 0.994 0.995	
227.59	27.65 55.16 140.65 262.00 441.27	0.017 0.030 0.070 0.119 0.180	0.992 0.994 0.996 0.996 0.997	
199.82	23.24 55.57 99.97 193.7 282.0 482.6	0.013 0.024 0.040 0.071 0.096 0.146	0.998 0.998 0.998 0.998 0.996 0.9985	
172.04	20.7 20.7 57.6 129.6 129.6 293.0 508.8	0.010 0.008 0.020 0.037 0.038 0.073 0.116	1.00 - 1.00 - 1.00 1.00	
144.26	37.6 141.3 286.1 286.1 493.0	0.010 0.030 0.050 0.053 0.067	1.00 1.00	

COMPONENTS:	ORIGINAL MEASUREMENTS:	
1. Hydrogen; H ₂ ; [1333-74-0] 2. Butane; C ₄ H ₁₀ ; [106-97-8]	Augood, D. R.  Trans. Instn. Chem. Engnrs.,  1957, 35, 394-408.	
VARIABLES:	PREPARED BY:	
Temperature, pressure	C. L. Young	

EXPERIMENTA	AL VALUES:			
T/K	P/psig ⁺	P/MPa	Mole fraction in liquid, $x_{ m H_2}$	n of hydrogen in gas, y _{H2}
273.2	2740	18.99	0.127	0.982
	1300	9.07	0.073	0.955
	1300	9.07	0.070	0.963
213.6	2715	18.82	0.087	0.996
	2715	18.82	0.081	-
	2640	18.31	0.074	-
	1300	9.07	0.054	-
	1300	9.07	0.047	-

### AUXILIARY INFORMATION

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The butane was condensed out and both components estimated volumetrically. Ratio of H₂/HD in liquid estimated by mass spectrometry.

METHOD/APPARATUS/PROCEDURE:

- SOURCE AND PURITY OF MATERIALS:
- 1. Electrolytic sample containing 0.09 mole per cent HD.
- 2. Shell Petroleum sample.

ESTIMATED ERROR:  $\delta T/K = \pm 0.1; \ \delta P/MPa = \pm 0.1;$   $\delta x_{H_2}, \ \delta y_{H_2} = \pm 4\% \ (\text{estimated by compiler})$ 

⁺ psig - pounds per square inch gauge pressure

Klink, A. E.; Chen, H. Y.; Amick, A. H. Jr.
Am. Inst. Chem. Eng. J. 1975, 21, 1142.
PREPARED BY:
C. L. Young

### Mole fraction of hydrogen P[†]/bar T/K P/bar in liquid, in vapor, yH2 327.65 25.13 0.025 31.27 0.777 36.15 42.54 0.036 0.828 49.28 55.85 0.047 0.863 68.69 61.54 0.063 0.879 83.76 76.20 0.074 0.896 84.67 92.48 0.086 0.903 104.31 96.11 0.094 0.910 117.42 108.75 0.110 0.916 130.31 121.28 0.123 0.922 138.04 128.70 0.128 0.924 138.21 128.94 0.129 0.925 157.77 147.81 0.147 0.930 168.47 156.02 0.160 0.932 344.25 0.022 27.78 19.11 0.638 41.77 32.69 0.036 0.741 54.97 45.53 0.053 0.791 69.30 59.40 0.068 0.825 73.05 83.46 0.081 0.846 96.79 85.89 0.098 0.860 0.109 106.28 95.20 0.871 111.01 99.81 0.113 0.875 124.64 112.76 127.30 0.129 0.881 139.81 0.141 0.888 (cont.)

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static cell fitted with stirrer. Pressure measured with dead weight piston gauge-diaphragm differential pressure indicator combination. Samples analysed by gas chromatography using a squalane column. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Ultra-pure sample; purity 99.999 mole per cent.
- Instrument grade sample; purity 99.5 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.05; \quad \delta P/\text{bar} = \pm 0.05;$   $\delta x_{\text{H}_2}, \quad \delta y_{\text{H}_2} = \pm 0.04.$ 

COMPONENTS:  1. Hydrogen; H ₂ ; [1333-74-0]			ORIGINAL MEASUREMENTS:  Klink, A. E.; Chen, H. Y.; Amick, A. H. Jr.		
EXPERIMENT	AL VALUES:				
T/K	P/bar	P [†] /bar	Mole fraction of hydrogen in liquid, in vapor,		
-7."	r/par	r /bai	x _{H₂}	y _{H₂}	
344.25	150.84 166.53	137.80 152.67	0.159 0.173	0.891 0.894	
360.95	27.93 41.17 56.17 68.09 83.19	15.62 28.42 43.16 54.56 68.91	0.021 0.037 0.058 0.069 0.090	0.483 0.619 0.706 0.743 0.772	
	98.68 110.85 123.56 138.47 149.97	83.93 95.66 107.82 122.07 132.92	0.108 0.122 0.134 0.158 0.166	0.799 0.814 0.825 0.835 0.839	
377.55	167.88 28.34 41.74 54.03 65.68 77.78 90.25	149.76 11.76 24.46 36.22 47.43 59.04 71.09	0.193 0.019 0.037 0.053 0.071 0.084 0.106	0.843 0.322 0.480 0.566 0.621 0.662 0.695	
	103.21 117.64 128.59 141.40 154.61 167.38	83.51 97.28 107.70 119.54 132.02 143.97	0.119 0.143 0.153 0.175 0.195 0.217	0.719 0.739 0.750 0.753 0.759 0.760	
394.25	34.31 48.62 61.46 77.17 88.65 101.50	143.97 11.23 25.07 37.17 52.27 63.41 75.79 86.65	0.21 0.021 0.049 0.066 0.095 0.109 0.135 0.149	0.213 0.367 0.444 0.514 0.555 0.588 0.609	
	112.87 125.33 138.91 138.99 152.89 168.76	98.74 111.58 111.63 124.77 140.24	0.149 0.172 0.193 0.194 0.228 0.266	0.609 0.632 0.637 0.638 0.633 0.615	

 $^{{\}it P}^{\dagger}$  partial pressure of hydrogen.

COMPONENTS:	EVALUATOR:
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Alkanes; C₅ to C₁₄</li> </ol>	Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.
	August 1980

### CRITICAL EVALUATION:

The solubility of hydrogen in n-alkanes at low pressures is treated separately. Data on the solubility of hydrogen in n-alkanes at high pressures are relatively scarce and it is not possible to recommend any data.

Hydrogen + Pentane

This system has been investigated by Frolich et al. (1). Their data were presented in graphical form and are classified as doubtful.

Hydrogen + Hexane

This system has been investigated by three groups of workers. Frolich et al. (1) presented their data at 298 K in a graphical form which are classified as doubtful. Nichols et al. (2) made an extensive study of this system over the temperature range 277 K to 477 K and at pressures up to 70 MPa. Sattler (3) investigated this system at 308 K at pressures up to 15 MPa and his mole fraction solubility data are considerably smaller than those obtained by interpolation of Nichols et al. data (2). et al. (1) data are larger than either Nichols et al. (2) or Sattler (3) when any reasonable estimate of the temperature dependence of solubility is used for extrapolation. A comparison with the low pressure data of Walter et al. (4) and Katayama and Nitta (5) when extrapolated to 308 K would indicate that Sattler's values (3) are too small, whereas Nichols' et al. (2) mole fractions are too large. However, such a comparison relies on an extrapolation to 1 atmosphere partial pressure and an extrapolation or interpolation to 308 K and must be made with caution. data of Sattler (3) and Nichols  $et \ \alpha l$ . (2) must nevertheless be considered in disagreement with each other and the low pressure data and are therefore classified as doubtful.

Hydrogen + Heptane
Deuterium + Heptane

Lachowicz (6), (7) studied the solubility of hydrogen and deuterium in heptane between 298 K and 323 K at pressures between 10 MPa and 30 MPa and found no difference in the solubility of the isotopes within the experimental error of about one per cent. The data of Lachowicz  $et\ al.$  (7) were given in graphical form and in terms of linear equations. Therefore no data table is given and the data are not evaluated in detail here. The equations given may be rewritten as:

COMPONENTS:	EVALUATOR:
1. Hydrogen; H ₂ ; [1333-74-0] 2. Alkanes; C ₅ to C ₁₄	Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.
	August 1980

CRITICAL EVALUATION:

The deuterium solubilities were identical, in terms of mole fractions to the hydrogen solubilities.

Peter and Reinhartz (8) studied hydrogen and heptane in the pressure range 424 K to 499 K at pressures up to 30 MPa. Although detailed comparison of the work of Lachowicz et al. (7) with that of Peter and Reinhartz (8) is not possible because of the difference in the temperature range studied, these two studies are, at least, in qualitative agreement. The data of Peter and Reinhartz (8) are classified as tentative.

Hydrogen + Octane Deuterium + Octane

Lachowicz (6), (7) studied the solubility of hydrogen and deuterium in octane between 298 K and 323 K at pressures between 5 MPa and 30 MPa and found no difference in the solubility of the isotopes within the experimental error of about one per cent (as in the case of heptane + hydrogen or + deuterium).

Lachowicz *et al*. (7) presented their data in graphical form and in terms of linear equations. The data were not compiled or evaluated in detail. The equations given may be rewritten as

 $\ln x_{\rm H_2}$ , 298.15 K = 6.78 × (p/atm)  $\ln x_{\rm H_2}$ , 310.65 K = 7.38 × (p/atm)  $\ln x_{\rm H_2}$ , 323.15 K = 7.89 × (p/atm)

The deuterium solubilities were identical, in terms of mole fractions, to the hydrogen solubilities.

The hydrogen + octane system has also been studied by Frolich  $et\ al.$  (1) and by Connolly (9). Connolly (9) studied the system between 463 K and 553 K and reported his data as K-values (mole fraction in the gas phase divided by mole fraction in the liquid phase). The temperature range of these results is sufficiently different from that both of other high pressure studies on this system and from low pressure measurements, to make meaningful comparison impossible. The data are classified as tentative

The data of Frolich  $\it et~al.$  (1) were presented in graphical form and are classified as doubtful.

Hydrogen + Decane

This system has been investigated by three groups of workers. The most recent data by Sebastian et  $\alpha l$ . (10) are thought to be reliable and cover the temperature range 462 K to 583 K and pressures up to 25 MPa.

(cont.)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Alkanes; C₅ to C₁₄

### **EVALUATOR:**

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

August 1980

### CRITICAL EVALUATION:

The considerably less extensive data of Sokolov and Polyakov (11) cover the temperature range 358 K to 483 K and pressure up to 30 MPa and are consistent with the data of Sebastian  $et\ al.$  (10).

Nederbragt (12) made some preliminary measurements on this system but was mainly concerned with the solubility of decane in the gas phase. His data are rejected.

The data of Sebastian et al. (10) and Sokolov and Polyakov (11) are both classified as tentative.

The gas-liquid critical temperature of decame is 617.7 K (13) and Young (14) has made a preliminary observation of gas-gas immiscibility in this system. The phase behaviour of this system needs to be further investigated and extreme caution needs to be exercised in extrapolating the solubility data to temperatures above 583 K.

Hydrogen + Dodecane

Hydrogen + 2-Methylpropane

The data of Dean and Tooke (15) are the only set of data on these systems. These workers' data on the system hydrogen + 2,2,4-trimethylpentane appear to be consistent with other data on that system. Therefore their data are classified as tentative for the hydrogen + dodecane system.

Hydrogen + Tetradecane

The data of Sokolov and Polyakov (11) are classified as tentative as their data appear to be reliable for the hydrogen + decane system (see above) and there are no other data available for this system.

Hydrogen + Hexadecane

The recent data of Chao and coworker appear to be reliable and the data of this group for this system are therefore classified as tentative. Hydrogen + 2,2,4-Trimethylpentane

The data of Dean and Tooke (15) and Peter and Reinhartz (8) are classified as tentative on the basis of the experimental techniques used and the agreement between the two sets at the common temperature of 423.95 K. The temperature range of the data of Laugier  $et\ al.$  (16) do not overlap with those of the measurements of Dean and Tooke (15) or Peter and Reinhartz (8).

### References:

- Frolich, P. K.; Trauch, E. J.; Hogan, J. J.; Peer, A. A. Ind. Eng. Chem. 1931, 23, 548.
- Nichols, W. B.; Reamer, H. H.; Sage, B. H. Am. Inst. Chem. Engnrs. J. 1957, 3, 262.
- 3. Sattler, Z. Tech. Physik. 1940, 21, 410.

(cont.)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Alkanes; C₅ to C₁₄

### **EVALUATOR:**

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

August 1980

### CRITICAL EVALUATION:

### References (cont.)

- Walters, J. A.; Mortimer, G. A.; Clements, H. E. J. Chem. Engng. Data 1970, 15, 174.
- 5. Katayama, T.; Nitta, T. J. Chem. Engng. Data 1976, 21, 194.
- 6. Lachowicz, S. K. Thesis, University of London, Dec. 1954.
- 7. Lachowicz, S. K.; Newitt, D. M.; Weale, K. E. Trans. Faraday Soc. 1955, 51, 1198.
- 8. Peter, S.; Reinhartz, K. Z. Phys. Chem. 1960, 24, 10.
- 9. Connolly, J. F. Amer. Petr. Inst. Report 1965, 45, (III), 62.
- Sebastian, H. M.; Simnick, J. J.; Lin, H. M.; Chao, K.-C.
   J. Chem. Engng. Data 1980, 25, 68.
- 11. Sokolov, B. I.; Polyakov, A. A. Zh. Prikl. Khim. 1977, 50, 1403.
- 12. Nederbragt, G. W. Appl. Sci. Res. 1948, A1, 237.
- 13. Ambrose, D. "Vapour-Liquid Critical Properties", 1980, N.P.L. Rep. 107. Teddington, U.K.
- 14. Young, C. L. Unpublished results.
- 15. Dean, M. R.; Tooke, J. W. Ind. Eng. Chem. 1946, 38, 389.
- 16. Laugier, S.; Richon, D.; Renon, H. J. Chem. Engng. Data 1980, 25, 274.

# ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Frolich, P.K.; Tauch, E.J.; Hogan, J.J.; Peer, A.A. 2. Pentane; C₅H₁₂; [109-66-0] Ind. Eng. Chem. 1931, 23, 548-550 VARIABLES: PREPARED BY: C.L. Young

EXPERIMENTAL VALUE	<i>P/</i> MPa	Solubility *	Mole fraction of hydrogen in liquid, $^+$ $^x_{ m H_2}$
298.15	1.0	2.4	0.0113
	2.0	4.5	0.0209
	3.0	6.7	0.0308
	4.0	9.0	0.0410

10.0 21.9 0.0942
 * Data taken from graph in original article. Volume of gas measured at 101.325 kPa pressure and 298.15 K dissolved by unit volume of liquid measured under the same conditions.

11.35

13.6

15.8

17.95

19.95

+ Calculated by compiler.

5.0

6.0

7.0

8.0

9.0

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for the vapor pressure of the liquid and the solubility of the gas at atmospheric pressure. Details in source.

### SOURCE AND PURITY OF MATERIALS:

Stated that the materials were the highest purity available. Pentane purity 98 to 99 mole per cent.

0.0511

0.0606

0.0698

0.0785

0.0865

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta x_{H_2} = \pm 5\%$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hexane;  $C_6H_{14}$ ; [110-54-3]

### ORIGINAL MEASUREMENTS:

Frolich, P.K.; Tauch, E.J.; Hogan, J.J.; Peer, A.A.

Ing. Eng. Chem. 1931, 23, 548-550.

VARIABLES:

PREPARED BY:

Pressure

C.L. Young

EXPERIMENTAL VALU	IES:		
т/к	P/MPa	Solubility*	Mole fraction of hydrogen $^+$ in liquid, $x_{ m H_2}$
298.15	1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0	1.85 3.65 5.5 7.3 9.1 10.95 12.8 14.6 16.4	0.0098 0.0193 0.0287 0.0378 0.0467 0.0556 0.0644 0.0728
	10.0	18.25 20.1	0.0894 0.0976

- * Data taken from graph in original article. Volume of gas measured at 101.325 kPa pressure and 298.15 K dissolved by unit volume of liquid measured under the same conditions.
- + Calculated by compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for the vapor pressure of the liquid and the solubility of the gas at atmospheric pressure. Details in source.

### SOURCE AND PURITY OF MATERIALS:

Stated that the materials used were the highest purity available. Purity of hexane 98 to 99 mole per cent.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta x_{H_2} = \pm 5\%$ 

COMPONENTS:		ORIGINAL MEASURE	MENITS.		
	,; [1333-74-0]	Sattler, H.			
-	-		z. Tech. Physik, 1940, 21,410-413.		
2. Hexane; C ₆ H	14; [110-54-3]	Z. Tech. Ph	ysik, <u>1940</u> , 21,410-413.		
		1			
VARIABLES:		PREPARED BY:			
Pre	ssure	C.L. Young			
EXPERIMENTAL VALUE	S:				
m /**	D //		Wala forables of		
T/K	P/bar Kue	nen Coefficient S	Mole fraction of hydrogen in liquid		
-			$x_{ m H_2}$		
308.35	51.0 51.5	8.84 8.96	0.03289 0.03332		
	94.1	16.09	0.05829		
	132.6 137.0	22.54	0.07980 0.08227		
	138.0	23.30 23.63	0.08333		
	148.3	25.23	0.08848		
	151.7	25.96	0.09080		
	AUXILIA	RY INFORMATION			
METHOD:/APPARATUS		SOURCE AND PURIT	Y OF MATERIALS:		
Rocking homb w	ith liquid sampling olvent and hydrogen				
charged into exof solvent in I gravimetrically liquid stripped	vacuated cell. Amount liquid sample estimate y and hydrogen in d out and estimated . Details in source.		ails given.		
		ESTIMATED ERROR.			
		ESTIMATED ERROR:			
		$\delta T/K = \pm 0.1; \delta$	$SP/bar = \pm 0.2;$		
		$\delta T/K = \pm 0.1; \delta$			

0.998 0.998 .

0.998

0.998

0.998

0.986

0.992

0.994

0.995

0.995

0.995

•		Saturated	Hydrocarbons	361
COMPONENTS:			ORIGINAL MEASUREMENTS:	
<ol> <li>Hydroger</li> </ol>	n; H ₂ ; [1333-	74-0]	Nichols, W. B.; Reamer	, н. н.;
2			Sage, B. H.	
4. Hexane;	C ₆ H ₁₄ ; [110-	54-3]	Am. Inst. Chem. Engnrs.	J .
			<u>1957</u> , 3, 262-7.	
VARIABLES:			PREDARED BY	
CABLES:			PREPARED BY:	
Temperature, pressure			C. L. Young	
EXPERIMENTAL	VALUES:			
m too		<b></b>	Mole fraction of	
T/K	$P/\mathtt{psia}$	P/MPa	$\begin{array}{c} \hbox{in liquid,} \\ x \end{array}$	in gas, y
			H ₂	H ₂
277.59	500	3.447	0.028	0.996
	1000	6.895	0.054	0.998
	1500	10.34	0.078 0.099	0.998 0.998
	2000 2500	13.79 17.24	0.099	0.998
	3000	20.68	0.140	0.998
	3500	24.13	0.160	0.998
	4000	27.58	0.179	0.998
	4500	31.03 34.47	0.199 0.218	0.998 0.998
	5000	34.4/	0.210	0.550

### AUXILIARY INFORMATION

41.37

48.26

55.16

62.05

68.95

10.34

13.79

17.24

20.68

24.13

3.447

6.895

### METHOD/APPARATUS/PROCEDURE:

310.93

PVT cell charged with mixture of known composition. Pressure measured with pressure balance and temperature measured with platinum resistance thermometer. Bubble Point and dew point determined for Various compositions from discontinuities in the pressure-volume isotherm. Co-existing liquid and gas phase properties determined by graphical means. Details in ref. (1) and source.

6000

7000

8000

9000

500

1000

1500

2000

2500

3000

3500

10000

### SOURCE AND PURITY OF MATERIALS:

0.256

0.294

0.334

0.376 0.422

0.031

0.059

0.084

0.108

0.131

0.153

0.175

1. Commercial electrolytic grade sample, purified by passage over platinum wire, dried, final purity 99.9 mole per cent.

(cont.)

Phillips Petroleum Co. sample, stated purity 99.7 mole per cent, dried and degassed.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$ ;  $\delta P/MPa = \pm 0.001$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 0.001$ .

### REFERENCES:

Sage, B. H.; Lacey, W. N.
 Trans. Am. Inst. Mining. Met.
 Engnrs. 1940, 136, 136.

Nichols, W. B.; Reamer, H. H.; 1. Hydrogen; H₂; [1333-74-0] Sage, B. H. Hexane; C₆H₁₄; [110-54-3] Am. Inst. Chem. Engnrs. J. 1957, 3, 262-7. EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/psia P/MPa in liquid, in gas,  $x_{\rm H_2}$  $y_{\rm H_2}$ 310.93 4000 27.58 0.196 0.995 4500 31.03 0.217 0.995 0.238 0.995 5000 34.47 6000 0.279 0.995 41.37 0.995 7000 48.26 0.322 0.366 0.995 8000 55.16 0.995 62.05 0.412 9000 10000 68.95 0.461 0.995 0.961 344.26 500 3.447 0.034 1000 6.895 0.064 0.978 0.983 1500 10.34 0.092 2000 13.79 0.119 0.986 2500 17.24 0.144 0.987 0.988 20.68 3000 0.169 3500 24.13 0.193 0.988 0.988 4000 27.58 0.216 4500 31.03 0.230 0.988 5000 34.47 0.988 0.262 0.988 6000 41.37 0.309 7000 48.26 0.356 0.988 55.16 8000 0.405 0.988 9000 62.05 0.456 0.988 10000 0.511 0.988 68.95 377.59 500 3.447 0.036 0.904 1000 6.895 0.070 0.946 0.960 1500 10.34 0.102 0.966 2000 13.79 0.132 2500 17.24 0.160 0.969 3000 20.68 0.187 0.971 3500 24.13 0.215 0.973 4000 27.58 0.241 0.974 0.974 4500 31.03 0.267 5000 34.47 0.293 0.974 0.974 0.345 6000 41.37 7000 0.396 0.974 48.26 0.974 0.450 8000 55.16 9000 62.05 0.508 0.974 0.570 0.973 10000 68.95 0.797 410.93 500 3.447 0.038 1000 6.895 0.078 0.886 10.34 0.115 0.914 1500 2000 13.79 0.149 0.927 17.24 0.181 0.934 2500 3000 20.68 0.213 0.939 0.244 0.942 3500 24.13 0.274 0.944 4000 27.58 0.945 0.304 4500 31.03 5000 34.47 0.334 0.946 6000 41.37 0.393 0.946 0.451 48.26 0.945 7000 8000 55.16 0.511 0.944 0.576 0.941 62.05 9000 0.649 0.931 10000 68.95 0.606 444.26 500 3.447 0.037 0.086 1000 6.895 0.772 1500 10.34 0.132 0.826 0.172 2000 13.79 0.851

17.24

2500

0.210

(cont.)

0.865

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hexane; C₆H₁₄; [110-54-3]

Nichols, W. B.; Reamer, H. H.; Sage, B. H.

Am. Inst. Chem. Engnrs. J.

<u>1957</u>, 3, 262-7

### EXPERIMENTAL VALUES:

T/K	P/psia	P/MPa	Mole fraction o in liquid, $^{x}_{\mathrm{H}_{2}}$	f hydrogen in gas, $y_{\rm H_2}$
444.26 477.59	3000 3500 4000 4500 5000 6000 7000 8000 9000 9200† 500 1000 1500 2000 2500 3500 4000 4500 5920†	20.68 24.13 27.58 31.03 34.47 41.37 48.26 55.16 62.05 63.43 3.447 6.895 10.34 13.79 17.24 20.68 24.13 27.58 31.03 34.47 40.82	0.249 0.285 0.322 0.359 0.394 0.461 0.528 0.597 0.691 0.768 0.032 0.103 0.165 0.224 0.283 0.341 0.396 0.448 0.500 0.555 0.688	0.873 0.878 0.882 0.884 0.885 0.884 0.885 0.865 0.768 0.768 0.768 0.7568 0.700 0.722 0.736 0.745 0.745 0.750 0.747 0.688

 $^{^{\}dagger}$  critical point

### COMPONENTS: ORIGINAL MEASUREMENTS:

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Heptane; C₇H₁₆; [142-82-5]
- Peter S.; Reinhartz, K.
- 2. Phys. Chem. 1960, 24, 103-18.

### VARIABLES:

Temperature, pressure

### PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

T/K	Mole fraction of hydrogen liquid, in $x_{\rm H_2}$		<i>P/</i> 10 ⁵ Pa	Mole fra of hydr in liquid, $x_{ m H_2}$	
49.0 0 98.1 0 147.1 0 196.1 0 294.2 0 392.2 0 588.4 0 784.5 0 471.65 24.5 0 49.0 0 98.1 0	.030 0.8 .062 0.9 .121 0.9 .171 0.9 .216 0.9 .295 0.9 .363 0.9 .482 0.9 .572 0.9 .020 0.5 .074 0.7 .150 0.8 .216 0.8	03 42 52 57 62 64 498.85 65 64 61 52	196.1 294.2 392.2 490.3 588.4 686.5 24.5 49.0 98.1 147.1 196.1 245.2 294.2 343.2	0.272 0.377 0.469 0.554 0.633 0.710 0.023 0.077 0.170 0.252 0.329 0.401 0.468 0.537	0.905 0.915 0.914 0.908 0.898 0.883 0.355 0.638 0.758 0.758 0.794 0.813 0.825 0.829

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static steel equilibrium cell fitted with magnetic stirrer and sampling ports. Temperature measured with a platinum resistance thermometer. Samples withdrawn after equilibrium established. The hydrocarbon component frozen out in a dry ice/acetone bath, hydrogen estimated volumetrically.

### SOURCE AND PURITY OF MATERIALS:

- Electrolytic grade, purity 99.9 mole per cent, 0.05 mole per cent methane.
- Phillips Petroleum Co. sample; pure grade, minimum purity 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$ ;  $\delta x_{\rm H_2} = \pm 3\%$ ;  $\delta y_{\rm H_2} = \pm 0.005$  (estimated by compiler).

## Saturated Hydrocarbons 365 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Frolich, P.K.; Tauch, E.J.; Hogan, J.J.; Peer, A.A. 2. Octane; C₈H₁₈; [111-65-9] Ind. Eng. Chem. 1931, 23, 548-550. VARIABLES: PREPARED BY: Pressure C.L. Young EXPERIMENTAL VALUES: Solubility,* T/K P/MPa Mole fraction of

-,	-,		hydrogen in liquid, $^+$
298.15	1.0	1.4	0.0093
	2.0	2.75	0.0181
	3.0	4.15	0.0270
	4.0	5.6	0.0361
	5.0	7.0	0.0447
	6.0	8.4	0.0532
	7.0	9.85	0.0618
	8.0	11.3	0.0702
	9.0	12.7	0.0783
	10.0	14.1	0.0861
	11.0	15.5	0.0939
	12.0	17.0	0.102
	13.0	18.4	0.110
	14.0	19.8	0.117
	15.0	21.3	0.125
	16.0	22.8	0.132
	17.0	24.3	0.140
	18.0	25.75	0.147
	19.0	27.2	0.154
* 5-1-1			1

- Data taken from graph in original article. Volume of gas measured at 101.325 kPa pressure and 298.15 K dissolved by unit volume of liquid measured under the same conditions.
- + Calculated by compiler.

METHOD/APPARATUS/PROCEDURE:

### AUXILIARY INFORMATION

### Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for the Vapor pressure of the liquid and the solubility of the gas at atmospheric pressure. Details in source.

SOURCE AND PURITY OF MATERIALS:

Stated that the materials were the highest purity available. Purity of octane 98 to 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \delta x_{H_2}$  $= \pm 5%$ 

COMPONENTS:		IOR	CINAL MEASURE	MENTS •	
			ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]			onnolly, J.	F.,	
2. Octane; C ₈ H ₁₈ ;	[111-65-9]	A (I	mer. Petr. II), 62-67.	Inst. Report,	<u>1965</u> , 45
VARIABLES:		PDI	PARED BY:	·	
Temperature,	nressure	1.2		L. Young	
10.mpc2ddd2c,	precodure			2	
EXPERIMENTAL VALUES:			K values		
T/K	P/bar	K _{C 8} H	18	^К н ₂	
463.15	4.55 6.89 13.8 20.7 27.6 34.5 51.7 68.9	1.00 0.70 0.38 0.27 0.21 0.17 0.12	5 7 3 2 5 7	14.2 79.8 42.5 29.2 22.4 18.2 12.5 9.57	
473.15	103.4 5.51 6.89 13.8 20.7 27.6 34.5 51.7 68.9 103.4	0.07 1.00 0.83 0.46 0.33 0.26 0.21 0.15 0.12	0 2 4 1 1 6 8	86.6 71.3 38.9 26.9 20.7 16.9 11.7 8.98 6.2+	
483.15	6.62 6.89 13.8 20.7 27.6 34.5 51.7	1.00 0.97 0.55 0.40 0.31 0.26 0.19	0 0 5 0 0 8	66.3 64.4 35.5 24.8 19.1 15.6	cont.
	AUXILI	IARY INF	ORMATION		!
METHOD/APPARATUS/PROCE Sample of known co over mercury. Mix constant temperatu bubble point deter Data smoothed.	mposition confin ture compressed re. Dew point a	ed at and	No definated Error: $\delta T/K = \pm 0.2 \\ \delta K/K = \pm 1 $	y OF MATERIALS: tails given.  ; δP/bar = ±0  by compiler).	.5;

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Connolly, J.F. 2. Octane; C₈H₁₈; [111-65-9] Amer. Petr. Inst. Report, 1965, 45 (III), 62-67. EXPERIMENTAL VALUES: K values T/K $K_{\rm H_2}$ P/bar $K_{C_8H_{18}}$ 8.39 0.159 483.15 68.9 0.123 103.4 5.87 137.9 0.106+ 493.15 7.93 1.000 50.0 13.8 0.653 31.7 20.7 0.475 22.4 27.6 0.380 17.4 34.5 0.320 14.2 51.7 0.237 10.0 7.76 0.195 68.9 103.4 0.154 5.47 4.30 137.9 0.133 503.15 9.38 1.000 37.5 13.8 0.759 27.7 20.7 0.560 20.0 0.452 15.7 27.6 34.5 0.384 12.9 51.7 0.287 9.11 7.12 68.9 0.237 103.4 0.188 5.04 137.9 0.163+ 3.97+ 11.0 1.000 28.1 513.15 13.8 24.1 0.863 20.7 0.647 17.6 27.6 0.527 13.9 34.5 0.450 11.5 51.7 8.19 0.343 68.9 0.287 6.42 4.59+ 103.4 0.228+ 20.7 523.15 12.9 1.000 13.8 0.960 20.0 20.7 0.742 15.0 0.614 12.0 27.6 34.5 0.532 10.0 51.7 7.23 0.4140.350 5.71 68.9 4.11 103.4 0.286 0.253+ 3.28+ 137.9 14.9 1.000 533.15 15.0 0.835 12.1 20.7 0.704 27.6 9.93 34.5 8.44 0.613 51.7 0.487 6.21 0.420 4.95 68.9 103.4 0.351 3.57+ 17.4 1.000 10.2 543.15 20.7 0.915 9.40 0.793 7.93 27.6 34.5 0.706 6.80 0.579 5.07 51.7 68.9 0.516 4.06 0.453 103.4 2.96 137.9 0.422 +2.36+ 0.879 5.68 553.15 27.6 0.802 4.98 34.5 51.7 0.691 3.80 0.631 3.08

68.9

obtained by extrapolation by authors.

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Sokolov, B. I.; Polyakov, A. A. Zh. Prikl. Khim. 1977, 50, 1403-5. VARIABLES: Temperature, pressure C. L. Young EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of hydrogen in liquid, ${}^x_{ m H_2}$
250 15	40 5	0.026
358.15	40.5 101.3	0.036 0.086
	202.6	0.158
	304.0	0.221
408.15	40.5	0.044
1	101.3	0.105
	202.6	0.191
	304.0	0.260
483.15	40.5	0.060
	101.3	0.147
	202.6	0.250
	304.0	0.345
ì		

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping gas out and measuring volume evolved. Remaining liquid estimated gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

### ESTIMATED ERROR:

 $\delta \mathbf{T}/\mathbf{K} = \pm \mathbf{1.0}; \quad \delta P/\mathrm{bar} = \pm \mathbf{0.5};$   $\delta \boldsymbol{\omega}_{\mathrm{H}_2} = \pm 3 \text{\$ (estimated by compiler).}$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Decane; C₁₀H₂₂; [124-18-5]

### ORIGINAL MEASUREMENTS:

PREPARED BY:

Sebastian, H. M.; Simnick, J. J.; Lin, H. M.; Chao, K-C.

J. Chem. Eng. Data 1980, 25, 68-70.

### VARIABLES:

Temperature, pressure

**}** 

C. L. Young

### EXPERIMENTAL VALUES:

			Mole fraction	
T/K	<i>P/</i> atm	<i>P/</i> MPa	in liquid,	in gas,
			[∞] H₂	у _{Н2}
462.5	1.4477	0.14669		
	19.01	1.926	0.0251	0.9216
	29.15	2.954	0.0408	0.9446
	49.4	5.01	0.0678	0.9676
	99.6	10.09	0.1309	0.9823
	148.3	15.03	0.1890	0.9860
	200.0	20.27	0.2406	0.9877
	251.9	25.52	0.2832	0.9891
503.4	3.485	0.3531		
	19.16	1.941	0.0289	0.8021
	32.46	3.289	0.0511	0.8786
	51.1	5.18	0.0818	0.9207
	99.9	10.12	0.1550	0.9539 ·
	149.5	15.15	0.2202	0.9657
	201.7	20.44	0.2760	0.9706
	250.4	25.37	0.3324	0.9740
543.0	7.132	0.7226		
	19.35	1.961	0.0286	0.6025
	30.92	3.133	0.0533	0.7367
	48.8	4.94	0.0903	0.8198
	99.5	10.08	0.1799	0.9001
	149.2	15.12	0.2582	0.9266
	• -		(con	t.)

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Details in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Airco sample, purity 99.95 mole per cent.
- Aldrich Chemical Co. sample, purity better than 99 mole per cent.

### ESTIMATED ERROR:

δT/K = ±0.2; δP/MPa = ±0.003 (below 3.5 MPa), ±0.02 (above 3.5 MPa);  $δx_{\rm H_2}$ ,  $δy_{\rm H_2} = ±1%$ .

### REFERENCES:

Simnick, J. J.; Lawson, C. C.;
 Lin, H. M.; Chao, K-C.
 Am. Inst. Chem. Engnrs. J.
 1977, 23, 469.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Decane;  $C_{10}H_{22}$ ; [124-18-5]

### ORIGINAL MEASUREMENTS:

Sebastian, H. M.; Simnick, J. J.; Lin, H. M.; Chao, K-C.

J. Chem. Eng. Data 1980, 25, 68-70.

### EXPERIMENTAL VALUES:

T/K	P/atm	P/MPa	Mole fraction o in liquid, $^{x}{ m H}_{2}$	f hydrogen in gas, ^y H ₂
F42 0	100.7	20.22	0. 2240	0.0201
543.0	199.7 251.8	20.23 25.51	0.3249 0.3825	0.9391 0.9446
583.5	13.378	1.3555	***************************************	
	49.9	5.06	0.1059	0.6355
	99.7	10.10	0.2220	0.7825
	150.1	15.21	0.3247	0.8303
	201.7	20.44	0.4098	0.8505
	243.7	24.69	0.5013	0.8581

## COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Dean, M. R.; Tooke, J. W. Ind. Eng. Chem. 1946, 38, 389-393. 2. Dodecane (isomeric mixture); Cl₂H₂₆; VARIABLES: Temperature, pressure PREPARED BY: C. L. Young

### **EXPERIMENTAL VALUES:**

T/K	P/bar	Mole fraction in liquid, "H ₂	of hydrogen in vapor, y _{H2}
366.5	36.2	0.0373	0.99831
	70.33	0.0684	0.99900
	139.6	0.124	0.99929
	209.3	0.169	0.99932
	277.9	0.215	0.99930
	347.2	0.254	0.99930
422.0	36.2	0.0442	0.9868
	80.33	0.0789	0.999227
	139.6	0.147	0.99520
	209.3	0.200	0.99602
	277.9	0.250	0.99633
	347.2	0.299	0.99652

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

Rocking equilibrium cell fitted with sampling valve which could be used for gas or liquid sample. Pressure measured with Bourdon gauge, temperature measured with mercury in glass thermometer. Hydrocarbon placed in cell, pressurized with hydrogen. Agitated and equilibrated samples withdrawn and hydrocarbon component frozen out in liquid nitrogen; hydrogen estimated Volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Electrolytic commercial sample, purity better than 99.8 mole per cent.
- Isomeric mixture prepared by polymerization of isobutylene.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.2$  (up to 70 bar);  $\pm 1.0$  (up to 400 bar);  $\delta x_{\rm H_2} = \pm 1\%$ ;  $\delta y_{\rm H_2} = \pm 0.1\%$  (estimated by compiler).

## ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sokolov, B. I.; Polyakov, A. A. 2h. Prikl. Khim. 1977, 50, 1403-5. 2. Tetradecane; C₁₄H₃₀; [629-59-4]

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

т/к	P/bar	Mole fraction of hydrogen in liquid, ${}^x_{ m H_2}$
328.15	40.5	0.033
	101.3	0.083
	202.6	0.146
	304.0	0.210
403.15	40.5	0.042
	101.3	0.104
	202.6	0.190
	304.0	0.258
473.15	40.5	0.059
•	101.3	0.131
	202.6	0.250
	304.0	0.326
1		

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping gas out and measuring volume evolved. Remaining liquid estimated gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0$ ;  $\delta P/bar = \pm 0.5$ ;  $\delta x_{\rm H_2} = \pm 3\%$  (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hexadecane; C16H34; [544-76-3]

### ORIGINAL MEASUREMENTS:

Lin, H.-M.; Sebastian, H.M.; Chao, K.-C.

J. Chem. Engng. Data. <u>1980</u>, 25, 252-257.

### VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

EXPERIMENTAL	VALUES:		Mole fra	ction
T/K	P/atm	P/MPa	in liquid,	in vapor,
			x CH $_4$	^y CH₄
461.65	20.05	2.032	0.0311	0.99666
	29.90	3.030	0.0468	0.99782
	50.0	5.07	0.0757	0.99850
	101.7	10.30	0.1428	0.99909
	149.5	15.15	0.1978	0.99929
	199.5	20.21	0.2468	0.99939
	249.4	25.27	0.2928	0.99945
542.25	19.83	2.009	0.0407	0.9648
	30.24	3.064	0.0617	0.9759
	50.7	5.14	0.1007	0.9849
	101.8	10.31	0.1854	0.99187
	149.7	15.17	0.2515	0.99362
	199.7	20.23	0.3104	0.99450
	248.9	25.22	0.3597	0.99503
622.85	19.97	2.023	0.0497	0.8083
	29.92	3.032	0.0764	0.8663
	50.4	5.11	0.1293	0.9179
	100.1	10.14	0.2354	0.9553
	150.9	15.29	0.3201	0.9665
	200.7	20.34	0.3903	0.9713
	249.3	25.26	0.4458	0.9757

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge. Details in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Airco sample, purity 99.95 mole per cent or better.
- Matheson Coleman and Bell sample purity better than 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta P/MPa = \pm 0.01; \ \delta x_{\rm H_2}, \ \delta y_{\rm H_2} < \pm 1.0$ 

### REFERENCES:

1. Simnick, J.J.; Lawson, C.C.; Lin, H.M.; Chao, K.C.

Am. Inst. Chem. Engnrs. J. <u>1977</u>, 23, 469.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hexadecane; C₁₆H₃₄; [544-76-3]

### ORIGINAL MEASUREMENTS

Lin, H.-M.; Sebastian, H.M.; Chao, K.-C.

J. Chem. Engng. Data. 1980, 25, 252-257.

EXPERIMENTAL	VALUES:

			Mole fra	ction	
T/K	P/atm	P/MPa	in liquid,	in vapor,	
			^x CH₄	y _{CH} ,	
664.05	19.69	1.995	0.0513	0.6054	
	30.02	3.042	0.0857	0.7205	
	50.2	5.087	0.1488	0.8224	
	100.7	10.20	0.2782	0.8977	
	100.4	10.17	0.2759	0.8988	
	150.4	15.24	0.3724	0.9271	
	199.9	20.25	0.4511	0.9378	
	250.5	25.38	0.5192	0.9452	

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>2. 2-Methylpropane; C₄H₁₀; [75-28-5]</li> </ol>	Dean, M. R.; Tooke, J. W.  Ind. Eng. Chem. 1946, 38, 389-393.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young

EXPERTM	ENTAL VALU	ES.		-L			
T/K	P/bar	Mole fr of hyd		T/K	P/bar	Mole from of hydronic of hydronic of $^{x}_{\mathrm{H}_{2}}$	rogen
310.9	34.47 68.95 103.4 137.9 172.4 206.8 34.47 68.95 103.4	0.0275 0.0592 0.0872 0.1112 0.142 0.179 0.0274 0.0676 0.0847	0.8631 0.9191 0.9423 0.9521 0.9571 0.9551 0.697 0.824 0.867	338.7 366.5	206.8 34.47 68.95 103.4 137.9 172.4 206.8 68.95 86.18	0.197 0.0225 0.0709 0.109 0.156 0.192 0.247 0.082 0.117	0.9018 0.407 0.615 0.719 0.758 0.758 0.565 0.370 0.406
	137.9 172.4	0.129 0.169	0.887 0.879		103.4	0.162	0.424

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

Rocking equilibrium cell fitted with sampling valve which could be used for gas or liquid sample. Pressure measured with Bourdon gauge, temperature measured with mercury in glass thermometer. Hydrocarbon placed in cell, pressurized with hydrogen. Agitated and equilibrated samples withdrawn and hydrocarbon component frozen out in liquid nitrogen; hydrogen estimated volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Electrolytic commercial sample; purity better than 99.8 mole per cent.
- Phillips Petroleum sample; purity 99.5 mole percent; major impurity n-butane.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 2$  (up to 70 bar);  $\pm 10$  (up to 400 bar);  $\delta x_{\rm H_2} = \pm 1\%$ ;  $\delta y_{\rm H_2} = \pm 0.1\%$  (estimated

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. 2,2,4 - Trimethylpentane; C₀H₁₀; [540-84-1] VARIABLES: Temperature, pressure ORIGINAL MEASUREMENTS: Dean , M. R.; Tooke, J. W. Ind. Eng. Chem. 1946, 38, 389-393. PREPARED BY: C. L. Young

em ekire	NTAL VALUE	Mole fraction of hydrogen				Mole fraction of hydrogen		
T/K	P/bar	in liquid,		T/K	P/bar	in liquid,		
310.9	12.1 36.2 70.33	0.0090 0.0272 0.0517	0.98950 0.99602 0.99764	366.5	208.6 276.5 348.5	0.174 0.218 0.258	0.9922 0.9930 0.9936	
366.5	139.3 208.6 276.5 346.5 17.1 40.2	0.0971 0.132 0.166 0.198 0.0165 0.0404	0.99831 0.99838 0.99840 0.99832 0.9490 0.9765	423.4	12.8 37.9 70.33 106.2 141.0 208.6	0.0122 0.0468 0.0910 0.129 0.167 0.238	0.6897 0.8969 0.9334 0.9511 0.9601 0.9676	
	71.36 104.8 142.7	0.0710 0.0974 0.130	0.9855 0.9888 0.9910		275.1 349.2	0.292 0.355	0.9725 0.9748	

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Rocking equilibrium cell fitted with sampling valve which could be used for gas or liquid sample. Pressure measured with Bourdon gauge, temperature measured with mercury in glass thermometer. Hydrocarbon placed in cell, pressurized with hydrogen. Agitated and equilibrated samples withdrawn and hydrocarbon component frozen out in liquid nitrogen; hydrogen estimated volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Electrolytic commercial sample; purity better than 99.8 mole per cent.
- Rohm and Haas Co. sample; "pure" sample.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 2$  (up to 70 bar);  $\pm 10$  (up to 400 bar);  $\delta x_{\rm H_2} = \pm 18$ ;  $\delta y_{\rm H_2} = \pm 0.18$  (estimated by compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Peter, S.; Reinhartz, K. Z. Phys. Chem. 1960, 24, 103-18. 2. 2,2,4 - Trimethylpentane; C₈H₁₈; [540 - 84 - 1]VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction Mole fraction of hydrogen of hydrogen T/K P/bar in liquid, T/K in gas, P/bar in liquid, in gas, $y_{\rm H_2}$ $y_{\rm H_2}$ $x_{\rm H_2}$ $x_{\rm H_2}$ 423.95 24.5 0.029 0.832 294.2 0.397 0.914 471.65 49.0 0.062 0.911 392.3 0.488 0.920 73.5 0.093 0.934 490.3 0.570 0.916 98.1 0.946 0.122 588.4 0.646 0.905 147.1 0.955 686.5 0.178 0.742 0.881 196.1 0.227 0.966 711.0 0.816 0.816 294.2 0.314 0.971 499.35 29.4 0.032 0.460 392.3 0.388 0.972 49.0 0.076 0.604 588.4 0.509 0.971 73.5 0.127 0.703 784.5 0.604 0.966 98.1 0.173 0.754 980.7 0.683 0.960 147.1 0.261 0.806 1078.8 0.707 196.1 0.958 0.340 0.828 471.65 0.591 24.5 0.029 245.2 0.413 0.839 49.0 0.072 0.758 294.2 0.483 0.843 73.5 0.114 0.824 343.2 0.557 0.840 98.1 0.153 0.854 372.6 0.601 0.825 147.1 0.225 0.886 387.4 0.729 0.729 196.1 0.290 0.903

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static steel equilibrium cell fitted with magnetic stirrer and sampling ports. Temperature measured with a platinum resistance thermometer. Samples withdrawn after equilibrium ^{established.} The hydrocarbon component frozen out in a dry ice/acetone bath, hydrogen estimated volumetrically.

### SOURCE AND PURITY OF MATERIALS:

- Electrolytic grade purity 99.9 mole per cent, 0.05 mole per cent methane.
- 2. Shell AG sample.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/bar = \pm 0.1;$  $\delta y_{\rm H_2} = \pm 0.005$  (estimated by compiler).

378		Hydrogen and D	euterium	Solubilities above 200kPa
COMPO	ONENTS:	· · · · · · · · · · · · · · · · · · ·		ORIGINAL MEASUREMENTS:
1.		[1333-74-0]		Laugier, S.; Richon, D.; Renon, H.
2.	2,2,4- Trimeth C ₈ H ₁₈ ; [540-84			J. Chem. Engng. Data. <u>1980</u> ,25, 274-276.
VARI	ABLES:			PREPARED BY:
	Temperature,	pressure		C.L. Young
EXPE	RIMENTAL VALUES:		<u></u>	
				ole fraction of hydrogen
1	T/K	P/MPa		iquid, in vapor,
			$x_{\rm H_2}$	2
	226.0	3.0 6.2 11.9 18.0 24.6 24.8 31.4 36.8	0.11 0.22 0.33 - 0.42 0.49	17 0.780 12 0.829 0.847 21 - 99 0.849
	250.0 ^a	3.15 8.00 10.20 13.00 15.05 16.05	0.03 0.1 0.23 0.34 0.3	71 – 32 – 0.704 45 –

### AUXILIARY INFORMATION

0.402

0.428 0.467

0.496 0.524

### METHOD APPARATUS / PROCEDURE:

Static equilibrium cell fitted with sampling valves which removed samples of  $10^{-9}$  m³. Samples analysed by gas chromatography. Temperature measured using thermocouples and pressure measured using pressure transducer calibrated against a dead weight gauge.

17.05

17.40

18.10

19.75

20.00

20.40

### SOURCE AND PURITY OF MATERIALS:

 L'Air Liquide sample, purity better than 99.95 mole per cent.

0.697

0.651

0.636

0.550

2. Fluka sample, guaranteed purity 99.5 mole per cent or better.

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.2$$
;  $\delta P/MPa = \pm 0.04$ ;  $\delta x_{H_2} = \pm 0.009$ ;  $\delta y_{H_2} = \pm 0.012$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 2,2,4-Trimethylpentane; C₈H₁₈; [540-84-1]

### ORIGINAL MEASUREMENTS:

Laugier, S.; Richon, D.; Renon, H.

J. Chem. Engng. Data. 1980, 25, 274-276.

### EXPERIMENTAL VALUES:

<i>P/</i> MPa	Mole fraction of hydrogen in liquid, in vapor,		
	x _{H2}	$y_{\rm H_2}$	
4.90	<u></u>	0.473	
5.05	0.093	-	
7.80	-	0.623	
10.40	_	0.670	
14.40	0.335	0.708	
18.70	0.444	_	
	5.05 7.80 10.40 14.40	4.90 - 5.05 0.093 7.80 - 10.40 - 14.40 0.335	

- a) First set of experiments
- b) Second set of experiments

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Cyclohexane; C₆H₁₂; [110-82-7]

### **EVALUATOR:**

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

August 1980

### CRITICAL EVALUATION:

This system, like hydrogen + benzene, has been studied fairly extensively under a wide range of conditions. The two most extensive studies are that of Berty, Reamer and Sage (1) who studied the system between 310 K and 407 K up to pressures of 62 MPa and that of Krichevskii and Sorina (2) who studied the system between 293 K and 333 K up to pressures of 67 MPa. While it is not possible to carry out a precise comparison because the system was not studied at a common temperature, there are some small discrepancies between the results of these workers. The limited data of Sattler (3) at 308 K agrees with that obtained by interpolation of Krichevskii and Sorina (2). The data of Thomson and Edmister (4) which was studied at 339 K and 394 K up to pressures of 69 MPa agree with the data of Krichevskii and Sorina (2) at the lower temperature and with that of Berty  $et \ al.$  (1) at the higher temperature. Comparison of the data of Ipatiev and Levina (5) with that of Krichevskii and Sorina (2) and Berty et al. (1) indicates that Ipatiev and Levina (5) data are slightly too low (as has been observed elsewhere; see, for example, the evaluation of hydrogen + 1,3-dimethylbenzene). The data of Brainard and Williams (6) were determined as part of a study of the quaternary system, hydrogen + benzene + cyclohexane + hexane. appears that their data are slightly high at 366 K the extent of their data is too limited for a meaningful comparison in view of the interpolation needed in both pressure and temperature. Frolich et al. (7)presented their data in graphical form and the mole fraction solubilities calculated from their results are almost 10 per cent greater than those of Krichevskii and Sorina (2).

The data of Ipatiev and Levina (5) and Frolich  $et\ al.$  (7) are classified as doubtful whereas those of Berty  $et\ al.$  (1), Krichevskii and Sorina (2), Sattler (3) and Thompson and Edmister (4) are classified as tentative.

### References:

- Berty, T. E.; Reamer, H. H.; Sage, B. H. J. Chem. Engng. Data 1966, 11, 25.
- Krichevskii, I. R.; Sorina, G. A. Zh. Fiz. Khim. 1958, 32, 2080.
- 3. Sattler, H. Z. Tech. Physik. 1940, 21, 410.
- 4. Thompson, R. E.; Edmister, W. C. Am. Inst. Chem. Engnrs. J. 1965, 11, 457.
- 5. Ipatiev, V. V.; Levina, M. I. Zh. Fiz. Khim. 1935, 6, 632.

(cont.)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Cyclohexane;  $C_6H_{12}$ ; [110-82-7]

### **EVALUATOR:**

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

### CRITICAL EVALUATION:

### References (cont.)

- 6. Brainard, A. J.; Williams, G. B. Am. Inst. Chem. Engnrs. J. 1967, 13, 60.
- 7. Frolich, P. K.; Trauch, E. J.; Hogan, J. J.; Peer, A. A.

  Ind. Eng. Chem. 1931, 23, 548.

### ORIGINAL MEASUREMENTS: COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Frolich, P. K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A. Ind. Eng. Chem. 1931, 23, 548-550. 2. Cyclohexane; $C_6H_{12}$ ; [110-82-7] VARIABLES: PREPARED BY: C. L. Young Pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen Solubility*, S T/K P/MPa in liquid, † $x_{\rm H_2}$ 298.15 1.0 1.0 0.0044 0.0088 2.0 2.0 3.0 3.0 0.013 4.0 3.9 0.017 5.0 4.9 0.021 5.9 0.025 6.0 7.0 6.9 0.030 7.9 8.0 0.034 9.0 8.9 0.038 10.0 9.9 0.042 11.0 10.9 0.046 12.0 11.9 0.050 13.0 13.0 0.055 14.0 14.0 0.059 15.0 15.05 0.063 16.0 16.1 0.067

17.2

18.25

17.0

18.0

### AUXILIARY INFORMATION

### METHOD APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for vapor pressure of liquid and the solubility of the gas at atmospheric pressure. Details in source.

### SOURCE AND PURITY OF MATERIALS:

Stated that the materials were the highest purity available. Purity of cyclohexane 98 to 99 mole per cent.

0.071

0.075

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta x_{H_2} = \pm 5\%.$ 

Data taken from graph in original article. Volume of gas measured at 101.325 kPa pressure and 298.15K dissolved by unit volume of liquid measured under the same conditions.

 $^{^{\}dagger}$  Calculated by compiler.

OMPONENTS:		ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333	-74-0]	Ipatiev, V.V.; Levina, M.I.
C. Cyclohexane; C ₆ H ₁₂ ; [110-82-7]		Zhur. Fiz. Khim. 1935, 6, 632-9.
VARIABLES:		PREPARED BY:
Temperature, pressure		C.L. Young
EXPERIMENTAL VALUES:		Mole fraction of
T/K	P/bar	hydrogen in liquid, $x_{\rm H_2}$
	<u> </u>	
298.15	44.1 91.2 196.1 294.2	0.01801 0.03401 0.06813 0.09889
423.15	44.1 91.2 196.1	0.03236 0.06836 0.1400
513.15	294.2	0.3668

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Hydrocarbon added to cell then pressurized at temperature of measurement. After 1-2 hours liquid samples removed. Analysed by stripping out hydrogen at low pressure.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Prepared by high pressure (150-200 atm) hydrogenation of benzene at 280°C in presence of nickel catalyst. Boiling pt. 80.6°C Density at 15°C = 0.7835.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta x_{H_2} = \pm 2\%$ . (estimated by compiler)

### 384 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sattler, H.; 2. Cyclohexane; C₆H₁₂; [110-82-7] Z. Tech. Physik, 1940, 21,410-413 VARIABLES: PREPARED BY: C.L. Young Pressure EXPERIMENTAL VALUES: T/K P/bar Kuenen Coefficient Mole fraction of hydrogen in liquid 308.35 54.9 6.21 0.02280 95.6 10.73 0.03875 96.1 10.84 0.03913 146.8 16.53 0.05848 147.1 0.05841 16.51 147.1 0.05811 16.42 AUXILIARY INFORMATION METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Rocking bomb with liquid sampling attachment. Solvent and hydrogen No details given.

Rocking bomb with liquid sampling attachment. Solvent and hydrogen charged into evacuated cell. Amount of solvent in liquid sample estimated gravimetrically and hydrogen in liquid stripped out and estimated volumetrically. Details in source.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.2$ ;

 $\delta x_{\rm H_2} = \pm 2$ %. (estimated by compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Krichevskii, I.R. and Sorina, G.A. Cyclohexane; $C_6H_{12}$ ; [110-82-7] Zhur. Fiz. Khim. 1958, 32,2080-6 VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: T/K T/K P/bar P/bar Mole fraction of Mole fraction hydrogen in liquid, of hydrogen in $liquid, x_{H_2}$ $x_{\rm H_2}$ 293.15 49.6 0.0215 313.15 50.6 0.0216 59.9 0.0257 59.8 0.0259 77.5 0.0307 68.7 0.0299 109.4 0.0438 75.1 0.0322 94.2 0.0407 119.6 0.0478 144.9 0.0526 99.1 0.0435 187.5 119.6 0.0718 0.0510 188.5 0.0691 150.0 0.0602 158.1 272.6 0.0651 0.0945 188.5 300.9 0.103 0.0731 318.2 0.102 198.6 0.0796 334.4 0.114 233.0 0.0910 379.0 0.117 280.7 0.105 382.0 0.119 296.9 0.112 403.3 0.129 359.7 0.133 379.0 424.6 0.130 0.139 389.1 448.9 0.136 0.141 479.3 0.149 436.7 0.152 512.7 0.151 457.0 0.155 547.2 0.162 462.0 0.165 491.4 601.9 0.176 0.171 609.0 0.177 539.0 0.177 643.4 0.184 565.4 0.186 658.6 0.188 601.9 0.196 AUXILIARY INFORMATION METHOD:/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static equilibrium cell fitted with 1. Dried by passing through silica gel stirrer. Pressure measured with and calcium chloride Bourdon gauge. Samples of liquid and Vapor phases analysed by stripping out 2. Boiling point 80.1°C at0.9710 bar; hydrogen and estimating volumetrically $n_4^{20} = 1.4263$ ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta P/bar = \pm 1$ (up to 300 bar), $\pm 5$ (above 300 bar); $\delta x_{\rm H_2} = \pm 0.0003$ or 1% (whichever is greater) (estimated by compiler). REFERENCES:

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Cyclohexane; C₆H₁₂; [110-82-7]

### ORIGINAL MEASUREMENTS:

Krichevskii, I.R. and Sorina, G.A.

Zhur. Fiz. Khim. 1958,32,2080-6

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EXPERIME	ENTAL VA	LUES:	· · · · · · · · · · · · · · · · · · ·		
т/к	P/bar	Mole fraction of hydrogen in liquid, $^{x}{\rm H}_{2}$	T/K	P/bar	Mole fraction of hydrogen in liquid, $x_{\rm H_2}$
313.15	677.9 50.1 71.1 92.2 117.5 154.0 181.4 207.7 229.0 245.2 251.3 260.4 290.8 329.3	0.217 0.0262 0.0367 0.0462 0.0571 0.0746 0.0841 0.0941 0.0983 0.108 0.110 0.114 0.125 0.141	333.15	363.8 400.2 417.5 434.7 445.8 474.2 486.4 513.7 545.1 576.5 603.9 653.5	0.156 0.164 0.170 0.170 0.178 0.189 0.192 0.202 0.214 0.217 0.266 0.241 0.246
T/K	P/bar	Mole fraction of hydrogen in vapor, ${}^{y}_{\mathrm{H}_{2}}$	T/K	P/bar	Mole fraction of hydrogen in vapor, ${}^{\mathcal{Y}}_{\text{H}_2}$
313.15	50.2 99.1 197.6 299.9 379.0 379.0 558.3 642.7 490.1 124.6 125.6 198.6 277.7 352.7 436.7 491.4	0.99738 0.99728 0.99830 0.99821 0.99858 0.99864 0.99853 0.99867 0.99803 0.99133 0.99133 0.99236 0.99559 0.99559 0.99555 0.99655 0.99681 0.99681 0.99713 0.99713 0.99713 0.99713 0.99702 0.99689 0.99665	313.15	491.4 599.8 603.9 688.0 50.1 102.3 104.4 193.5 193.5 290.8 388.1 388.1 484.3 486.4 574.5 576.5 688.0	0.99666 0.99653 0.99654 0.99621 0.99584 0.9858 0.99203 0.99192 0.99402 0.99466 0.99466 0.99466 0.99461 0.99451 0.99441 0.99441 0.99429 0.99322 0.99296

## COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Thompson, R. E.; Edmister, W. C. Am. Inst. Chem. Engnrs. J. 2. Cyclohexane; C₆H₁₂; [110-82-7] 1965, 11, 457-461. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

EXPERIMENTAL	VALUES:
--------------	---------

T/K	P/bar	Mole fraction in liquid, $x_{\rm H_2}$	of hydrogen in vapor, ^y H ₂
338.7	6.88	0.00362	0.9027
	13.78	0.00710	0.9523
	34.60	0.0182	0.9773
	34.58	-	0.9793
	68.66	0.0345	0.9880
	116.8	0.0563	0.99132
394.3	207.0	0.102	0.99320
	413.4	0.178	0.99330
	690.4	0.262	0.99358
	690.4	-	0.99315
	6.98	0.00317	0.451
	13.78	0.00802	0.237
	34.47	0.0225	0.101
	68.94	0.0456	0.0565
	117.2	0.0774	0.0377
	206.8	0.131	0.0269
	413.4	0.236	0.0213
	689.4	0.350	0.0188

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

Equilibrium cell fitted with glass fiber packing and grooved cone to assist equilibrium being established. Pressure measured with dead weight tester and temperature with thermocouple. Sample analysed by freezing out hydrocarbon and gas measured volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.8 mole per cent.
- Phillips Petroleum sample, purity 99.94 mole per cent or better.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ ;  $\delta P/bar = \pm 0.1$ %,  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 3$ % (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Cyclohexane; C₆H₁₂; [110-82-7]

### ORIGINAL MEASUREMENTS:

Berty, T. E.; Reamer, H. H.;

Sage, B. H.

J. Chem. Engng. Data <u>1966</u>, 11, 25-30.

### VARIABLES:

Temperature, pressure

EXPERIMENTAL VALUES:

### PREPARED BY:

C. L. Young

		Mole fra of hydr				Mole fra of hydr	
T/K	P/bar	in liquid,	in gas,	T/K	P/bar	in liquid,	_
		$x_{ m H_{2}}$	$y_{ m H_{2}}$			$x_{ m H_{2}}$	$y_{ m H_{2}}$
310.9	34.5	0.0135	0.9921	344.3	413.7	0.1760	0.9920
1	68.9	0.0269	0.9949		482.6	0.2030	0.9919
ļ	103.4	0.0400	0.9964		551.6	0.2273	0.9918
	137.9	0.0530	0.9969		620.5	0.2520	0.9917
	172.4	0.0658	0.9970	377.6	34.5	0.0189	0.9350
	206.8	0.0784	0.9971		68.9	0.0384	0.9622
	241.3	0.0906	0.0072		103.4	0.0574	0.9716
	275.8	0.1028	0.9973		137.9	0.0760	0.9763
	310.3	0.1145	0.9973		172.4	0.0941	0.9789
	344.7	0.1260	0.9972		206.8	0.1119	0.9804
	413.7	0.1480	0.9970		241.3	0.1281	0.9815
	482.6	0.1692	0.9967		275.8	0.1446	0.9822
}	551.6	0.1893	0.9960		310.3	0.1599	0.9827
344.3	34.5	0.0157	0.9734		344.7	0.1758	0.9830
1	68.9	0.0316	0.9851		413.7	0.2058	0.9832
	103.4	0.0473	0.9888		482.6	0.2362	0.9834

### AUXILIARY INFORMATION

407.6

0.9903

0.9912

0.9915

0.9919

0.9920

0.9920

0.9920

### METHOD/APPARATUS/PROCEDURE:

137.9

172.4

206.8

241.3

275.8

310.3

344.7

Static PVT cell fitted with dead weight pressure balance and platinum resistance thermometer. Bubble point determined from discontinuity in slope of pv isotherm. Gas phase compositions determined by analysis using partial condensation techniques. Details in source and ref. 1.

0.0627

0.0774

0.0927

0.1068

0.1215

0.1357

0.1494

### SOURCE AND PURITY OF MATERIALS:

551.6

34.5

68.9

103.4

137.9

172.4

206.8

1. Electrolytic hydrogen passed over hot platinum wire. Final purity better than 99.86 mole per cent.

0.2644

0.0244

0.0466

0.0697

0.0914

0.1118

0.1340

0.9835

0.8582

0.9196

0.9402

0.9503

0.9564

0.9603

 Phillips Petroleum research grade sample. Purity 99.94 mole per cent minimum. Dried.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.01; \quad \delta P/bar = \pm 0.03;$ 

 $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 0.001$ .

### REFERENCES:

Sage, B. H.; Lacey, W. N.
 Trans. Am. Inst. Mining Met.
 Engnrs. 1940, 136, 136.

- Hydrogen; H₂; [1333-74-0]
- 2. Cyclohexane; C₆H₁₂; [110-82-7]

### ORIGINAL MEASUREMENTS:

Berty, T. E.; Reamer, H. H.; Sage, B. H.

J. Chem. Engng. Data 1966, 11, 25-30.

### EXPERIMENTAL VALUES:

T/K	P/bar	Mole frac of hydro in liquid, "H ₂	ogen
407.6	241.3 275.8 310.3 344.7 413.7 482.6 551.6	0.1505 0.1673 0.1858 0.2020 0.2343 0.2652 0.2919	0.9630 0.9651 0.9664 0.9673 0.9681 0.9681

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Cyclohexane;  $C_6H_{12}$ ; [110-82-7]

### ORIGINAL MEASUREMENTS:

Brainard, A. J.; Williams, G. B. Am. Inst. Chem. Engnrs. J.

1967, 13, 60-69.

### VARIABLES:

PREPARED BY:

Temperature, pressure

C. L. Young

### EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction in liquid,  **H ₂	of hydrogen in vapor, ^y H ₂	
366.48 422.04	146.86 37.92 139.07 37.78	0.0853 0.0231 0.1097 0.0300	0.985 0.959 0.949 0.859	

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Stirred equilibrium cell. Pressure measured with Bourdon gauge. Analysis of samples carried out by expanding into an expansion cylinder and freezing out the hydrocarbon; hydrogen measured volumetrically and then hydrocarbon estimated volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Matheson ultrapure sample, purity better than 99.998 mole per cent.
- Phillips Petroleum sample,
   purity 99.99 mole per cent;
  2,4-dimethylpentane and 2,2 dimethylpentane major impurities

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3$ ;  $\delta P/bar = \pm 0.15$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 1.0$ % (estimated by compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Ipatiev, V.V.; Levina, M.I. 2. Methylcyclohexane; C7H14; Zhur. Fiz. Khim. 1935, 6, 632-9. [108-87-2] VARIABLES: PREPARED BY: Pressure. C.L. Young EXPERIMENTAL VALUES: T/K P/bar Mole fraction of hydrogen in liquid, $x_{\rm H_2}$ 298.15 44.1 0.02250 91.2 0.04400 196.1 0.08264 294.2 0.1398 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static equilibrium cell. Hydrocarbon 1. No details given. added to cell then pressurized at temperature of measurement. After Prepared by high pressure (150-200 atm) hydrogenation of toluene at 280°C in presence of nickel 1-2 hours liquid samples removed. Analysed by stripping out hydrogen at low pressure. catalyst. Boiling pt. $100.8^{\circ}$ C. Density at $15^{\circ}$ C = 0.7783. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \delta x_{H_2} = \pm 2\%.$ (estimated by compiler). REFERENCES:

### COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Peter, S.; Reinhartz, K. Z. Phys. Chem. 1960, 24, 103-18. VARIABLES: Temperature, pressure PREPARED BY: C. L. Young

### EXPERIMENTAL VALUES:

т/к	P/bar	Mole fraction of hydroin liquid, $x_{\rm H_2}$	ogen	T/K	P/bar	Mole fra of hydr in liquid, $x_{\rm H_2}$	ogen
424.15	24.5 49.0 98.1 147.1 196.1 294.2 490.3 686.5 882.6 24.5 49.0 98.1 147.1 196.1	0.022 0.044 0.085 0.124 0.161 0.226 0.335 0.421 0.492 0.023 0.023 0.055 0.112 0.163 0.209	0.925 0.955 0.965 0.970 0.972 0.974 0.977 0.978 0.978 0.707 0.858 0.912 0.925 0.931	471.65 498.85	294.2 490.3 686.5 882.6 24.5 49.0 98.1 147.1 196.1 294.2 392.3 588.4 784.5	0.292 0.363 0.519 0.597 0.017 0.054 0.121 0.180 0.233 0.329 0.411 0.543 0.638	0.938 0.941 0.938 0.935 0.464 0.735 0.855 0.885 0.893 0.899 0.900 0.899

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static steel equilibrium cell fitted with magnetic stirrer and sampling ports. Temperature measured with a platinum resistance thermometer. Samples withdrawn after equilibrium established. The hydrocarbon component frozen out in a dry ice/acetone bath, hydrogen estimated volumetrically.

### SOURCE AND PURITY OF MATERIALS:

- 1. Electrolytic grade, purity 99.9 mole per cent, 0.05 mole per cent methane.
- Phillips Petroleum Co. sample; pure grade, minimum purity 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$ ;  $\delta x_{H_2} = \pm 3\%$ ;  $\delta y_{H_2} = \pm 0.005$  (estimated by compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sokolov, B. I.; Polyakov, A. A. Zh. Prikl. Khim. 1977, 50, 1403-5. Decahydronaphthalene, (Decalin); $C_{10}H_{18}$ ; [9 $\bar{1}$ -17-8] VARIABLES: PREPARED BY: C. L. Young Temperature, pressure

Mole fraction of hydrogen

### EXPERIMENTAL VALUES:

T/K	P/bar	in liquid, "H ₂	
338.15	40.5	0.014	
	101.3	0.038	
	202.6	0.076	
	304.0	0.123	
398.15	40.5	0.020	
	101.3	0.054	
	202.6	0.105	
	304.0	0.158	
473.15	40.5	0.025	
	101.3	0.069	
	202.6	0.136	
	304.0	0.195	

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping out gas and measuring volume evolved. Remaining liquid estimated gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0$ ;  $\delta P/bar = \pm 0.5$ ;  $\delta x_{\rm H_2}$  = ±3% (estimated by compiler).

541.85

COMPONENT	rs:			ORIGINAL MEASUREMENTS:			
1. Hydrogen; H ₂ ; [1333-74-0]				Sebasti	an, H.	M.; Yao, J.	; Lin,
				нм.;	Chao,	кс.	
2. 1,1'-Bicyclohexy1; $C_{12}H_{22}$ ;				J. Chem	. Engng	. Data <u>1978</u>	., <i>23</i> , 167.
	[92-51	-3]					
VARIABLE	S:	<del></del>		PREPARED	BY:		
Temperature, pressure				C. L. Young			
EXPERIME	NTAL VALU	JES:		1		<u>-</u> <u>-</u>	
		Mole fra of hydr				Mole fra	
т/к	P/bar		in vapor,	T/K	P/bar		in vapor,
462.15	20.3	0.0181	0.9842	621.75			0.6117
	30.4 50.7	0.0262 0.0443	0.9889 0.9929		30.4 50.7		0.7322 0.8296
	101.3		0.9958		101.3	0.1398	
		0.1158	0.9969		152.0		
	202.7 253.3	0.1418 0.1718	0.9974 0.9977		202.7 253.3	0.2578 0.3112	0.9445 0.9533
	2,3,3	0.1/10	0.5377		233.3	0.3112	0.5555

0.8988

0.9312

0.9558

0.9748

0.9813

0.9845

0.9866

### AUXILIARY INFORMATION

701.65

### METHOD/APPARATUS/PROCEDURE:

20.3

30.4

50.7

101.3

152.0

202.7

253.3

0.0212

0.0329

0.0543

0.1031

0.1480

0.1899

0.2268

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge.

### SOURCE AND PURITY OF MATERIALS:

20.3

30.4

50.7

101.3

152.0

202.7

253.3

 Air Products Co. sample; purity 99.95 mole per cent.

0.0054

0.0289

0.0793

0.1818

0.2680

0.3494

0.4239

0.0602

0.2463 0.4885

0.6720

0.7467

0.7857

0.8050

Fischer Scientific Co. sample; purity about 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.7$ ;  $\delta P/bar = \pm 0.3$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 1\%$  (estimated by compiler).

### REFERENCES:

Simmick, J. J.; Lawson, C. C.;
 Lin, H.-M.; Chao, K.-C.
 Am. Inst. Chem. Engnrs. J. 1977,
 23, 469.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ethene;  $C_2H_4$ ; [74-85-1]

### **EVALUATOR:**

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

### CRITICAL EVALUATION:

This system has been investigated by four groups. The early data of Likhter and Tikhonovich (1) are of limited accuracy; the mole fraction of hydrogen in the liquid was found to be proportional to the fugacity of hydrogen, f, up to 8 MPa. The constants, k, in the equation

$$f = kx$$

were 1450, 1607, 1845 and 2152 atm at 188, 178, 168 and 158 K, respectively. It appears that the mole fraction solubilities from these equations are higher than more recent data. The mole fraction solubility data of Hiza et al. (2) which cover the temperature range 121 to 170 K and pressures between 2 and 15 MPa are consistently a few per cent higher than those given by Sagara et al. (3) which cover the temperature range 123 to 248 K and pressures between 2 and 8 MPa. Both sets of data are classified as tentative.

The data of Williams and Katz (4) are mostly reported as K-values (K = gas phase mole fraction/liquid phase mole fraction) or in graphical form. K-values calculated from the data of Sagara  $et\ al.$  (3) are in agreement with those quoted by Williams and Katz (4).

### References:

- 1. Likhter, A. I.; Tikhonovich, N. P. Zh. Tekh. Fiz. 1939, 9, 1916.
- 2. Hiza, M. J.; Heck, C. K.; Kidnay, A. J. Chem. Eng. Progr. Symp. Ser. 1968, 64, no. 88, 57.
- 3. Sagara, H.; Arai, Y.; Saito, S. J. Chem. Engng. Japan 1972, 5, 339.
- 4. Williams, R. B.; Katz, D. L. Ind. Eng. Chem. 1954, 46, 2512.

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Williams, R.B.; Katz, D.L. 2. Ethene, (Ethylene); C₂H₄; Ind. Eng. Chem. 1954, 46, 2512-20. VARIABLES: Temperature, pressure C.L. Young EXPERIMENTAL VALUES:

EXPERIMENTAL VALUES:				
т/к	p/psi	p/10 ⁵ Pa	K value of hydrogen	
255.37	500	34.47	17.1	
	1000	68.95	8.10	
	2000	137.90	3.94	
241.48	500	34.47	23.1	
	1000	68.95	11.25	
	2000	137.90	5.50	
	4000	275.79	2.43	
227.59	250	17.24	56.0	
	500	14.47	28.2	
	1000	68.95	14.4	
	2000	137.90	7.35	
	4000	275.79	3.51	
199.82	250	17.24	84.2	
	500	34.47	41.3	
	1000	68.95	21.2	
	2000	137.90	10.8	
	4000	275.79	5.75	
172.04	250	17.24	123.6	
	500	34.47	62.0	
	1000	68.95	31.8	

### AUXILIARY INFORMATION

137.90

### METHOD/APPARATUS/PROCEDURE:

Flow system described in ref. (1). Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Vapor recirculated by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room temperature and pressure; analysed by gas density measurements. K-values for ethylene given in source.

2000

### SOURCE AND PURITY OF MATERIALS:

16.5

- 1. Purity 99.9 mole %. Dried.
- 2. 99.6% pure as estimated by mass spectrometry.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.6$ ;  $\delta p/psi = \pm 0.5$ %;  $\delta K < 1$ %.

### REFERENCES:

Aroyan, H.J.; Katz, D.L.
 Ind. Eng. Chem., <u>1951</u>, 43, 185.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ethene, (Ethylene);  $C_2H_4$ ; [74-85-1]

ORIGINAL MEASUREMENTS:

Williams, R.B.; Katz, D.L.

Ind. Eng. Chem. 1954, 46, 2512-20

### EXPERIMENTAL VALUES:

т/к	p/psi	p/10 ⁵ Pa	K value of hydrogen
172.04	4000	275.79	8.82
	8000	551.58	4.95
158.15	250	17.24	147
	500	34.47	75.1
	1000	68.95	38.6
	2000	137.90	20.2
	4000	275.79	10.9
	8000	551.58	6.25
144.26	250	17.24	188
	500	34.47	96.4
	1000	68.95	50.3
	2000	137.90	26.6
	4000	275.79	14.60
	8000	551.58	8.75
116.48	250	17.24	308
	500	34.47	159
	1000	68.95	82.7
	2000	137.90	44.8
	4000	275.79	28.5
	8000	551.58	18.7

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Hiza, M. J.; Heck, C. K.; Kidnay, A. J.
2. Ethene; C ₂ H ₄ ; [74-85-1]	Chem. Eng. Progr. Symp. Ser. No. 88 1968, 64, 57-65.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young
DADDINGNESS AND A Second on	Molo fragtic

EXPERIMENTAL VALUES: Mole fraction of hydrogen					Mole fra of hydr		
T/K	P/bar	in liquid,	in vapor,	T/K	P/bar	in liquid,	
	•	$x_{ m H_{2}}$	^у н ₂			$x_{ m H_{2}}$	$y_{ m H_{2}}$
169.90	23.8	0.0117	0.9460	129.62	33.9	0.00929	_
169.93	48.4	0.0235	0.9696	130.0	43.8	_	0.99811
169.72	61.6	0.0303	_	129.85	61.0	0.0161	-
	62.6	_	0.9733	130.00	76.4	_	0.99831
169.75	81.1	_	0.9764	129.82	80.4	0.0205	-
169.73	105.4	0.0507	-	130.00	92.8	-	0.99831
	106.9	_	0.9784	129.78	105.7	0.0266	_
169.72	136.8	0.0638	-	130.00	129.5	-	0.99818
169.76	147.9	_	0.9796	129.79	131.2	0.0320	-
149.71	30.4	-	0.9884	122.00	10.76	-	0.99813
149.93	31.7	0.0121	-		25.58	-	0.99896
149.68	56.1	-	0.99177		37.0	0.00800	-
149.84	60.2	0.0224	-		39.28	-	0.999142
149.69	77.4	0.0289	-	121.79	61.10	0.0133	-
149.67	84.1	-	0.99249	122.00	71.33	-	0.999223
149.55	94.2	0.0340	-	121.77	90.69	0.0192	-
149.70	113.0	-	0.99269	122.00	100.1	-	0.999166
150.00	133.2	-	0.99275	121.77	120.6	0.0246	-
149.55	149.5	0.0512	-	122.00	131.7	-	0.999060
130.0	23.15	-	0.99736	121.69	159.1	0.0310	-

Additional vapor compositions in source at lower temperatures including vapor-solid equilibrium data.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Closed loop flow system with pump at ambient temperature. Temperature measured with platinum resistance thermometer and pressure with Bourdon gauge. Samples of both phases analysed by gas chromatography.

### SOURCE AND PURITY OF MATERIALS:

- Purified (no other details given).
- 2. Research grade, purity 99.98 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/bar = \pm 0.1$  (up to 100 bar);  $\pm 0.3$  (above 100 bar);  $\delta x_{\rm H_2} = \pm 2\%$ ;  $\delta (1-y_{\rm H_2}) = \pm 3\%$ .

### COMPONENTS: 1. Hydrogen; H₂; [1333-74-0]

2. Ethene; C₂H₄; [74-85-1]

ORIGINAL MEASUREMENTS:

Sagara, H.; Arai, Y.; Saito, S. J. Chem. Engng. Japan 1972, 5, 339-348.

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMENTAL	VALUES:	Mole fraction of	hvdrogen
T/K	P/bar	in liquid,	in gas,
	-,		-
_		$x_{ m H_{2}}$	$y_{\rm H_2}$
123.15	20.3	0.00531	0.996
	40.5	0.00932	0.997
	60.8	0.0127	0.998
	81.1	0.0146	0.998
148.15	20.3	0.00743	0.979
	40.5	0.0131	0.985
	60.8	0.0185	0.988
_	81.1	0.0266	0.990
173.15	20.3	0.00865	0.921
	40.5	0.0164	0.954
	60.8	0.0281	0.964
	81.1	0.0361	0.968
198.15	20.3	0.0100	0.747
	40.5	0.0207-	0.863
	60.8	0.0370	0.890
200	81.1	0.0489	0.909
223.15	20.3	0.00843	0.438
	40.5	0.0265	0.673
	60.8	0.0448	0.760
340	81.1	0.0603	0.797
248.15	30.4	0.00988	0.209
	81.1	0.0212	0.331

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

Static stainless steel cell of capacity  $5 \times 10^5$  mm³ fitted with magnetic stirrer and sampling valves. Cell enclosed in cryostat. Temperature measured with thermocouple. Pressure measured using Bourdon gauge. Gases added to cell and equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Nippon Sanso Co. Ltd. sample; purity 99.99 mole per cent.
- Takachiho Chemical Co. Ltd. sample; purity 99.5 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/bar = \pm 0.1;$  $\delta x_{H_2}, \quad \delta y_{H_2} = \pm 1%.$ 

COMPONENTS:	EVALUATOR:
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Olefins</li> </ol>	Colin L. Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia.
	August 1980

### CRITICAL EVALUATION:

Apart from the ethene + hydrogen system, no hydrogen + olefin system has been studied at high pressures by more than one group. Therefore the evaluations are limited to inferring the reliability or otherwise of the data from the evaluation of solubility data on other systems by the same workers.

### Hydrogen + Propene

This system has been studied by Williams and Katz (1) and their data are classified as tentative on the basis of the evaluation of these workers' results for the systems ethene, ethane and propane + hydrogen.

Hydrogen + 1-Hexene, + 1-Heptene, + 1-Octene

Sokolov and Polyakov's data (2) on hydrogen + decane appears to be reliable (see evaluation), therefore their data on 1-hexene, 1-heptene and 1-octene + hydrogen are expected to be fairly reliable and are classified as tentative.

### References:

- l. Williams, R. B.; Katz, D. L. Ind. Eng. Chem. 1954, 46, 2512.
- 2. Sokolov, B. I.; Polyakov, A. A. Zh. Prikl. Khim. 1977, 50, 1403.

- Hydrogen; H₂; [1333-74-0]
- 1-Propene, (Propylene); C3H6; [115-07-1]

### ORIGINAL MEASUREMENTS:

Williams, R.B.; Katz, D.L.

Ind. Eng. Chem. 1954, 46, 2512-20

VARIABLES:

PREPARED BY:

Temperature, pressure

C.L. Young

EAPERIMENTAL V	ALUES:
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T/K	p/psi	<i>p</i> /10 ⁵ Pa	K value of hydrogen	
297.04	250	17.24	46.0	
	500	34.47	24.9	
	1000	68.95	13.4	
	2000	137.90	7.12	
	4000	275.79	3.67	
	8000	551.58	1.81	
283.15	250	17.24	57 <b>.</b> 0	
	500	34.47	30.9	
	1000	68.95	16.1	
	2000	137.90	8.39	
	4000	275.79	4.38	
	8000	551.58	2.31	
255.37	250	17.24	79.4	•
	500	34.47	40.4	
	1000	68.85	21.1	
	2000	137.90	11.0	
	4000	275.79	5.82	
	8000	551.58	3.20	
277.59	250	17.24	112	
	500	34.47	57.6	
	1000	68.95	29.2	
	2000	137.90	14.7	

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Flow system described in ref. (1). Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Vapor recirculated by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room temperature and pressure; analysed by gas density measurements. K-values for propene given in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.9 mole %. Dried.
- 2. Stated purity better than 99 mole %.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.6$ ;  $\delta p/psi = \pm 0.5$ %;  $\delta K < 1%$ .

### REFERENCES:

1. Aroyan, H.J.; Katz, D.L. Ind. Eng. Chem. 1951, 43, 185.

1. Hydrogen; H₂; [1333-74-0]

2. 1-Propene, (Propylene);  $C_3H_6$ ; [115-07-1]

ORIGINAL MEASUREMENTS:

Williams, R.B.; Katz, D.L.

Ind. Eng. Chem. 1954, 46, 2512-20.

### EXPERIMENTAL VALUES:

т/к	p/psi	p/10 ⁵ Pa	K value of hydrogen	
277.59	4000 8000	275.79 551.58	7.65 4.31	
199.82	250	17.24	156	
	500	34.47	79.6	
	1000	68.95	40.2	
	2000	137.90	20.3	
	4000	275.79	10.4	
	8000	551.58	5.93	
172.04	250	17.24	201	
	500	34.47	103	
i	1000	68.95	52.9	
	2000	137.90	27.1	
	4000	275.79	14.7	
	8000	551.58	8.63	
158.15	250	17.24	306	
	500	34.47	159	
	1000	68.95	82.8	
	2000	137.90	43.2	
	4000	275.79	23.2	
	8000	551.58	13.8	
144.26	250	17.24	596	
	500	34.47	318	
	1000	68.95	165	
	2000	137.90	89.0	
	4000	275.79	48.5	
	8000	551.58	28.6	

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sokolov, B. I.; Polyakov, A. A. Zhur. Prikl. Khim. 1977, 50, 1403-5. 2. 1-Hexene; $C_6H_{12}$ ; [592-41-6] VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/bar in liquid, x H 2

### 0.086 101.3 0.159 202.6 0.228 304.0 403.15 40.5 0.047 101.3 0.114 0.215 202.6 304.0 0.303 443.15 40.5 0.050 101.3 0.141 202.6 0.263 304.0 0.380

0.040

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

40.5

333.15

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping gas out and measuring volume evolved. Remaining liquid estimated gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0; \quad \delta P/\text{bar} = \pm 0.5;$   $\delta x_{\text{H}_2} = \pm 3 \text{% (estimated by compiler)}.$ 

### COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Sokolov, B. I.; Polyakov, A. A. 2. 1-Heptene; C₇H₁₄; [592-76-7] VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

### EXPERIMENTAL VALUES:

т/к	P/bar	Mole fraction of hydrogen in liquid, "H ₂
333.15	40.5	0.028
	101.3	0.073
	202.6	0.137
	304.0	0.201
403.15	40.5	0.041
	101.3	0.108
	202.6	0.190
	304.0	0.261
473.15	40.5	0.049
	101.3	0.146
	202.6	0.255
	304.0	0.353

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping gas out and measuring volume evolved. Remaining liquid estimated gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0$ ;  $\delta P/bar = \pm 0.5$ ;

 $\delta x_{\rm H_2} = \pm 3\%$  (estimated by compiler).

ORIGINAL MEASUREMENTS:
Sokolov, B. I.; Polyakov, A. A. Zh. Prikl. Khim. 1977, 50, 1403-5.
PREPARED BY: C. L. Young

### EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of hydrogen in liquid, $^{x}_{\mathrm{H}_{2}}$
328.15	40.5	0.024
1	101.3	0.070
	202.6	0.120
	304.0	0.186
393.15	40.5	0.038
	101.3	0.094
	202.6	0.179
	304.0	0.243
463.15	40.5	0.049
	101.3	0.131
	202.6	0.255
	304.0	0.318
L		

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping gas out and measuring volume evolved. Remaining liquid estimated gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

### ESTIMATED ERROR:

$$\begin{split} \delta T/K &= \pm 1.0; \quad \delta P/\text{bar} = \pm 0.5; \\ \delta x_{\text{H}_2} &= \pm 3 \text{\% (estimated by compiler).} \end{split}$$

COMPONENTS:		EVALUATOR:
<ol> <li>Hydrogen; H₂;</li> <li>Benzene; C₆H₆;</li> </ol>	[1333-74-0] [71-43-2]	Colin Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia. August 1980
<b>L</b>		3

### CRITICAL EVALUATION:

This system has been studied fairly extensively under a wide range of conditions. The data of Brainard and Williams (1) were determined as part of a study of the quaternary system hydrogen + benzene + cyclohexane + hexane. While it appears that their data are consistent with those of Connolly (2) and Thompson and Edmister (3) the data are too limited for a meaningful comparison in view of the interpolation in pressure and temperature needed for such a comparison. Hence the Brainard and Williams (1) results are not considered further.

The data of Connolly (2) cover the temperature range 433 K to 533 K and pressures up to 18 MPa. These data are in reasonable agreement with those of Thompson and Edmister (3) at the common temperature of 433 K. The latter data cover the temperature range 339 K to 433 K and when interpolated to 345.75 K are in fair agreement with the data of Sattler (4).

The data of Ipatiev and Levina (5) cover the temperature range from 298 K to 513 K and the mole fractions in the liquid are smaller than the values given by Connolly (2) and Thompson and Edmister (3). It appears, in general, that Ipatiev and Levina (5) data are slightly too small (see, for example, evaluation of hydrogen + 1,3-dimethylbenzene). Therefore, in the present evaluation the data of Ipatiev and Levina (5) are classified as doubtful.

The higher pressure data of Ipatiev and coworkers (6) are more or less consistent with the work of Ipatiev and Levina (5).

The data of Krichevskii and Efremova (7) are limited to the temperature of 288.15 K and are slightly smaller than values obtained by extrapolation of the data of either Ipatiev and Levina (5) or Thompson and Edmister (3). The data of Krichevskii and Efremova (7) are classified as doubtful.

This system was also studied by Frolich et al. (8) but no table or graph of result was given. It was stated that the curve of solubility of hydrogen in benzene coincided with that of hydrogen in isopropyl alcohol. (The curve was a plot of Ostwald coefficient x pressure against pressure.) The data are not considered further in the present context.

The data of Connolly (2), Thompson and Edmister (3) and Sattler (4) are classified as tentative.

### References:

- Brainard, A. J.; Williams, G. B. Am. Inst. Chem. Engnrs. J. <u>1967</u>, 13, 60.
- 2. Connolly, J. F. J. Chem. Phys. 1962, 36, 2897.
- Thompson, R. E.; Edmister, W. C. Am. Inst. Chem. Engnrs. J. 1965, 11, 457.

(cont.)

### COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Benzene; C₆H₆; [71-43-2] EVALUATOR: Colin Young, School of Chemistry, University of Melbourne, Parkville, Victoria 3052, Australia. August 1980

### CRITICAL EVALUATION:

### References (cont.)

- 4. Sattler, H. Z. Tech. Physik. 1940, 21, 410.
- 5. Ipatiev, V. V.; Levina, M. I. Zh. Fiz. Khim. 1935, 6, 632.
- Ipatiev, V. V.; Teodorovich, V. P.; Brestkin, A. P.; Artemovich,
   V. S. Zh. Fiz. Khim. <u>1948</u>, 22, 834.
- 7. Krichevskii, I. R.; Efremova, G. D. Zh. Fiz. Khim. 1948, 22, 1116.
- Frolich, P. K.; Trauch, E. J.; Hogan, J. J.; Peer, A. A.
   Ind. Eng. Chem. 1931, 23, 548.

### ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Ipatiev, V.V.; Levina, M.I. 2. Benzene; C₆H₆; [71-43-2] Zhur. Fiz. Khim. 1935, 6, 632-9. VARIABLES: PREPARED BY: Temperature, pressure. C.L. Young

EXPERIMENTAL VALUES:  * Mole fraction of hydrogen				
T/K	P/bar	in liquid, $x_{\rm H_2}$		
298.15	49.0 98.1 294.2	0.01253 0.02516 0.07140		
373.15	49.0 98.1 294.2	0.01842 0.03694 0.1063		
423.15	49.0 98.1 196.1 294.2	0.02496 0.05497 0.1058 0.1563		
473.15	49.0 98.1 196.1 294.2	0.02760 0.06327 0.1313 0.1976		
513.15	49.0 98.1 196.1 294.2	0.04553 0.07320 0.1682 0.2455		

### calculated by compiler.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell.
Hydrocarbon added to cell then
pressurized at temperature of
measurement. After 1-2 hours liquid
samples removed. Analysed by stripping out hydrogen at low pressure.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Fractionally crystalised, distilled. Boiling pt. 80.2°C, Melting pt. 5.3°C, Density (at 15°C) = 0.8803.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta x_{\rm H_2} = \pm 2$ %. (estimated by compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sattler, H.; 2. Benzene, $C_6H_6$ ; [71-43-2] Z. Tech. Physik, 1940, 21,410-413. VARIABLES: PREPARED BY: Temperature, pressure C.L. Young EXPERIMENTAL VALUES: T/K P/bar Kuenen coefficient Mole fraction of hydrogen in $liquid, x_{H_2}$ 50.5 4.15 0.01427 308.15 4.33 0.01487 54.9 98.8 7.88 0.02674 99.7 0.02734 8.06 100.2 8.19 0.02777 11.77 147.3 0.03943 147.8 11.55 0.03872 0.01808 5.28 345.75 51.0 54.4 5.78 0.01976 10.97 0.03684 104.9 106.9 11.25 0.03775 0.05005 145.1 15.11 151.0 0.05200 15.73 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Rocking bomb with liquid sampling attachment. Solvent and hydrogen No details given. charged into evacuated cell. Amount of solvent in liquid sample estimated gravimetrically. Amount of hydrogen in liquid stripped out and estimated volumetrically. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta P/bar = \pm 0.2; \ \delta x_{H_2} =$ ±2%. (estimated by compiler). REFERENCES:

## COMPONENTS: 1. Hydrogen, H₂; [1333-74-0] 2. Benzene, C₆H₆; [71-43-2] VARIABLES: Pressure ORIGINAL MEASUREMENTS: Krichevskii, I. R.; Efremova, G. D. Zhur. Fiz. Khim. 1948, 22, 1116-25. C. L. Young

### EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of hydrogen in liquid, "H ₂
288.15	50.1 99.1 199 235 242 285 298 393	0.0114 0.0228 0.0436 0.0509 0.0520 0.0608 0.0642 0.0851
	435 460	0.0904 0.0969
	493	0.102

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Pressure measured with Bourdon gauge. Sample of liquid analysed by separating the two components, weighing the benzene and estimating the hydrogen volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Dried.
- Dried and purified by fractional crystallisation; final purity 99.65 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/bar = \pm 0.35%;$ 

 $\delta x_{\rm H_2} = \pm 0.5\%$ 

COMPONE	ENTS:			ORIGINAL MEA	ASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]				ł .		odorovich, V.P.;	
_				Brestkin,	A.P.; A	rtemovich, V.S.	
2. B	enzene; C ₆ H ₆ ;	[/1-43-2]		Zh. Fiz.	Khim. <u>194</u>	<u>8</u> , 22, 834-845.	
VARIABI	LES:			PREPARED BY	PREPARED BY:		
Temperature, pressure				C.L. Young			
EXPERI	MENTAL VALUES:			l			
T/K	P/atm	P/MPa		olubility, / cm ³ g-1	in liqui	ction of hydrogen d in vapour,	
298	250	25.3		18.3	x _{H2}	y _{H2} 0.9984	
1	500	50.7	3	36.9	0.114	0.9982	
323	1000 250	101.3 25.3	Ž	75.0 20.8	0.207 0.067	0.9976 0.9980	
	500 1000	50.7 101.3		12.0 35.0	0.127 0.229	0.9964 0.9948	
	2000	202.7	17	72.0	0.375	0.9920	
343	3000 250	304.0 25.3	262.5 23.5		0.461 0.076	0.9888 0.9929	
	500 1000	50.7 101.3		17.5 96.5	0.142 0.252	0.9939 0.9921	
1	2000	202.7	19	95.0	0.406	0.9878	
373	3000 250	304.0 25.3	300.0 28.5		0.511 0.090	0.9830 0.9844	
	500 1000	50.7 101.3		59.0	0.170	0.9861	
	2000	202.7		25.0 54.0	0.303 0.480	0.9858 0.9764	
423	3000 250	304.0 25.3		20.0 2.5	0.594 0.129	0.9668 0.9505	
	500	50.7	8	37.5	0.234	0.9588	
	1000 2000	101.3 202.7		30.0 32.0	0.385 0.571	0.9528 0.9230	
+ Vo:	lume of hydrogen nzene.	, reduced to	273k	and 101.3	kPa, diss	olved unit mass of	
METRICO	,		ILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:				SOURCE AND PURITY OF MATERIALS:			
Single	e pass flow metho	od		No detail	s availab	le	
	,						
				ESTIMATED E	RROR:		
1						+	
			$\delta T/K = \frac{1}{2}0.2$ ; $\delta x_{H_2}$ , $\delta y_{H_2} = \frac{1}{2}4$ % estimated by compiler				
			REFERENCES:				

COMPONENTS:				ORIGINAL MEASUREMENTS:			
1. Hydrogen; H ₂ ; [1333-74-0]			Connolly, J. F. J. Chem. Phys.				
2. Benzene; C ₆ H ₆ ; [71-43-2]			<u>1962</u> , 30	6, 2897-2	2904.		
VARIABLES	3:			PREPARED	BY:		
Temperature, pressure			C. L. Young				
EXPERIMEN	TAL VALUES:			· · · · · · · · · · · · · · · · · · ·		Mole fra	
T/K	P/bar i	of hydroin liquid, $x_{ m H_2}$	ogen in gas, ^y H ₂	T/K	P/bar	of hydre in liquid,  **H ₂	
400.15	22.24		0.6345	400.15	22.42	0.01207	0 2002
433.15	20.94 32.38 52.12 90.18 115.11	0.00890 0.01615 0.02846 0.05145 0.06601	0.6147 0.7376 0.8285 0.8897 0.9081	483.15	32.42 40.97 57.99 95.77 178.03	0.02136 0.03605 0.06764 0.13175	0.3902 0.4921 0.6147 0.7376 0.8285
443.15	19.00 25.88 40.30 65.79 117.13	0.00715 0.01182 0.02149 0.03822 0.07053	0.4921 0.6147 0.7376 0.8285 0.8897	493.15 503.15	38.72 49.37 70.95 120.78 46.24	0.01825 0.02824 0.04811 0.09212 0.02425	0.3902 0.4921 0.6147 0.7376 0.3902
453.15	152.19 23.13 31.80 49.99 83.15	0.09159 0.00938 0.01562 0.02853 0.05139	0.9081 0.4921 0.6147 0.7376 0.8285	513.15	59.70 87.49 155.94 37.21 55.51	0.03779 0.06510 0.12863 0.01253 0.03282	0.4921 0.6147 0.7376 0.2027 0.3902
463.15	153.71 22.47 28.07 38.89	0.09734 0.00801 0.01233 0.02061	0.8897 0.3902 0.4921 0.6147	523.15	72.67 109.53 35.83 43.80	0.05147 0.09030 0.00741 0.01725	0.4921 0.6147 0.0998 0.2027
473.15	61.91 105.58 33.94 47.46 76.80 135.78	0.03787 0.06937 0.01621 0.02718 0.05042 0.09478	0.7376 0.8285 0.4921 0.6147 0.7376 0.8285	533.15	86.66 141.96 41.58 82.67 114.70	0.06839 0.13163 0.01041 0.06602 0.10802	0.4921 0.6147 0.0998 0.3902 0.4921
				INFORMATIO	IN .		
METHOD //	APPARATUS/	PROCEDURE:				F MATERIALS.	
METHOD /APPARATUS/PROCEDURE:  Lime-glass capillary in which mixture could be pressurized over mercury.  Details in refs. 1 and 2. Dew point and bubble point observed visually.			SOURCE AND PURITY OF MATERIALS:  No details given.				
			Both substances thought to be better than 99.9 mole per cent.				
-							
				ESTIMATED δT/K = ±		P/bar = ±0.1	per cent;
				$\delta x_{\rm H_2} = \pm$		$\delta y_{\rm H_2} = \pm 0$ . ed by compil	
			İ		S: olly, J.	F.; Kandali 1960, 3, 46	c, G. A.
					11	<b>.</b> 7.1	17. • 7-

2. Connolly, J. F. Phys. Fluids 1961, 4, 1494.

### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Thompson, R. E.; Edmister, W. C. Am. Inst. Chem. Engnrs. J. Benzene: C₆H₆: [71-43-2] 1965, 11, 457-461. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction Mole fraction of hydrogen of hydrogen T/K P/bar in liquid, in vapor, T/K P/bar in liquid, in vapor, $x_{\rm H_2}$ $y_{\rm H_2}$ $x_{\rm H_2}$ $y_{\rm H_2}$ 338.7 5.25 0.00166 0.875 394.3 13.86 0.00536 0.753 13.40 0.9500 34.43 0.0153 0.897 0.0117 0.9797 69.15 0.9443 34.69 0.0321 69.15 0.9429 34.68 0.9802 0.0238 0.0541 70.74 0.9889 117.3 0.9621 0.9617 70.74 0.9887 117.3 117.7 0.0389 0.99150 206.8 0.0937 0.9732 117.7 0.99157 206.8 0.9736 172.9 0.0536 0.99321 413.3 0.167 0.9792 275.8 0.0812 0.99425 688.3 0.243 0.9820 0.708 0.794 0.99503 482.5 0.131 433.1 29.45 0.0144 689.3 0.176 0.99494 41.49 0.0214 0.180 0.0291 689.3 0.99557 53.64 0.833 394.3 6.69 0.00186 0.514 90.25 0.0506 0.890

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Equilibrium cell fitted with glass fiber packing and grooved cone to assist equilibrium being established. Pressure measured with dead weight tester and temperature with thermocouple. Sample analysed by freezing out hydrocarbon and gas measured Volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.8 mole per cent.
- Phillips Petroleum sample, purity 99.94 mole per cent or better.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ ;  $\delta P/bar = \pm 0.1$ %;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 3$ % (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Benzene; C₆H₆; [71-43-2]

### ORIGINAL MEASUREMENTS:

Brainard, A. J.; Williams, G. B.

Am. Inst. Chem. Engnrs. J.

1967, 13, 60-69.

### VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

т/к	P/bar	Mole fraction of in liquid,  **H2	hydrogen in vapor, ^y H ₂
366.48 422.04	77.91 33.16 139.89 36.68	0.0332 0.0142 0.0785 0.0200	0.977 0.956 0.949 0.851

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

Stirred equilibrium cell. Pressure measured with Bourdon gauge. Analysis of samples carried out by expanding into an expansion cylinder and freezing out the hydrocarbon; hydrogen measured volumetrically and then hydrocarbon estimated volumetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Matheson ultrapure sample, purity better than 99.998 mole per cent.
- Phillips Petroleum sample, purity 99.89 mole per cent; major impurity toluene.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3; \quad \delta P/bar = \pm 0.15;$   $\delta x_{\rm H_2}, \quad \delta y_{\rm H_2} = \pm 1.0 \%$  (estimated by compiler).

1. Hydrogen; H.; [1333-74-0]

2. Methylbenzene; C7H8; [108-88-3]

### EVALUATOR:

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

August 1980

### CRITICAL EVALUATION:

This system has been studied at elevated pressures by Ipatiev and Levina (1) and more recently by Simnick et al. (2). The data of Ipatiev and Levina (1) cover the temperature range 208 K to 573 K and pressures up to 29 MPa (although the data at any one temperature are not extensive) whereas that of Simnick et al. (2) cover the temperature range range 461 K to 575 K and pressures up to 25 MPa. There is broad agreement between these two sets of data although Ipatiev and Levina (1) mole fraction solubility data are, in general, slightly smaller than those of Simnick et al. (2).

The gas-liquid critical temperature of methylbenzene is 591.8 K (3) and it is probable that this system exhibits the phenomenon of gas-gas immiscibility (4) above this temperature. Furthermore, methylbenzene may thermal decompose (5) or react with hydrogen at temperatures above 550 K and workers investigating this system should be aware of these possibilities.

The data of Simnick et al. (2) are classified as tentative.

### References:

- Ipatiev, V. V.; Levina, M. I. Zhur. Fiz. Khim. 1935, 6, 632.
- 2. Simnick, J. J.; Sebastian, H. M.; Lin, H. M.; Chao, K.-C. J. Chem. Engng. Data 1978, 23, 339.
- З. Ambrose, D. "Vapour-Liquid Critical Properties", 1980, N.P.L. Rep. 107. Teddington, U.K.
- Schneider, G. M. Chem. Soc. Spec. Per. Report No. 22, Vol. 2, ed. McGlashan, M. L., Chapter 4, 1978.
- 5. Johns, I. B.; McElhill, E. A.; Smith, J. O. J. Chem. Engng. Data 1962, 7, 277.

#### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Ipatiev, V.V.; Levina, M.I. 2. Zhur. Fiz. Khim. 1935, 6,632-9. Methylbenzene, (toluene); C₇H₈; [108-88-3] VARIABLES: PREPARED BY: Temperature, pressure. C.L. Young EXPERIMENTAL VALUES: Mole fraction of hydrogen in liquid, $x_{\rm H_2}$ T/K P/bar 49.0 0.00629 208.15 98.1 0.01251 0.01435 217.15 98.1 248.15 49.0 0.01010 98.1 0.01984 0.01259 273.15 49.0 0.02456 98.1 298.15 49.0 0.01539 98.1 0.02911 294.2 0.08077 373.15 49.0 0.02094 98.1 0.04140 423.15 49.0 0.02651 98.1 0.05265 0.1076 196.1 0.1579 294.2 473.15 49.0 0.02977 98.1 0.06643 196.1 0.1382 294.2 0.1964 513.15 49.0 0.03155 98.1 0.07717 196.1 0.1661 294.2 0.2388 573.15 98.1 0.09311 AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static equilibrium cell. Hydrocarbon | 1. No details given. added to cell then pressurized at 2. Washed with water and sodium temperature of measurement. After hydroxide solution. Dried and 1-2 hours liquid samples removed. distilled. Boiling pt. 110.0 °C.; Density at 15 °C = 0.8655. Analysed by stripping out hydrogen at low pressure. ESTIMATED ERROR: $\delta T/K = \pm 0.1$ up to 250°C, $\pm 1.0$ at 300°C; $\delta x_{\rm H_2} = \pm 2\%$ . (estimated by compiler). REFERENCES:

- 1. Hydrogen; H₂; [1333-74-0]
- Methylbenzene, (toluene);
  C₇H₈; [108-88-3]

#### ORIGINAL MEASUREMENTS:

Simnick, J.J.; Sebastian, H.M.; Lin, H.M.; Chao, K.-C.

J. Chem. Engng. Data. <u>1978</u>, 23, 339-340.

# VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:			
T/K	P/bar	Mole fraction	of hydrogen
_,	-,-	in liquid, x _{H2}	in gas,y _{H2}
		H ₂	3 10 H ₂
461.83	20.3	0.0113	0.6674
102102	30.3	0.0187	0.7678
	50.4	0.0342	0.8425
	101.1	0.0704	0.9064
	151.9	0.1023	0.9284
	202.9	0.1331	0.9374
	253.7	0.1645	0.9430
502.15	20.2	0.0082	0.3491
44-1-2	30.3	0.0181	0.5356
	50.7	0.0375	0.6863
	100.6	0.0812	0.8182
·	152.2	0.1227	0.8645
	203.0	0.1649	0.8831
	252.6	0.2015	0.8905
542.15	30.4	0.0120	0.2100
	51.1	0.0385	0.4555
	100.8	0.0977	0.6668
	151.6	0.1545	0.7357
	202.8	0.2088	0.7789
	253.1	0.2581	0.7986
575.15	50.2	0.0332	0.2410
	101.2	0.1196	0.4824
	151.7	0.2005	0.5527
	205.1	0.2844	0.5890
	253.5	0.3935	0.6145

#### AUXILIARY INFORMATION

# METHOD: /APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separate under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Air Products, minimum purity 99.95 mole per cent.
- Fischer Scientific Co. sample, designated high purity reagent grade, no impurity detected by GC.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.5$ %;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 0.001$  (estimated by compiler).

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Methylbenzene, (Toluene); C₇H₈; [108-88-3] VARIABLES: Temperature, pressure ORIGINAL MEASUREMENTS: Laugier, S.; Richon, D.; Renon, H. J. Chem. Engng. Data. 1980, 25, 274-276. PREPARED BY: C.L. Young

PERIMENTAL VALI	JES:	Mole fraction o	of Hydrogen
T/K	P/MPa	in liquid, $x_{\rm H_2}$	in vapor, y _{H2}
269.0	3.46	0.019	-
	6.23	-	0.521
	7.60	0.070	-
	10.30		0.668
	12.90	0.128	-
	14.05	-	0.718
	15.35	-	0.733
	16.20	0.172	_
	22.25	-	0.789
	22.30	0.232	-
	28.10	<del>-</del>	0.796
	28.40	0.289	_
	32.30	0.327	-
	32.70	-	0.792
295.0	6.45	<del>-</del>	0.385
	7.40	0.074	_
	10.10	-	0.527
	13.00	0.162	_
	18.05	0.237	-
	18.40	-	0.648
	20.00	<del>-</del>	0.665
	22.95	0.311	_
	23.00	-	0.673
	23.90	<del></del>	0.686
	25.70	-	0.689
	28.45	0.415	<del>-</del>
	28.90	<del>-</del>	0.675
	30.80	0.514	

#### AUXILIARY INFORMATION

#### METHOD APPARATUS / PROCEDURE:

Static equilibrium cell fitted with sampling valves which removed samples of  $10^{-9}$  m³. Samples analysed by gas chromatography. Temperature measured using thermocouples and pressure measured using pressure transducer calibrated against a dead weight gauge.

#### SOURCE AND PURITY OF MATERIALS:

- L'Air Liquide sample, purity better than 99.95 mole per cent.
- 2, Merck sample, guaranteed purity 99.5 mole per cent or better.

ESTIMATED ERROR:  $\delta T/K = \pm 0.2$ ;  $\delta P/MPa = \pm 0.04$ ;  $\delta x_{H_2} = \pm 0.009$ ;  $\delta y_{H_2} = \pm 0.012$ .

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 1,3-Dimethylbenzene;  $C_8H_{10}$ ; [108-38-3]

#### **EVALUATOR:**

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

#### CRITICAL EVALUATION:

This system has been investigated at elevated pressures by Ipatiev and Levina (1), Sattler (2) and more recently by Simnick  $et\ al$ . (3). The data of Ipatiev and Levina (1) cover the temperature range 298 K to 513 K at pressures up to 20 MPa. The data of Sattler (2) are restricted to 308 K and pressures near 15 MPa whereas the data of Simnick  $et\ al$ . (3) are estensive and cover the temperature range 462 K to 582 K and pressures up to 25 MPa. The data of Simnick  $et\ al$ . (3) are considered the most reliable and are classified as tentative. The mole fraction solubility data of Ipatiev and Levina are, in general, smaller than those inter-Polated from the data of Simnick  $et\ al$ . (3).

The gas-liquid critical temperature of 1,3-dimethylbenzene is 617 K (4) and above this temperature this system may exhibit the Phenomenon of gas-gas immiscibility (5). 1,3-Dimethylbenzene also Probably decomposes slowly above about 550 K and/or reacts with hydrogen. Workers investigating this system at high temperatures should be aware of the existence of possible reactions of "unusual" phase behaviour.

# References:

- 1. Ipatiev, V. V.; Levina, M. I. Zhur. Fiz. Khim. 1935, 6, 632.
- 2. Sattler, H. Z. Tech. Physik. 1940, 21, 410.
- 3. Simnick, J. J.; Sebastian, H. M.; Lin, H. M.; Chao, K.-C.
  J. Chem. Thermodyn. 1979, 11, 531.
- 4. Ambrose, D. "Vapour-Liquid Critical Properties", 1980, N.P.L. Rep. 107. Teddington, U.K.
- Schneider, G. M. Chem. Soc. Spec. Per. Report No. 22, Vol. 2, ed. McGlashan, M. L., Chapter 4, 1978.

ORIGINAL MEASUREMENTS:

<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>1,3 - Dimethylbenzene, (m-xylene)</li> </ol>		Ipatiev, V.V.; Levina, M.I.  Zhur. Fiz. Khim. 1935, 6, 632-9	
C ₈ H ₁₀ ; [108-38-3]			
VARIABLES: Temperature, pr	essure	PREPARED BY: C.L. Young	
EXPERIMENTAL VALUES:	P/bar	Mole fraction of	
T/A	P/par	hydrogen in liquid,  xH2	
298.15	49.0 98.1 294.2	0.01678 0.03322 0.08950	
373.15	49.0 98.1	0.02360 0.04439	
423.15	49.0 98.1 196.1	0.02451 0.05593 0.1116	
473.15	49.0 98.1 196.1	0.03300 0.06926 0.1360	
513.15	49.0 98.1 196.1	0.03917 0.08500 0.1673	
313.13	98.1	0.08500	

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Hydrocarbon added to cell then pressurized at temperature of measurement. After 1-2 hours liquid samples removed. Analysed by stripping out hydrogen at low pressure.

# SOURCE AND PURITY OF MATERIALS:

- No details given.
- Meta isomer distilled from mixture of isomers, sulfonated and steam distilled. Dried and then fractionally distilled. Boiling pt. 138.5°C. Density at 15°C = 0.8590.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta x_{H_2} = \pm 2\%$ . (estimated by compiler).

COMPONENTS	3:			ORIGINAL MEASU	REMENTS:		
1. Hydr	ogen; H ₂ ; [	[1333-74-0]		Sattler, H.;			
<pre>2. 1,3-Dimethylbenzene, (m-Xylene);     C₈H₁₀; [108-38-3]</pre>		Z. Tech. Physik, <u>1940</u> , 21,410-413					
VARIABLES	:			PREPARED BY:			
Temperature, pressure			e	C.L. Young	r		
EXPERIMEN	TAL VALUES:						
	T/K	P/bar	Kuenen	Coefficient S	Mole fraction of Hydrogen in liquid, $^{x}{\rm H}_{2}$		
30	08.15	147.8 148.3 149.7 152.7	1 1	1.52 1.61 1.65 1.87	0.05178 0.05216 0.05233 0.05326		
			AUXILIARY	INFORMATION			
METHOD: /	APPARATUS/P	ROCEDURE:	<del></del>	SOURCE AND PUR	ITY OF MATERIALS:		
Rocking attachm charged of solv gravime liquid	bomb with ent. Solve into evacu ent in liqu trically an stripped ou rically. D	liquid samp nt and hydr ated cell. id sample e d hydrogen	Amount estimated in	No detai	ls given.		
				1	R: ; $\delta P/\text{bar} = \pm 0.2$ ; (estimated by compiler).		
				REFERENCES:			

#### 422 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Simnick, J. J.; Sebastian, H. M.; 1. Hydrogen; H₂; [1333-74-0] Lin, H. M.; Chao K.-C. 2. 1,3-Dimethylbenzene, (m-xylene); $C_8H_{10}$ ; [108-38-3] J. Chem. Thermodyn., 1979, 11, 531-7. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/MPa in liquid, $x_{\rm H_2}$ in vapor, $y_{\rm H_2}$ 462.4 0.3193* 0.0134 0.8264 1.986 3.04 0.0217 0.8809 5.08 0.0373 0.9227 10.07 0.0735 0.9550 15.23 0.1092 0.9644 20.21 0.1416 0.9698 0.1724 25.13 0.9720 502.3 0.6960* 1.996 0.0131 0.6148 3.04 0.0231 0.7353

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

542.6

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Details in ref. (1).

5.10

10.09

15.20

20.34

25.26

1.321*

1.986

3.05

5.07 10.07

15.27

20.28

25.44

#### SOURCE AND PURITY OF MATERIALS:

0.0420

0.0856

0.1309

0.1676 0.2041

0.0091

0.0221

0.0465

0.1034

0.1550

0.2042

0.2494

- 1. Air Products sample, purity 99.95 mole per cent.
- Aldrich Chemical Co. gold label grade, purity 99 mole per cent.

0.8332

0.9087

0.9264

0.9409

0.9477

0.2870

0.4842

0.6659

0.7974

0.8562

0.8769

0.8899

#### ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.5; \ \delta \text{P/MPa} = \pm 0.02;$   $\delta x_{\text{H}_2}, \ \delta y_{\text{H}_2} = \pm 1 \text{% (estimated by compiler)}$ 

#### REFERENCES:

 Sebastian, H. M.; Simnick, J. J.; Lin H-M.; Chao K.-C.
 J. Chem. Engng. Data, 1978, 23, 305-8.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
	H ₂ ; [1333-74-0] hylbenzene, (m-xylene); 108-38-3] contd.	Simnick, J. J.; Sebastian, H. M.; Lin H. M.; Chao KC. J. Chem. Thermodyn., 1979, 11, 531-7.		
VARIABLES:		PREPARED BY:		
Temperature, pressure		C. L. Young		
EXPERIMENTAL VAL	UES:	<u> </u>		
T/K	P/MPa	Mole fraction of hydrogen in liquid, $x_{\rm H_2}$ in vapor, $y_{\rm H_2}$		
582.1	2.269* 3.04 5.01 10.09 15.13 20.33 25.44	0 0 0.0142 0.1741 0.0470 0.3901 0.1257 0.6147 0.1959 0.7077 0.2560 0.7545 0.3241 0.7851		

^{*} Vapor pressure of m-xylene.

# 424 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H2; [1333-74-0] Ipatiev, V.V.; Levina, M.I. 1,3,5-Trimethylbenzene, 2. Zhur, Fiz. Khim. 1935, 6, 632-9. (mesitylene); $C_9H_{12}$ ; [108-67-8] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young EXPERIMENTAL VALUES: Mole fraction of T/K P/bar hydrogen in liquid, $x_{\rm H_2}$ 0.01508 298.15 49.0 98.1 0.03390 294.1 0.08968 423.15 98.1 0.06002 473.15 98.1 0.07403 513.15 98.1 0.08808 Calculated by compiler

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Hydrocarbon added to cell then pressurized at temperature of measurement. After 1-2 hours liquid sample removed. Analysed by stripping out hydrogen at low pressure.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Sample made from acetone using catalyst and hydrochloric acid at high pressure. Purified. Boiling pt. 135.0°C, density = 0.7783 at 15°C.

# ESTIMATED ERROR:

 $\delta x_{\rm H_2} = \pm 2 \%.$  $\delta T/K = \pm 0.1;$ (estimated by compiler)

# 

#### EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of hydrogen in liquid, $^{x}{\rm H}_{2}$
343.15	40.5	0.020
	101.3 202.6	0.047 0.089
	304.0	0.131
413.15	40.5	0.025
	101.3	0.062
	202.6 304.0	0.119 0.174
488.15	40.5	0.033
	101.3	0.094
	202.6	0.180
	304.0	0.287

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping out gas and measuring volume evolved. Remaining liquid estimated gravimetrically.

#### SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 1.0$ ;  $\delta P/bar = \pm 0.5$ ;  $\delta x_{H_2} = \pm 3$ % (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]

#### ORIGINAL MEASUREMENTS:

Simnick, J. J.; Lawson, C. C.; Lin, H. M.; Chao, K. C. Am. Inst. Chem. Engnrs. J. 1977, 23, 469-476.

#### VARIABLES:

Temperature, pressure

#### PREPARED BY:

C. L. Young

l			<b>I</b>	
EXPERIMENT.	AL VALUES:	Molo function	- F h	
T/K	P/bar	Mole fraction of in liquid,		
1/10	1 / Dal	in riquid,	in vapor,	
- ·· · · · · · · · · · · · · · · · · ·		ж _{Н 2}	^у н ₂	
462.75	20.3	0.0118	0.9652	
	30.4	0.0176	0.9748	
	50.7	0.0297	0.9828	
	101.3	0.0571	0.9897	
	152.0	0.0823	0.9927	
	202.6	0.1051	0.990	
	253.3	0.1289	0.9948	
541.85	20.3	0.0143	0.8028	
	30.4	0.0221	0.8676	
	50.7	0.0373	0.9155	
	101.3	0.0732	0.9538	
	152.0	0.1046	0.9657	
1	202.6	0.1373	0.9714	
	253.3	0.1640	0.9748	
621.75	50.7	0.0452	0.7066	
	101.3	0.0925	0.8346	
	152.0	0.1390	0.8827	
l	202.6	0.1884	0.9038	
	253.3	0.2314	0.9167	
662.25	50.7	0.0482	0.4810	
	101.3	0.1170	0.7008	
İ	152.0	0.1760	0.7808	
	202.6	0.2303	0.8174	
	253.3	0.2824	0.8399	
	253.3	0.2824	0.8399	

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Air products sample, stated purity 99.95 mole per cent.
- Aldrich Chemical Co., purity about 99 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ ;  $\delta P/bar = \pm 0.1$ % or  $\pm 0.3$  whichever is the greater;

$$\delta x_{\rm H_2}, \ \delta y_{\rm H_2} = \pm 1\%.$$

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Sokolov, B. I.; Polyakov, A. A. Zhur. Prikl. Khim. 1977, 50, 1403-5.
2. 1-Methylnaphthalene; C ₁₁ H ₁₀ ; [90-12-0]	
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young

#### EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of hydrogen in liquid, "H ₂
220 15	40 5	0.010
328.15	40.5 101.3	0.010 0.023
	202.6	0.046
	304.0	0.071
393.15	40.5	0.014
	101.3	0.029
	202.6	0.057
472 75	304.0	0.089
473.15	40.5	0.019
	101.3	0.045
	202.6	0.090 0.132
	304.0	V.132

#### AUXILIARY INFORMATION

METHOD / APPARATUS / PROCEDURE:	
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Static equilibrium cell with stirrer. Solvent placed in cell then pressurized with hydrogen at room temperature, heated to experimental temperature and equilibrated. Liquid samples removed and cooled; analysed by stripping out gas and measuring volume evolved. Remaining liquid estimated gravimetrically.

# SOURCE AND PURITY OF MATERIALS:

1 and 2 "Pure" grade samples.

## ESTIMATED ERROR:

 $\delta T/K = \pm 1.0; \quad \delta P/\text{bar} = \pm 0.5;$   $\delta x_{\text{H}_2} = \pm 3 \text{% (estimated by compiler)}.$ 

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. 1-Methylnaphthalene; C₁₁H₁₀; [90-12-0] VARIABLES: Temperature, pressure ORIGINAL MEASUREMENTS: Yao, J.; Sebastian, H.M.; Lin, H.M.; Chao, K.C. PREPARED BY: C.L. Young

#### EXPERIMENTAL VALUES:

T/K	P/atm	P/MPa	Mole fraction o in liquid, x _{H2}	f hydrogen in gas,y _{H2}
462.15	0.250	0.0253	0.0	0.0
	20	2.03	0.0103	0.9863
	30	3.04	0.0153	0.9906
	50	5.07	0.0250	0.9939
	100	10.13	0.0479	0.9965
	150	15.20	0.0692	0.9974
	200	20.27	0.0887	0.9978
	250	25.33	0.1060	0.9980
541.85	1.68	0.170	0.0	0.0
	20	2.03	0.0127	0.9007
	30	3.04	0.0202	0.9360
	50	5.07	0.0342	0.9596
	100	10.13	0.0641	0.9778
	150	15.20	0.0931	0.9838
	200	20.27	0.1191	0.9867
	250	25.33	0.1452	0.9883
621.75	6.34	0.642	0.0	0.0
	20	2.03	0.0132	0.6153
	30	3.04	0.0225	0.7384
	50	5.07	0.0406	0.8368
	100	10.13	0.0814	0.9113
	150	15.20	0.1180	0.9350

#### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Flow apparatus with both liquid and gaseous components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge.

#### SOURCE AND PURITY OF MATERIALS:

- Air Products sample, purity 99.95 mole per cent or better.
- Distilled, purity 98 mole per cent.

#### ESTIMATED ERROR:

 $\begin{array}{lll} \delta \mathrm{T/K} &= \pm 0.05 ^{\circ} \mathrm{C}; & \delta P/\mathrm{MPa} &= \pm 1 \% & \mathrm{or} \\ \pm 0.02 & \mathrm{(whichever is greater)}; \\ \delta x_{\mathrm{H}_2}, & \delta y_{\mathrm{H}_2} &= \pm 0.5 \% \end{array}$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. l-Methylnaphthalene;  $C_{11}H_{10}$ ; [90-12-0]

# ORIGINAL MEASUREMENTS:

Yao, J.; Sebastian, H.M.; Lin, H.M.; Chao, K.C. Fluid Phase Equilibrium, 1978, 1, 293-304

#### EXPERIMENTAL VALUES:

T/K	P/atm	P/MPa	Mole fraction in liquid, $x_{\rm H_2}$	of hydrogen in gas,y _{H2}
621.75	150	20.27	0.1564	0.9481
	250	25.33	0.1923	0.9541
701.65	17.33	1.756	0.0	0.0
	30	3.04	0.0184	0.3084
	50	5.07	0.0459	0.5169
	100	10.13	0.1051	0.7111
	150	15.20	0.1615	0.7881
	200	20.27	0.2126	0.8263
	250	25.33	0.2590	0.8500

COMPONENTS:	COMPONENTS:				
<ol> <li>Hydrogen; F</li> <li>1-Methylnar</li> <li>C₁₁H₁₀; [90]</li> </ol>		·0]	Lin, H.M.; Sebastian, H.M.; Chao, K.C.  Fluid Phase Equilibria, 1980, 4, 321		
VARIABLES:	ssure		PREPARED BY: C.L. Young		
EXPERIMENTAL VALUES	S:		Mole fraction	of hydrogen	
т/к	P/atm	P/MPa	in liquid,  **H ₂		
730.05	50.2 76.2 96.4 126.5 151.0 176.2 199.8 248.7 274.2	5.09 7.72 9.77 12.82 15.30 17.85 20.24 25.20 27.78	0.0431 0.0842 0.1149 0.1593 0.1916 0.2252 0.2604 0.3070 0.3362	0.3717 0.5350 0.6103 0.6806 0.7229 0.7478 0.7703 0.7850 0.7954	

#### AUXILIARY INFORMATION

#### METHOD APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

No details given.

#### ESTIMATED ERROR:

 $\begin{array}{l} \delta \text{T/K} = \pm 0.3; \; \delta P/\text{MPa} = \pm 0.02; \\ \delta x_{\text{H}_2}, \; \delta y_{\text{H}_2} < \text{1.0%} \\ \text{(estimated by compiler).} \end{array}$ 

# REFERENCES:

Simnick, J.J.; Lawson, C.C.;
 Lin, H.M.; Chao, K.C.

Am. Inst. Chem. Engnrs. J. 1977, 23, 469.

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				J			
EXPERIMEN	TAL VALUE	S:					
T/K	P/bar	Mole fra of hydr		T/K	P/bar	Mole fra of hydr in liquid, $x_{H_2}$	ogen
				<del> </del>			<del></del>
462.75	20.3	0.0123	0.9903	621.75	20.3	0.0184	0.7362
1	30.4	0.0183	0.9935		30.4	0.0296	0.8144
	50.7	0.0300	0.9963		50.7	0.0516	0.8825
l	101.3	0.0591	0.9980		101.3	0.0985	0.9362
	152.0	0.0830	0.9985		152.0	0.1450	0.9533
	202.7	0.1055	0.9988		202.7	0.1880	0.9615
~	253.3	0.1240	0.9989		253.3	0.2272	0.9675
541.85	20.3	0.0159	0.9390	701.65	30.4	0.0306	0.4497
	30.4	0.0244	0.9580		50.7	0.0630	0.6360
	50.7	0.0408	0.9741		101.3	0.1380	0.7881
	101.3	0.0785	0.9861		152.0	0.2030	0.8469
l	152.0	0.1105	0.9895		202.7	0.2577	0.8799
ļ	202.7	0.1416	0.9912		253.3	0.3056	0.8964
	253.3	0.1724	0.9921				

# AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrially and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Air Products sample with minimum purity of 99.95 mole per cent.
- Aldrich Chemical Co. sample purified by vacuum distillation, purity better than 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.7; \quad \delta P/\text{bar} = \pm 0.3;$   $\delta x_{\text{H}_2}, \quad \delta y_{\text{H}_2} = \pm 1 \text{% (estimated by compiler)}.$ 

# REFERENCES:

Simnick, J. J.; Lawson, C. C.;
 Lin, H.-M.; Chao, K.-C.
 Am. Inst. Chem. Engnrs. J. 1977.
 23, 469.

ORIGINAL MEASUREMENTS:

<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>9,10-Dihydrophenanthrene; C₁₄H₁₂; [776-35-2]</li> <li>VARIABLES: Temperature, pressure</li> </ol>		Lin, H.M.;  J. Chem. En  PREPARED BY:	Sebastian, H.M.; Simnick, J.J. Lin, H.M.; Chao, K-C.  J. Chem. Eng. Data. 1979, 24,343-5.  PREPARED BY:  C.L. Young		
EXPERIMENTAL VALUES:	P/MPa	Mole fractio in liquid, $^{x}{ m H}_{2}$	on of hydrogen in vapor, ${}^{y}_{\mathrm{H}_{2}}$		
461.45	1.968 3.071 5.022 10.11 15.23 20.37 25.54	0.0093 0.0141 0.0231 0.0446 0.0649 0.0843 0.1032	0.99776 0.99860 0.99920 0.99957 0.99964 0.99973		
542.15	2.038 3.037 5.030 10.06 15.21 20.28 25.16	0.0126 0.0191 0.0308 0.0595 0.0868 0.1139	0.9796 0.9864 0.9916 0.9953 0.9967 0.9971		
622.85	2.044 3.027 4.774 10.18 15.21 20.54 25.40	0.0156 0.0233 0.0375 0.0769 0.1121 0.1462 0.1720	0.8992 0.9306 0.9548 0.9769 0.9834 0.9867 0.9888		
METHOD/APPARATUS/PROCEDI		LIARY INFORMATION	TY OF MATERIALS:		

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Details in ref. (1).

- 1. Airco sample, purity 99.95 mole per cent or better.
- Sample prepared by zone refining of Aldrich sample.
   Further purified by distillation under nitrogen at reduced pressure. Final purity better

than 99 mole per cent.

ESTIMATED ERROR:  $\delta T/K = \pm 0.5$ ;  $\delta P/MPa = \pm 0.02$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 1$ % (at 3 lower temperatures)  $\pm 2$ % (at 703.05K) (estimated by compiler).

#### REFERENCES:

 Sebastian, H.M.; Simnick, J.J. Lin, H.M.; Chao, K-C.
 J. Chem. Engng. Data. 1978, 23, 305-8.

- Hydrogen; H₂; [1338-74-0]
- 9,10- Dihydrophenanthrene;
   C₁₄H₁₂; [776-35-2]

#### ORIGINAL MEASUREMENTS:

Sebastian, H.M.; Simnick, J.J. Lin, H-M.; Chao, K-C.

J. Chem. Eng. Data. 1979, 24, 343-5.

## EXPERIMENTAL VALUES:

т/к	P/MPa	Mole fraction in liquid, "H ₂	of hydrogen in vapor, y _{H2}
703.05+	2.021	0.0161	0.6500
	3.024	0.0280	0.7597
	5.037	0.0492	0.8497
	10.15	0.0984	0.9191
	15.27	0.1446	0.9443
	20.34	0.1815	0.9575
	25.27	0.2184	0.9629

⁺ Some conversion of dihydrophenanthrene to phenanthrene occured at this temperature. The percentage conversion was about 4-5 per cent and this amount was thought to not to alter the results from the true equilibrium conditions substantially.

COMPONENTS:	EVALUATOR:
l. Hydrogen; H ₂ ;	Colin L. Young, Department of Physical Chemistry,
2. Carbon monoxide; CO;	University of Melbourne, Parkville, Victoria 3052,
3. Hydrocarbons	Australia.
	November 1980

#### CRITICAL EVALUATION:

The only study of gas solubility for these systems for which numerical details have been published is that of Trust and Kurata (1) whose data are classified as tentative.

Tyvina and coworkers (2-5) have made extensive measurements for some hydrogen + carbon monoxide + hydrocarbon systems but, in general, report numerical values for gas-liquid critical properties and graphs for gas-liquid equilibria data. These data are not considered further here except for inclusion of the reference and title of papers.

- Trust, D. B.; Kurata, F. Am. Inst. Chem. Engnrs. J. <u>1971</u>, 17, 86-91.
- 2. Tyvina, T. N.; Kharchenko, A. A.; Pryanikova, R. O. Phase-volume relations in the toluene-carbon monoxide-hydrogen system.
  Zh. Prikl. Khim. 1976, 49, 1638-1640 (J. Appl. Chem. USSR 1976, 49, 1665-1667).
- 3. Tyvina, T. N.; Kharchenko, A. A.; Pryanikova, R. O. Phase and volume relations in the propylene-carbon monoxide-hydrogen system. Zh. Prikl. Khim. 1976, 49, 1640-1642 (J. Appl. Chem. USSR 1976, 49, 1667-1669).
- 4. Tyvina, T. N.; Kharchenko, A. A.; Pryanikova, R. O. Phase and volume relations in the toluene-propylene-carbon monoxide-hydrogen mixture. Zh. Prikl. Khim. 1977, 50, 186-188
  (J. Appl. Chem. USSR 1977, 50, 186-188).
- 5. Naumova, A. A.; Tyvina, T. N.; Kharchenko, A. A. Phase and volume relations in the system isobutylene-carbon monoxide-hydrogen.
  Zh. Prikl. Khim. 1979, 52, 1416-1419 (J. Appl. Chem. USSR 1979, 52, 1347-1349).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methanol; CH₄O; [67-56-1]

#### **EVALUATOR:**

Colin L. Young, Department of Physical Chemistry, University of Melbourne, Parkville, Victoria 3052,

Australia.

October 1980

#### CRITICAL EVALUATION:

The high pressure solubility of hydrogen in methanol has been studied by a number of workers but it is not possible to recommend any particular set of data. Measurements at 25 °C (298.15 K) have been carried out by Frolich  $et\ al$ . (1) at pressures up to 19 MPa, by Ipat'ev  $et\ al$ . (2) at the pressure of 10.1 MPa and by Krichevskii and Efremova (3) at pressures up to 60 MPa. The isolated value of Ipat'ev  $et\ al$ . (2) is in reasonable agreement with the values of Krichevskii and Efremova (3) but is not considered further in view of its isolated nature. The data of Krichevskii and Efremova (3) are 10-15 per cent higher than those of Frolich  $et\ al$ . (1) but are in reasonable agreement but slightly lower than values given by Michels  $et\ al$ . (4) at 297.55 K. Therefore the values of Frolich  $et\ al$ . (1) are classified as doubtful.

The data of Michels  $et\ al.$  (4) over the temperature range 297 K to 373 K and pressures up to 8.1 MPa are in reasonable agreement with the data of Krichevskii  $et\ al.$  (5) at the temperature of 294 K, 363 K and 413 K and pressures up to 30 MPa and therefore both sets of data and those of Krichevskii and Efremova (3) are classified as tentative.

The data of Yorizane  $et~\alpha l$ . are of low precision and the mole fractions appear to be too large when compared with the data of Michels  $et~\alpha l$ . (4) and the low pressure data of Katayama and Nitta (7).

# References

- Frolich, K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A. Ind. Eng. Chem. 1931, 23, 548.
- Ipat'ev, V. V.; Druzhina-Artemovich, S. I.; Tikhomirova, V. I.
  Zh. Obshchei Khim. 1931, 1, 594.
- Krichevskii, I. R.; Efremova, G. D. Zh. Fiz. Khim. 1951, 25, 577.
- 4. Michels, A.; de Graaff, W.; van der Somme, J. Appl. Sci. Res. 1953, A4, 105-8.
- 5. Krichevskii, I. R.; Zhavoronokov, N. M.; Tsiklis, D. S. Zh. Fiz. Khim. 1937, 9, 317.
- Yorizane, M.; Sadamoto, S.; Masuoka, H.; Eto, Y.
   Kogyo Kagaku Zasshi 1969, 72, 2174-7.
- 7. Katayama, T.; Nitta, T. J. Chem. Engng. Data 1976, 21, 194-6.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methanol, (Methyl alcohol);
   CH₄O; [67-56-1]

# ORIGINAL MEASUREMENTS:

Frolich, P.K.; Tauch, E.J.; Hogan, J.J.; Peer, A.A.

Ind. Eng. Chem. 1931, 23, 548-550.

**VARIABLES:** 

Pressure

PREPARED BY:

C.L. Young

ERIMENTAL VALUI T/K	ES: <i>P/</i> MPa	Solubility*	Mole fraction of hydrogen in liquid, +
1/1	r/mra	SOLUDILLEY	"CH ₄ O
298.15	1.0	0.9	0.0015
	2.0	1.8	0.0030
	3.0	2.55	0.0042
	4.0	3.35	0.0055
	5.0	4.15	0.0069
	6.0	4.9	0.0081
	7.0	5.8	0.0096
	8.0	6.7	0.0110
	9.0	7.5	0.0123
	10.0	8.3	0.0136
	11.0	9.1	0.0149
	12.0	9.9	0.0162
	13.0	10.55	0.0172
	14.0	11.45	0.0187
	15.0	12.25	0.0200
	16.0	13.0	0.0212
	17.0	13.8	0.0225
	18.0	14.5	0.0236
	19.0	15.3	0.0248

- * Data taken from graph in original article. Volume of gas measured at 101.325 kPa and 298.15 K dissolved by unit volume of liquid measured under the same conditions.
- + Calculated by compiler.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for the vapor pressure of the liquid and the solubility of the gas at atmospheric pressure. Details in source.

# SOURCE AND PURITY OF MATERIALS:

Stated that materials were the highest purity available.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta x_{H_2} = \pm 5\%$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Krichevskii, I. R.; Zhavoronokov, N. M.; Tsiklis, T. S.
2. Methanol; CH ₄ O; [67-56-1]	Zh. Fiz. Khim. <u>1937</u> , 9, 317-328.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young

T/K	P/atm	<i>P/</i> MPa	Solubility [#] , S /cm ³ g ⁻¹	Mole fraction* of hydrogen, $^{x}_{\mathrm{H}_{2}}$
294	76	7.7	8.1	0.0114
294	178	18.0	19.5	0.0271
294	179	18.1	19.7	0.0274
294	272	27.6	29.7	0.0407
363	71	7.2	11.1	0.0157
363	74	7.5	11.7	0.0165
363	134	13.6	20.6	0.0286
363	186	18.8	29.2	0.0401
363	300	30.4	46.5	0.0624
413	78	7.9	16.0	0.0186
413	196	19.9	39.9	0.0540
413	281	28.5	57.7	0.0762

[#] measured at 273.15 K and at a pressure of 101.3 kPa.

#### AUXILIARY INFORMATION

# No details available. Numerical data taken from Stephan and Stephan (ref. (1)).

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

# REFERENCES:

1. Stephan, H.; Stephan, T. Solubilities of Inorganic and Organic Compounds, Vol. 1, Pergamon, Oxford, 1963, p.540.

^{*} calculated by compiler.

COMPONENTS:	The second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second second secon		ORIGINAL MEASUREMENTS:
1. Hydroge	en; H ₂ ; [1333-74-0]		Krichevskii, I. R.; Efremova,
1	2,, (2000 / 5 0)		G. D.
2 Methano	ol; CH ₄ O; [67-56-1]		Zh. Fiz. Khim.
z. Rechan	51, ento, [0, 30 1]		1951, 25, 577-583.
			1551, 20, 511 550
ARIABLES:			PREPARED BY:
Pr	essure		C. L. Young
EXPERIMENTAL	VALUES:		
T/K	P/atm	P/MPa	Mole fraction of hydrogen, $x_{ m H_2}$
298.2	48.2	4.88	
	91.7 113	9.29 11.4	0.0142 0.0175
	129	13.1	0.0198
	147	14.9 17.0	0.0227 0.0255
	168 183	18.5	0.0235
	212	21.5	0.0316
	246 260	24.9 26.3	0.0362 0.0374
	292	29.6	0.0411
	424	43.0	0.0555
	437 493	44.3 50.0	0.0581 0.0640
	507 582	51.4 59.0	0.0656 0.0747
	Α	UXILIARY	INFORMATION
METHOD 'APPARA	ATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:
	s available. data taken from Step	han	
and Stepha	an (ref. (1)).		
			ESTIMATED ERROR:
			REFERENCES:
			1. Stephan, H.; Stephan, T.
			Solubilities of Inorganic and
			Solubilities of Inorganic and

Organic Compounds, Vol. 1,
Pergamon, Oxford, 1963, p.541.

COMPONENT	rs:			ORIGINAL	MEASUREME	NTS:	<del></del>
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Methanol; CH₃OH; [67-56-1]</li> </ol>				Somme,	J.	le Graaff, W	N.; van der 105-8.
							·
VARIABLE	S:			PREPARED	BY:		
-	Tempera	ature, pressu	re		C. L. 3	oung?	
	NTAL VALUE	ES: Mole for of hydronic in liquid, $x_{\rm H_2}$		T/K	P/bar	of h	fraction nydrogen , in vapor,
297.55	152 304 405 507 608 811	0.0253 0.0475 0.0594 0.0726 0.0831 0.1058	- - - -	348.15 372.45	405 507 608 811 101 122	0.0917	0.9931 
322.55	304 507 811	0.1038 0.0519 0.0798 0.1224	- - -		152 203 253	-	0.9734 0.9763 0.9790
348.15	85 123 152 253 304	0.0184 0.0256	0.9801 0.9845 0.9869 0.9905		304 405 507 608 811	0.0635 - 0.1046 - 0.1566	0.9821 0.9847  0.9871

#### AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

One pass flow method. Hydrogen passed through methanol for several hours. Samples of both phases analysed by passing through silica gel and collecting hydrogen in calibrated flask. Methanol determined from increase in weight of silica gel adsorption vessel. Details in source and ref. 1.

#### SOURCE AND PURITY OF MATERIALS:

No details given

# ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.1; \quad \delta P/\text{bar} = \pm 0.5; \quad \delta x_{\text{H}_2}, \\ \delta y_{\text{H}_2} = \pm 2 \text{\$ (estimated by compiler).}$ 

#### REFERENCES:

Michels, A.; Skelton, G. F.;
 Dumoulin, E.
 Physica 1950, 16, 831.

		ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-	74-0]	Yorizane, M.; Sadamoto, S.;		
	-	Masuoka, H.; Eto, Y.		
2. Methanol; CH ₃ OH; [67-56-1]		Kogyo Kagaku Zasshi 1969, 72,		
	<b>-</b>	2174-7.		
ARIABLES:		PREPARED BY:		
Temperature, pres	ssure	C. L. Young		
XPERIMENTAL VALUES:		· <del></del>		
T/K	P/MPa	Mole fraction of hydrogen in liquid,		
27.11	- / 111 4	x _{H2}		
		2		
273.15	1.11 3.14	0.005 0.011		
	5.17	0.015		
258.15	1.01	0.005		
	2.03 3.04	0.007 0.009		
	5.07	0.013		
243.15	1.01	0.003		
	2.03	0.005		
	3.04 4.05	0.006 0.007		
	5.07	0.008		
	AUXILIARY	INFORMATION		
ETHOD 'APPARATUS/PROCEDURE:	AUXILIARY	INFORMATION SOURCE AND PURITY OF MATERIALS:		
Vapor-liquid equilibrium o		SOURCE AND PURITY OF MATERIALS:		
Vapor-liquid equilibrium o Details given in source.		SOURCE AND PURITY OF MATERIALS:		
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METHOD APPARATUS/PROCEDURE:  Vapor-liquid equilibrium of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the control of the contr		SOURCE AND PURITY OF MATERIALS:  1. Purity 99.9 mole per cent.  ESTIMATED ERROR:		
Vapor-liquid equilibrium o Details given in source.		SOURCE AND PURITY OF MATERIALS:  1. Purity 99.9 mole per cent.		
Vapor-liquid equilibrium o Details given in source.		SOURCE AND PURITY OF MATERIALS:  1. Purity 99.9 mole per cent.  ESTIMATED ERROR: $\delta T/K = \pm 0.1;  \delta x_{\rm H_2} = \pm 0.001$		
Vapor-liquid equilibrium o Details given in source.		SOURCE AND PURITY OF MATERIALS:  1. Purity 99.9 mole per cent.  ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta x_{\rm H_2} = \pm 0.001$ (estimated by compiler).		
Vapor-liquid equilibrium o Details given in source.		SOURCE AND PURITY OF MATERIALS:  1. Purity 99.9 mole per cent.  ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta x_{\rm H_2} = \pm 0.001$ (estimated by compiler).		

- 1. Hydrogen; H; [1333-74-0]
- C₂ to C₁₆Alcohols, ethers and esters

#### **EVALUATOR:**

Colin L. Young.
Department of Chemistry,
University of Melbourne
Parkville,
Victoria, 3052
AUSTRALIA:

The most extensive study of the solubility of hydrogen in alcohols at high pressures is that of Brunner (1). Androsov and Loktev (2) studied the solubility of hydrogen, carbon monoxide and ethyne (acetylene) in several aliphatic alcohols and hydrocarbons. However, even in the deposited article the data were presented in unclear graphs and therefore the data are not considered further. Frolich et al (3) have studied the solubility of hydrogen in 1-propanol, 2-propanol and 1-butanol. The data for 1-butanol are in fair agreement with those of Brunner (1) whereas the hydrogen solubilities for the other two alcohols are about 10 per cent smaller than those of Brunner (1). The solubility of hydrogen in 1-butanol and 2-methyl - 1-propanol have also been studied by Tyvina et al (4). The latter data cover the temperature range 313 K to 473 K and pressures up to 30 MPa whereas those of Brunner (1) are restricted to a temperature range of 298 K to 373 K and pressures below 10 MPa. The interpolated values in overlapping ranges of temperatures and Pressures from these two sets of data are only in fair agreement, the mole fraction of hydrogen in the liquid given by Tyvina et al (4) being about 5 per cent smaller than those of Brunner (1). Schroder (5) investigated the solubility of hydrogen in 1-butanol at 323.15 K at Pressures up to 5 MPa and his results are in good agreement with those of Brunner (1). However, the numerical data of Schroder were not available to us and are not considered further.

Brunner (1) quoted partial molar volumes of hydrogen at infinite dilution,  $V^{\infty}$  and partial molar heats of solution,  $\Delta h$ , where these were calculated from the equation.

$$\ln \ (p_{\rm H_2}/{\rm bar}) \ /x_{\rm H_2} = \ln \ {\it H/bar} + {\rm V^{\infty}} \ p_{\rm H_2}/{\rm RT}$$

$$\frac{\partial \ln x_{\text{H}_2}}{\partial (1/\text{T})} = \frac{-\Lambda h}{R}$$

where H is Henry's law constant at zero partial pressures of hydrogen.

Values of  $H/10^5$ Pa,  $V^{\infty}/\text{cm}^3$  mol⁻¹ and  $\Delta h/J$  mol⁻¹ are given below for Brunner data. Values in parentheses are those calculated from other worker's data as indicated in the footnotes of the table.

Alcohol	T/K	<i>H</i> /10 ⁵ Pa	$V^{\infty}/cm^3 \text{ mol}^{-1}$	Δh/J mol ⁻¹
1,2-Ethanediol	298.15 323.15 373.15	24700 20750 15390	31 35 36	5850
l-Propanol	298.15 323.15 373.15 298.15 253.15 273.15 298.15	4125 3681 2783 (4403) a (5550) b (4970) b (4270) b	36 35 35	4920
2-Propanol	298.15 323.15 373.15 298.15 298.15	3693 3160 2324 (4300) a (3760) e	34 37 48	5750

Alcohol	T/K	<i>H</i> /10 ⁵ Pa	$V^{\infty}/cm^3 \text{ mol}^{-1}$	Δh/J mol
2-Methoxyethanol	298.15 323.15 373.15	6941 5620 4006	18 23 23	6780
l-Butanol	298.15 323.15 373.15 298.15 253.15 273.15 298.15 323.15 323.15 373.15 298.15	3609 3154 2470 (3597) a (4770) b (4320) b (3750) b (3090) c (3670) d (2740) d (3800) f	36 41 43	4695
2-Methyl-l-propanol	298.15 323.15 373.15 323.15 373.15	3545 2921 2257 (3100) d (2500) d	26 48 50	6200
2-Butanol	298.15 323.15 373.15	3729 3178 2212	17 23 37	6510
2-Ethoxyethanol	298.15 323.15 373.15	4448 3735 2785	42 50 51	5780
l-Pentanol	298.15 323.15 373.15 298.15	3375 2881 2269 (3730) f	24 36 36	4880
l-Hexanol	298.15 323.15 373.15 298.15	2948 2536 2080 (3320) f	37 40 26	4270
2-Butoxyethanol	298.15 323.15 373.15	3169 2754 2070	36 41 38	5290
2-Ethyl-l-hexanol	298.15 323.15 373.15 393.15	2529 2146 1708 1512	35 40 42 55	5110
.,3-Propanediol	298.15 323.15 373.15	1558 1360 1038	19 20 25	5045
1,4-Butanediol	298.15 323.15 373.15	1167 1009 777.3	13 19 22	5030
1,2-Dimethoxyethane	298.15 323.15 373.15	272.6 224.9 161.4	32 38 59	6480

Alcohol	T/K	<i>H</i> /10 ⁵ Pa	V [∞] /cm³ mol⁻¹	Δh/J mol ⁻¹
2,2'-Oxybisethanol	298.15 323.15 373.15	1312 1099 808.8	23 25 30	5980
2-(2-Methoxyethoxy) ethanol	298.15 323.15 373.15	580.8 473.9 334.8	23 26 32	6805
2,2'-[1,2-ethanediylbis- (oxy)]bisethanol	298.15 323.15 373.15	971.2 796.0 555.7	19 24 31	6910
2-[2-(2-methoxyethoxy)- ethoxy]ethanol	298.15 323.15 373.15	500.7 406.8 286.2	21 25 32	6910

- a) values for data of Frolich et al (3) quoted by Brunner (1)
- b) values for low pressure data of Katayama and Nitta (6) quoted by Brunner (1)
- c) values for data of Schröder (5) quoted by Brunner (1)
- d) values for data of Tyvina  $et \ al(4)$  quoted by Brunner (1).
- e) Values for low pressure data of Puri and Ruether (6) calculated by evaluator.
- f) values for low pressure data of Makranczy  $et\ al$  (7) calculated by evaluator.

There are some discrepancies between Henry's law constants calculated from the data of Brunner and from low pressure measurements. However, some of the discrepancy arises from the extrapolation of Brunner data to low pressures. The data of Brunner are classified as tentative.

- 1. Brunner, E. J. Chem. Thermodynamics, 1980, 12,993.;
  Brunner, E. Ber Bunsenges. Phys. Chem. 1979, 83, 715.
- Androsov, D.I.; Loktev, S.M. Zh. Fiz. Khim. 1978, 52, 1348. Complete article VINITI No. 4463-77.
- Frolich, K.; Tauch, E.J.; Hogan, J.J.; Peer, A.A.; Ind. Eng. Chem. 1931, 23, 548.
- Tyvina, T.N.; Valuev, K.I.; Vasileva, I.I.; Sokolov, B.I.; Kharchenko, A.A.; Zhur. Prikl. Khim. 1977, 50, 2578.
- 5. Schröder, W. Z. Naturforsch. 1969, 24B, 500.
- 6. Puri, P.S.; Ruether, J.A. Can. J. Chem. Eng. 1974, 7, 41.
- 7. Makranczy, J.; Rusz, L. Balog-Megyery, K.; Hung. J. Ind. Chem. 1979, 7, 41.

# COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. Ber. Bunsenges. Phys. Chem. <u>1979</u>, 83, 715-721. 1,2-Ethanediol; C2H6O2; [107-21-1] VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: $p^*/10^5$ Pa T/K 10 x Mole fraction of hydrogen, 104x_{H2} 298.15 25.3 10.03 51.5 20.26 69.6 26.95 85.9 32.73 323.15 26.8 12.69 48.3 22.30 28.78 62.6 89.7 40.40 373.15 39.4 25.02 55.4 34.71 75.0 46.85 87.4 53.88 total pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static cell fitted with stirrer. 1. No details given. After equilibrium established liquid sample withdrawn and analysed by 2. Merck AG sample purity stripping out hydrogen. better than 99 mole per cent. Details in source and ref. (1). ESTIMATED ERROR: $\delta T/K = \pm 0.1; \delta p/MPa = \pm 0.01;$ $\delta x_{\rm H_2} = \pm 2.0\%.$ (estimated by compiler) REFERENCES: 1. Brunner, E. Ber. Bunsenges. Phys. Chem. 1978, 82,798.

446	Hydrogen and Deuterium Solubilities above 200kPa				
COMPC 1. 2.			Brunner, Ber. Buns	ORIGINAL MEASUREMENTS: Brunner, E. Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721.	
VARI	ABLES:	<u> </u>	PREPARED BY	:	
	Temperatu	re, pressure		C.L. Young.	
EXPE	RIMENTAL VALUES:				
	T/K	r ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4  ext{x}$ Mole fraction of hydrogen, $10^4 x_{ m H_2}$	
	298.15	0.03 24.6 49.8 77.4 99.3	0 24.5 49.8 77.3 99.3	0 58.24 115.3 176.0 220.0	
	323.15	0.11 23.7 36.0 51.8 74.7 106.0	0 23.6 35.9 51.7 74.6 105.9	0 62.96 94.90 135.7 191.5 266.0	
	373.15	1.11 22.9 47.5 86.2 97.7	0 21.8 46.4 85.1 96.4	0 74.41 162.0 289.1 327.0	
	+ total p	pressure			
	* partial	l pressure			
		AUX	ILIARY INFORMATION		
METH	OD APPARATUS/PRO	CEDURE:	SOURCE AND	PURITY OF MATERIALS:	
Sta	Static cell fitted with stirrer			etails given.	

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

Details in source and ref.(1).

- 2. Merck AG sample, purity better than 99 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \delta p/MPa = \pm 0.01;$   $\delta x_{\rm H_2} = \pm 2.0\%$  (estimated by compiler).

# REFERENCES.

1. Brunner, E.

Ber. Bunsenges. Phys. Chem. <u>1978</u>, 82, 798.

COMPONENTS:			ORIGINAL MEASUREMENTS:		
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>2-Propanol; C₃H₈O; [67-63-0]</li> </ol>			Frolich, P. K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A.		
ARIABLES:			PREPARED BY:		
	Pressure	Ì	C. L. Young		
EXPERIMENTAL V	ALUES:		. Mole fraction of hydrogen		
T/K	P/MPa	Solubility			
-/	- / ••• u	<del></del>			
298.15	1.0	0.7	0.0024		
	2.0	1.5			
	3.0	2.2			
	4.0 5.0	3.0 3.7			
	6.0	4.4			
	7.0	5.2	0.0161		
	8.0	5.9			
	9.0	6.6 7.4			
	10.0 11.0	8.1	• • • • • • • • • • • • • • • • • • • •		
	12.0	8.9	•		
	13.0	9.6			
	14.0	10.3			
	15.0	11.1			
	16.0 17.0	11.8 12.6			
	18.0	13.3			
	19.0	14.0	0.0423		
† Cal	culated by comp	iler.			
* Data	a taken from gr	aph in origi:	nal article. Volume of gas		
mea	sured at 101.32	5 kPa and 29	8.15 K dissolved by unit volume conditions.		
OI .		under the s			
		AUXILIARY	INFORMATION		
METHOD/APPARA	rus/procedure:		SOURCE AND PURITY OF MATERIALS:		
Static equ	ilibrium cell.	Liquid			
_			Stated that the materials		
saturated with gas and after equilibrium established samples			were the highest purity		
	removed and analysed by volumetric		available.		
	<del>-</del>				
	sure of liquid		1		
=	of the gas at				
pressure.	Details in so				
	Security in Se		ESTIMATED ERROR:		
			$\delta T/K = \pm 0.1;  \delta x_{H_2} = \pm 5\%.$		
			n ₂		
			REFERENCES:		

#### Hydrogen and Deuterium Solubilities above 200kPa 448 COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. 2. 2-Propanol; C₃H₈O; [67-63-0] Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721. VARIABLES: PREPARED BY: Temperature, pressure C.L. Young 10 x Mole fraction EXPERIMENTAL VALUES: $p^{*}/10^{5}$ Pa of hydrogen, 10 "xH2" $p^{+}/10^{5}$ Pa T/K 298.15 0.057 20.68 7.45 7.51 10.2 27.71 10.1 10.8 10.7 29.33 15.9 42.40 15.8 20.2 20.1 53.85 56.58 21.2 21.2 36.5 36.4 96.26 45.1 45.0 116.5 117.4 45.2 45.2 63.5 63.4 163.4 74.1 188.6 74.2 97.2 97.2 245.4 323.15 0.234 0 0 6.74 21.20 6.98 12.2 11.9 37.14 74.67 24.3 24.1 27.0 84.69 26.8 40.4 40.1 121.1 53.1 160.8 53.3 73.3 73.1 219.3 83.1 82.8 245.3 92.4 92.1 245.5 total pressure * partial pressure AUXILIARY INFORMATION

# ${\tt METHOD/APPARATUS/PROCEDURE:}$

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

Details in source and ref. (1).

#### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Merck AG sample, purity 99.7 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{\rm H_2} = \pm 2.0\%$ . (estimated by compiler).

#### REFERENCES:

1. Brunner, E.

Ber. Bunsenges. Phys. Chem. 1978, 82, 798.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 2-Propanol; C₃H₈O; [67-63-0]

# ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721.

#### EXPERIMENTAL VALUES:

т/к	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4$ x Mole fraction of hydrogen, $10^4x_{ m H_2}$
373.15	1.98	0	0
	9.35	7.37	31.98
	12.0	10.0	42.89
	26.1	24.1	102.1
	30.9	28.9	120.1
	36.7	34.7	142.9
	61.7	59.8	240.3
	89.2	87.3	344.6

- + total pressure
- * partial pressure

450	Hydrogen and Deuterium Solubilities above 200kPa			ove 200kPa		
СОМРО	<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>2-Methoxyethanol; C₃H₈O₂; [109-86-4]</li> </ol>		ORIGINAL MEASU	ORIGINAL MEASUREMENTS:		
			Brunner, E. Ber. Bunsenges. Phys. Chem. <u>1979</u> , 83 715-721.			
VARIA	BLES:		PREPARED BY:	PREPARED BY:		
	Temperature	, pressure	C. L. Young			
EXPER	IMENTAL VALUES:		<u>_</u>			
	T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4 x$ Mole fraction of hydrogen, $10^4 x_{ m H_2}$		
	298.15	0.02 34.2 56.9 101.0	0 34.2 56.9 101.0	0 49.00 82.00 143.0		
	323.15	0.06 33.6 56.5 71.6 81.0	0 33.6 56.5 71.6 80.9	0 59.11 98.65 125.3 139.9		
	373.15	0.46 27.5 45.4 87.8	0 27.0 44.9 87.4	0 67.00 110.0 211.7		
	+ total pressure		* p	artial pressure		
		AUXIL	IARY INFORMATION			
METHO	DD/APPARATUS/PRO	CEDURE:	SOURCE AND PUR	ITY OF MATERIALS:		
Aft liq	Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.		2. BASF Ak	ils given. tiengesellschaft purity 99.8 mole t.		

Details in source and ref. (1).

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/MPa = \pm 0.01; \\ \delta x_{\rm H_2} = \pm 2.0 \%$  (estimated by compiler)

#### REFERENCES:

1. Brunner, E. Ber. Bunsenges. Phys. Chem. 1978, 82, 798.

COMPONENTO		Larrania		
COMPONENTS:		ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]		Brunner, E.		
		J. Chem. Thermodyn. 1980, 12,		
2. 1,3-Propanedi	ol; $C_3H_8O_2$ ;	993-1002.		
[504-63-2]				
VARIABLES:		PREPARED BY:		
Temper	ature, pressure	C. L. Young		
EXPERIMENTAL VALUES:		<del></del>		
T/K	p*/MPa	Mole fraction of hydrogen in liquid,		
<u> </u>	• •	$x_{ m H_2}$		
		_		
	<u></u>			
298.15	1.93	0.001238		
	4.507	0.002868		
	4.674 7.26	0.002960 0.004621		
	10.31	0.006502		
323.15	1.706	0.001250		
	4.519 7.53	0.003281 0.005486		
	10.32	0.007404		
373.15	1.877 4.607	0.001808 0.004343		
	7.58	0.004343		
	10.22	0.009577		
	* total pressu	re.		
	AUXILIARY	INFORMATION		
METHOD/APPARATUS/PROC	FDURF.	SOURCE AND PURITY OF MATERIALS:		
	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	TOOKOL MID TOKETT OF IMPERIALS.		
		1 Marrier Guidachain anns 1 anns 1		
Static		1. Messer-Griesheim sample, purity		
Static cell fitte		99.997 mass per cent.		
After equilibrium	a established	2. Riedel-de-Haem sample, purity		
liquid sample wit		99.5 mass per cent.		
analysed by strip	pping out hydrogen.			
Details in source	and ref. (1).			
1				
1		ESTIMATED ERROR:		
		$\delta T/K = \pm 0.1;  \delta p/MPa = \pm 0.2%;$		
		$\delta x_{\rm H_2} = \pm 2  \text{\$}  .$		
		П2		
		REFERENCES:		
		1. Brunner, E.		
		Ber. Bunsenges. Phys. Chem.		
I		1		

1978, 82, 798.

COMPONENTS:	· · · · · · · · · · · · · · · · · · ·		ORIGINAL MEASUREMENTS:		
	gen; H ₂ ; [l		Tyvina, T. N.; Valuev, K. I.; Vasil'eva, I. I.; Sokolov, B. I.; Kharchenko, A. A. Zh. Prikl. Khim. 1977, 50, 2578- 2581; J. Appl. Chem. USSR 1977, 50, 2446- 2449.		
VARIABLES:			PREPARED BY:		
	Temperature,	pressure	C. L	. Young	
EXPERIMENTAL	L VALUES:		<u> </u>		
T/K	P/atm	P/MPa	Mole fraction of in liquid, $^{x}{ m H}_{2}$	of hydrogen in gas, ^y H ₂	
313.2	300 200 100 50 25	30.4 20.3 10.1 5.07 2.53 1.01	0.0750 0.0512 0.0268 0.0135 0.0065 0.0013	0.9992 0.9991 0.9989 0.9985 0.9980 0.9942	
353.2	300 200 100 50 25 10	30.4 20.3 10.1 5.07 2.53 1.01 0.405	0.0889 0.0614 0.0320 0.0162 0.0082 0.0032 0.0013	0.9959 0.9955 0.9941 0.9925 0.9899 0.9763 0.9386	
393.2	300 200 100 50 25 10	30.4 20.3 10.1 5.07 2.53 1.01 0.405	0.1090 0.0752 0.0387 0.0194 0.0098 0.0032 0.0009	0.9895 0.9884 0.9839 0.9778 0.9561 0.8902	
			(con-	t.)	
		AUXILIARY	INFORMATION		
METHOD/APPAI	RATUS/PROCEDURE:		SOURCE AND PURITY OF MAT	ERIALS:	
ŀ	ositions of c		1. Purity 99.8 mole	e per cent.	
phases were determined by analysis and a static apparatus was employed. However, other details and references given in the source are ambiguous.			2. Analytical grade	e.	
	_		ESTIMATED ERROR: $\delta T/K = \pm 0.1;  \delta x_{H_2}$ $\delta (1-y_{H_2}) = \pm 6\%$ (esterior)		

- 1. Hydrogen;  $H_2$ ; [1333-74-0]
- 2. Butanol; C₄H₁₀O; [71-36-3]

# ORIGINAL MEASUREMENTS:

Tyvina, T. N.; Valuev, K. I.; Vasil'eva, I. I.; Sokolov, B. I.; Kharchenko, A. A. Zh. Prikl. Khim. 1977, 50, 2578-2581; J. Appl. Chem. USSR 1977, 50, 2446-2449.

# EXPERIMENTAL VALUES:

T/K	P/atm	P/MPa	Mole fraction of in liquid, $^{^{lpha}\mathrm{H}_{2}}$	E hydrogen in gas, ^y H ₂
433.2 473.2	300 200 100 50 25 10 300 200 100 50	30.4 20.3 10.1 5.07 2.53 1.01 30.4 20.3 10.1 5.07 2.53	0.1419 0.0984 0.0503 0.0251 0.0117 0.0032 0.1769 0.1230 0.0620 0.0282 0.0107	0.9761 0.9744 0.9622 0.9253 0.8642 0.7371 0.9595 0.9566 0.9068 0.8213

## Hydrogen and Deuterium Solubilities above 200kPa 454 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Brunner, E. 2. 1-Butanol; C₄H₁₀0; [71-36-3] Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721. VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: 10 x Mole fraction $p^{+}/10^{5}Pa$ $p^*/10^5 Pa$ of hydrogen, 10 xH2 T/K 298.15 0.01 15.95 5.79 5.78 9.08 9.05 24.92 13.41 13.40 36.87 13.42 13.41 36.97 28.5 28.5 76.00 77.1 77.1 199.0 80.7 80.7 209.6

97.3

Λ

4.88 8.29

11.67

15.57

21.7

25.3

30.4

43.5

68.2

99.7

+ total pressure

* partial pressure

248.8

0

15.61

25.99

36.69

48.44

67.34

78.02

92.93

130.5

200.6

288.0

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

323.15

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

97.3

0.04

4.92

8.33

11.71

15.61

21.7

25.4

30.4

43.5

68.2 99.3

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Merck AG sample, purity 99.5 mole per cent.

# ESTIMATED ERROR:

 $\begin{array}{lll} \delta T/K &=& \pm 0.1; & \delta p/\text{MPa} &=& \pm 0.01; \\ \delta x_{\text{H}_2} &=& \pm 2.0 \text{\%}. \\ \text{(estimated by compiler).} \end{array}$ 

# REFERENCES:

- 1. Hydrogen; H₂; [1333-74-0]
- 2. l-Butanol; C₄H₁₀O; [71-36-3]

# ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721.

# EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p [*] /10 ⁵ Pa	$10^4  imes  ext{Mole fraction}$ of hydrogen, $10^4 x_{ ext{H}_2}$
373.15	0.51	0	0
	9.82	9.28	37.93
	12.83	12.29	50.24
	18.8	18.23	71.39
	21.7	21.1	82.43
	22.3	21.8	85.04
	28.9	28.4	111.0
	30.4	29.9	120.2
	33.8	33.3	129.4
	78.0	77.5	287.4

- + total pressure
- * partial pressure

# 456 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Tyvina, T. N.; Valuev, K. I.; Vasil'eva, I. I.; Sokolov, B. I.; Kharchenko, A. A. Zh. Prikl. Khim. 1977, 50, 2578-2. 2-Methyl-1-propanol, (isobutane); C₄H₁₀O; [78-83-1] J. Appl. Chem. USSR 1977, 50, 2446-2449. VARIABLES: PREPARED BY: C. L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/atm P/MPa in liquid, in gas, $x_{\rm H_2}$ $y_{\rm H_2}$ 300 30.4 0.0830 0.9987 313.2 0.9983 0.0572 20.3 200 0.0300 0.9978 100 10.1 0.0155 0.9968

# AUXILIARY INFORMATION

# METHOD 'APPARATUS / PROCEDURE:

50

25

10

300

200 100

50

25

10

300

200

100

50

25

10

4

4

353.2

393.2

4

5.07

2.53

1.01

30.4

20.3

10.1

5.07

2.53

1.01

30.4

20.3

10.1

5.07

2.53

1.01

0.405

0.405

0.405

The compositions of coexisting phases were determined by analysis and a static apparatus was employed. However, other details and references given in the source are ambiguous.

# SOURCE AND PURITY OF MATERIALS:

0.0080

0.0965

0.0680

0.0345

0.0175

0.0085

0.0030

0.0014

0.1194

0.0820

0.0427

0.0217 0.0105

0.0036

0.0007

1. Purity 99.8 mole per cent.

(cont.)

0.9954

0.9913

0.9800

0.9938

0.9932

0.9912

0.9887

0.9850 0.9645

0.9080

0.9842

0.9831

0.9767 0.9678

0.9324

0.8574

0.7148

2. Analytical grade.

ESTIMATED ERROR:  $\delta T/K = \pm 0.1; \quad \delta x_{H_2} = \pm 4%;$  $\delta(1-y_{\rm H_2}) = \pm 6\%$  (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 2-Methyl-l-propanol, (isobutane);
  C4H100; [78-83-1]

# ORIGINAL MEASUREMENTS:

Tyvina, T. N.; Valuev, K. I.; Vasil'eva, I. I.; Sokolov, B. I.; Kharchenko, A. A. Zh. Prikl. Khim. 1977, 50, 2578-2581; J. Appl. Chem. USSR 1977, 50, 2446-2449.

# EXPERIMENTAL VALUES:

T/K	P/atm	P/MPa	Mole fraction of in liquid, $^{x}{ m H}_{2}$	hydrogen in gas, $y_{ m H_2}$
433.2	300	30.4	0.1579	0.9650
	200 100	20.3 10.1	0.1096 0.0565	0.9622 0.9430
	50	5.07	0.0363	0.9430
	25	2.53	0.0118	0.8013
	10	1.01	0.0026	0.6476
	4	0.405	0.0007	0.4572
473.2	300	30.4	0.2015	0.9350
	200	20.3	0.1407	0.9245
	100	10.1	0.0698	0.8641
	50	5.07	0.0302	0.7454
	25	2.53	0.0089	0.5775

- 1. Hydrogen; H₂; [1333-74-0]
- 2-Methyl-l-propanol, (isobutanol); C₄H₁₀O; [78-83-1]

# ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721.

# VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

# EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	10 x Mole fraction of hydrogen, 10 xH2
298.15	0.02	0	0
	26.5	26.5	74
	52.8	52.8	145
	97.2	97.2	263
323.15	0.07	0	0
	34.5	34.4	113
	82.5	82.4	255
373.15	0.75	0	0
	26.5	25.8	111
	88.9	88.2	354

- + total pressure
- * partial pressure

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Merck AG sample, purity better than 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/\text{MPa} = \pm 0.01; \\ \delta x_{\text{H}_2} = \pm 2.0 \text{\$.}$  (estimated by compiler).

# REFERENCES:

- Hydrogen; H₂; [1333-74-0]
- 2. 2-Butanol; C₄H₁₀O; [78-92-2]

# ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721.

# VARIABLES:

Temperature, pressure

# PREPARED BY:

C.L. Young

# EXPERIMENTAL VALUES:

EXPERIMENTAL VALUES	p [†] /10 ⁵ Pa	p [*] /10 ⁵ Pa	10 x Mole fraction of hydrogen, 10 x _{H2}
298.15	0.02	0	0
	28.1	28.1	75
	52.1	52.1	139
	76.8	76.8	205
	98.6	98.6	261
323.15	0.11	0	0
	30.0	30.1	93
	50.7	50.6	158
	98.6	98.5	300
373.15	0.75	0	0
	19.8	19.1	85.1
	52.6	51.8	226.6
	100.0	99.3	419.0

- + total pressure
- * partial pressure

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Merck AG sample, purity better than 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{\rm H_2} = \pm 2.0$ %. (estimated by compiler).

# REFERENCES:

1. Brunner, E.

Ber. Bunsenges. Phys. Chem. 1978, 82, 798.

COMPONENTS:		ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ;	[1333-74-0]	Brunner, E.
2. 1,2-Dimethoxyethane,		J. Chem. Thermodyn. 1980, 12,
(ethylene glycol dimethyl ether);		993-1002.
$C_4H_{10}O_2$ ; [110-71-4]		775-1002.
C4H10O2; [LLC	J~/1-4]	
VARIABLES:		PREPARED BY:
Tempera	ture, pressure	C. L. Young
EXPERIMENTAL VALUES:		
<u> </u>	* .	
T/K	p*/MPa	Mole fraction of hydrogen in liquid,
		$x_{ m H_{2}}$
298.15	0.009	0.0
296.13	1.159	0.004189
	4.582	0.01623
	7.43	0.02570
202.15	9.53	0.03272
323.15	0.0288 1.707	0.0 0.007352
	1.782	0.007352
1	4.479	0.01880
j .	4.916	0.02085
1	7.08	0.02947
272	9.82	0.04028
373.15	0.165	0.0
1	2.127 2.219	0.01183 0.01280
	4.516	0.01280 . 0.02583
1	7.96	0.04501
	9.73	0.05473
	* total pressure	e.

# AUXILIARY INFORMATION

# METHOD APPARATUS / PROCEDURE:

Static cell fitted with stirrer.

After equilibrium established
liquid sample withdrawn and
analysed by stripping out hydrogen.

Details in source and ref. (1).

- SOURCE AND PURITY OF MATERIALS:
  - Messer-Griesheim sample, purity
     99.997 mass per cent.
  - BASF Akteingesellschaft sample, purity 99.7 mass per cent.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.1; \quad \delta p/MPa = \pm 0.2%; \\ \delta x_{H_2} = \pm 2%.$$

# REFERENCES:

### Organic Compounds Containing Oxygen 461 COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. 2-Ethoxyethanol; C4H10O2; Ber. Bunsenges. Phys. Chem. 1979, 1110-80-51 83. 715-721. VARIABLES: PREPARED BY: Temperature, pressure C.L. Young. EXPERIMENTAL VALUES: $p^{+}/10^{5}$ Pa p*/10⁵Pa 10 4x Mole fraction T/K of hydrogen, 10 x_{H2} 0.007 298.15 0 23.9 23.9 52.41 40.4 40.4 86.61 124.7 59.3 59.3 108.2 108.2 216.0 323.15 0.03 0 26.2 26.2 67.92 104.9 41.4 41.4 66.0 160.1 66.0 75.6 75.6 184.8 103.0 103.0 240.10

+ total pressure,

0.31

56.1 101.7

102.0

* partial pressure,

# AUXILIARY INFORMATION

0 55.8

101.4 101.7

# METHOD /APPARATUS / PROCEDURE:

373.15

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. BASF Aktiengesellschaft sample purity 99.8 mole per cent.

188.0

326.0 323.0

ESTIMATED ERROR:  $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{\rm H_2} = \pm 2.0\%$ .

(estimated by compiler).

# REFERENCES:

1. Brunner, E.

Ber. Bunsenges. Phys. Chem. 1978, 82, 798.

COMPONENTS:		ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]		Brunner, E.		
2. 1,4-Butanediol [110-63-4]	;C4H ₁₀ O ₂ ;	J. Chem. Thermodyn. <u>1980</u> , 12, 993-1002.		
VARIABLES:		PREPARED BY:		
Temperature, pressure		C. L. Young		
EXPERIMENTAL VALUES:				
T/K	p [*] /MPa	Mole fraction of hydrogen in liquid, ${}^{x}_{ m H_{2}}$		
298.15	1.542 4.46 7.58 7.86 9.89	0.001320 0.003827 0.006535 0.006794 0.008470		
323.15 2.169 3.608		0.002149 0.003559		

total pressure.

4.648

5.080

6.27 6.41

9.60

5.47 8.03

8.13 9.42

2.529 5.25

# AUXILIARY INFORMATION

# METHOD APPARATUS / PROCEDURE:

373.15

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

1. Messer-Griesheim sample, purity 99.997 mass per cent.

0.004535

0.005000

0.006155

0.006221 0.009300

0.003243

0.006668 0.006937

0.01014 0.01034

0.01187

2. BASF Akteingesellschaft sample, purity 99.7 mass per cent.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.1; \quad \delta p/MPa = \pm 0.2%;$$
  
 $\delta x_{H_2} = \pm 2%.$ 

# REFERENCES:

COMPONENTS:		ORIGINAL MEASUREMENTS:	
1. Hydrogen; H2;	[1333-74-0]	Brunner, E.	
2. 2,2'-Oxybiseth glycol); C ₄ H ₁ [111-46-6]	anol, (ethylene	J. Chem. Thermodyn. <u>1980</u> , 12, 993-1002.	
ARIABLES:		PREPARED BY:	
Tempera	ture, pressure	C. L. Young	
EXPERIMENTAL VALUES:			
T/K	p [*] /MPa	Mole fraction of hydrogen in liquid, $x_{\rm H_2}$	
298.15	1.916 4.547	0.001452 0.003411	
	7.29 8.91	0.005417 0.006557	
323.15	7.29	0.005417	

^{*} total pressure.

# AUXILIARY INFORMATION

# Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and

analysed by stripping out hydrogen. Details in source and ref. (1).

METHOD/APPARATUS/PROCEDURE:

# SOURCE AND PURITY OF MATERIALS:

- Messer-Griesheim sample, purity
   99.997 mass per cent.
- BASF Akteingesellschaft sample, purity 99.7 mass per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta p/MPa = \pm 0.2%;$  $\delta x_{\rm H_2} = \pm 2%.$ 

# REFERENCES:

- 1. Hydrogen; H₂; [1333-74-0]
- 2. l-Pentanol,  $C_5H_{12}O$ ; [71-41-0]

# ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem.

1979, 83, 715-721.

VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

# EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p [*] /10 ⁵ Pa	$10^4  imes  ext{Mole fraction}$ of hydrogen, $10^4 x_{ ext{H}_2}$
298.15	0.003	0	0
	27.2	27.2	80
	59.7	59.7	171
	78.6	78.6	230
	98.0	98.0	279
323.15	0.02	0	0
	25.4	25.4	0 87
	55.3	55.3	181
	88.4	88.4	288
373.15	0.25	0	0
	33.4	33.2	143
	60.5	60.3	256
	79.7	79.5	333

- + total pressure
- * partial pressure

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen.

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Merck AG sample, purity 98.5 mole per cent.

# ESTIMATED ERROR:

 $\begin{array}{lll} \delta T/K &=& \pm 0.1; & \delta p/\text{MPa} &=& \pm 0.01; \\ \delta x_{\text{H}_2} &=& \pm 2.0 \text{\%}. \\ \text{(estimated by compiler)} \end{array}$ 

# REFERENCES.

OMPONENTS:	ì	ORIGINAL MEASUREMENTS:	
1. Hydrogen; H ₂	; [1333-74-0]	Brunner, E.	
2. 2-(2-Methoxy	ethoxy)ethanol,	J. Chem. Thermodyn. 1980, 12,	
(diethylene glycol, monomethyl		993-1002.	
	I ₁₂ O ₃ ; [111-77-3]		
ARIABLES:		PREPARED BY:	
Temperature, pressure		C. L. Young	
EXPERIMENTAL VALUES:	······································	<u> </u>	
T/K	p [*] /MPa	Mole fraction of hydrogen in liquid, $^{x}_{\mathrm{H}_{2}}$	
298.15	$3.4 \times 10^{-5}$	0.0	
	1.441 4.185	0.002478 0.007176	
	6.97	0.01176	
	6.97 10.19	0.01176 0.01691	
323.15	6.97 10.19 2.0 × 10 ⁻⁴	0.01176 0.01691 0.0	
323.15	6.97 10.19 2.0 × 10 ⁻⁴ 1.486	0.01176 0.01691 0.0 0.003119 0.008947	
323.15	6.97 10.19 2.0 × 10 ⁻⁴	0.01176 0.01691 0.0 0.003119 0.008947 0.01489	
	6.97 10.19 2.0 × 10 ⁻⁴ 1.486 4.32 7.25 10.41	0.01176 0.01691 0.0 0.003119 0.008947 0.01489 0.02107	
323.15 373.15	6.97 10.19 2.0 × 10 ⁻⁴ 1.486 4.32 7.25 10.41 3.5 × 10 ⁻³	0.01176 0.01691 0.0 0.003119 0.008947 0.01489 0.02107	
	6.97 10.19 2.0 × 10 ⁻⁴ 1.486 4.32 7.25 10.41 3.5 × 10 ⁻³ 2.11	0.01176 0.01691 0.0 0.003119 0.008947 0.01489 0.02107 0.0	
	6.97 10.19 2.0 × 10 ⁻⁴ 1.486 4.32 7.25 10.41 3.5 × 10 ⁻³	0.01176 0.01691 0.0 0.003119 0.008947 0.01489 0.02107	

^{*} total pressure.

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer.

After equilibrium established
liquid sample withdrawn and
analysed by stripping out hydrogen.

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- Messer-Griesheim sample, purity
   99.997 mass per cent.
- BASF Akteingesellschaft sample, purity 99.7 mass per cent.

# ESTIMATED ERROR:

$$\begin{split} \delta \mathbf{T}/\mathbf{K} &= \pm 0.1; \quad \delta p/\mathbf{MPa} = \pm 0.2\%; \\ \delta x_{\mathrm{H}_2} &= \pm 2\%. \end{split}$$

# REFERENCES:

466	Hydrogen and Deuterium Solubilities above 200kPa				
COMPONENTS:  1. Hydrogen; H; [1333-74-0]  2. 1-Hexanol; C ₆ H ₁₄ O; [111-27-3]		Brunner	ORIGINAL MEASUREMENTS: Brunner, E.  Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721.		
VARIABLES: Tempe	rature, pressure	PREPARED B	Y: C.L. Young.		
EXPERIMENTAL VALUES T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	10 x Mole fraction of hydrogen, 10 x H2		
298.15	0.001 30.1 57.0 57.1 79.9 98.7	0 30.1 56.9 57.1 79.9 98.7	0 99.50 182.2 185.0 251.9 305.8		
323.15	0.01 34.0 44.3 66.6 83.1 103.4	0 34.0 44.2 66.6 83.0 103.4	0 113.5 164.6 250.4 296.4 374.1		
373.15	0.11 32.6 73.7 87.1 102.4	0 32.5 73.6 87.0 102.3	0 155.2 340.4 406.2 478.2		
	pressure,				
	AU	XILIARY INFORMATION	I		
METHOD/APPARATUS/PRO	OCEDURE:	SOURCE AND	PURITY OF MATERIALS:		

Static cell fitted with stirrer.
After equilibrium established
liquid sample withdrawn and analysed
by stripping out hydrogen.

Details in source and ref. (1).

- 1. No details given.
- 2. Merck AG sample, purity better than 98 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{H_2} = \pm 2.0$ %.

(estimated by compiler)

# REFERENCES:

1. Brunner, E.

Ber. Bunsenges. Phys. Chem. 1978, 82, 798.

# COMPONENTS: ORIGINAL MEASUREMENTS: Brunner, E. Hydrogen; H₂; [1333-74-0] Ber. Bunsenges. Phys. Chem. 1979, 83, 715-721. 2. 2-Butoxyethanol; C6H14O2; [111-76-2] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young EXPERIMENTAL VALUES: $p^{*}/10^{5}$ Pa $p^+/10^5$ Pa 10 x Mole fraction T/K of hydrogen, 10 xH2 0 298.15 0.002 134.1 44.1 44.1 191.1 63.8 63.8 208.6 70.7 70.7 248.4 84.4 84.4 0 Λ 323.15 0.008 34.4 120.7 34.4 35.5 35.5 124.5 56.8 195.4 56.8 77.0 77.1 260.8 336.7 102.7 102.7 373.15 0.09 0 n 36.2 170.1 36.2 65.9 65.8 303.1 84.0 83.9 381.5 total pressure partial pressure AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static cell fitted with stirrer. 1. No details given. After equilibrium established liquid sample withdrawn and 2. BASF Aktiengesellschaft analysed by stripping out hydrogen. sample, purity 99.5 mole per cent. Details in source and ref. (1). ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta p/MPa = \pm 0.01$ ; $\delta x_{\rm H_2} = \pm 2.0\%$ (estimated by compiler) REFERENCES: 1. Brunner, E.

Ber. Bunsenges. Phys. Chem. 1978,

82, 798.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Brunner, E.
2. 2,2'-[1,2-Ethanediylbis(oxy)]bis-	J. Chem. Thermodyn. <u>1980</u> , 12,
ethanol, (triethylene glycol);  C ₆ H ₁₄ O ₄ ; [112-27-6]	993-1002.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young
EXPERIMENTAL VALUES:	

T/K	<i>p</i> */MPa	Mole fraction of hydrogen in liquid, ${}^{x_{ m H_{2}}}$
298.15	2.05 4.617 6.97	0.002096 0.004710 0.007076
323.15	10.06 1.994 4.456 7.67	0.01009 0.002502 0.005517 0.00938
373.15	10.41 2.59 4.574 7.48 9.97	0.01261 0.004600 0.008050 0.01296 0.01705

^{*} total pressure

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer.

After equilibrium established
liquid sample withdrawn and
analysed by stripping out hydrogen.

Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. Messer-Griesheim sample, purity 99.997 mass per cent.
- BASF Akteingesellschaft sample, purity 99.7 mass per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta p/MPa = \pm 0.2\%;$   $\delta x_{\rm H_2} = \pm 2\%.$ 

# REFERENCES:

Organic Compounds Containing Oxygen			
ethanol, (Ti	e; [1333-74-0]  exyethoxy)-ethoxy]-  riethylene glycol  cher); C ₇ H ₁₆ O ₄ ;	ORIGINAL MEASUREMENTS:  Brunner, E.  J. Chem. Thermodyn. 1980, 12, 993-1002.	
VARIABLES:		PREPARED BY:	
Temper	ature, pressure	C. L. Young	
EXPERIMENTAL VALUES:	<del></del>	<u></u>	
T/K	p [*] /MPa	Mole fraction of hydrogen in liqu $^{x}{ m H}_{2}$	ıid,
298.15	1.759 4.649 6.83	0.003469 0.009193 0.01349	
323.15	10.26 1.66 3.138 6.68	0.01993 0.004061 0.007623 0.01598	
373.15	10.33 1.805 3.76 6.81 10.30	0.02447 0.006270 0.01280 0.02303 0.03399	,
	* total pressu	re.	
	AUXILIARY	INFORMATION	

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source and ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. Messer-Griesheim sample, purity 99.997 mass per cent.
- 2. BASF Akteingesellschaft sample, purity 99.7 mass per cent.

# ESTIMATED ERROR:

$$\delta T/K = \pm 0.1; \quad \delta p/MPa = \pm 0.2%; \\ \delta x_{H_2} = \pm 2%.$$

# REFERENCES:

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Brunner, E. 2. 2-Ethoxy-1-hexanol; C₈H₁₈O; Ber. Bunsenges. Phys. Chem. 1979, [104-76-7] 83, 715-721. VARIABLES: PREPARED BY: C.L. Young. Temperature, pressure EXPERIMENTAL VALUES: $p^{*}/10^{5}$ Pa $p^{+}/10^{5}$ Pa 10 x Mole fraction T/K of hydrogen, 10 xH2 0 298.15 0.0002 n 75.80 19.72 19.72 34.3 34.3 132.1 44.2 44.2 170.8 77.4 77.4 289 94.6 343 94.6 0.002 0 323.15 0 50.3 222 50.3 97.8 97.8 410 373.15 0.04 0 349 62.6 62.6 524 96.5 96.5 393.15 0.11 0 0 171.3 26.7 26.9 46.1 46.0 287.7 total pressure, partial pressure AUXILIARY INFORMATION METHOD APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: 1. No details given. Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and BASF Aktiengesellschaft sample, purity better than analysed by stripping out hydrogen. 98 mole per cent. Details in source and ref. (1).

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \delta p/MPa = \pm 0.01;$  $\delta x_{\rm H_2} = \pm 2.0\%$ 

# (estimated by compiler)

# REFERENCES:

# Organic Compounds Containing Oxygen 471 COMPONENTS: ORIGINAL MEASUREMENTS: Loktev, S. M.; Androsov, D. I.; 1. Hydrogen; H₂; [1333-74-0] Zuev, A. A. Zh. Prikl. Khim. 1978, 51, 2023-2. Carbon Monoxide; CO; [630-08-0] 2027; J. Appl. Chem. USSR 1978, 51, 1914-3. Alcohols 1917. VARIABLES: PREPARED BY: Temperature, pressure, gaseous composition C. L. Young EXPERIMENTAL VALUES:

T/K	Mole fraction of hydrogen in gas before saturation		pressure	Bunsen coe	efficients
_		p/atm	p/MPa	α _{H₂}	^α co
315	0.690	20	2.03	0.77	0.73
i -		40	4.05	1.62	1.40
		60	6.08	2.20	1.80
		80	8.11	2.85	2.15
		100	10.13	3.55	2.91
	0.515	20	2.03	0.55	1.10
		40	4.05	1.17	2.00
		60	6.08	1.63	2.97
		80	8.11	2.12	4.00
		100	10.13	2.87	4.90
	0.43	20	2.03	0.46	1.25
		40	4.05	0.95	2.33
		60	6.08	1.47	3.55
		80	8.11	1.91	4.67
		100	10.13	2.30	5.70
371	0.69	20	2.03	1.06	0.72
		40	4.05	2.06	1.52
		60	6.08	2.98	2.16
		80	8.11	3.99	2.83
		100	10.13	4.67	3.55
			(0	ont )	

(cont.)

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Liquid saturated with gaseous mixture by bubbling gas through liquid in a stirred vessel. Samples of liquid analysed by Volumetric technique and gas chromatography.

# SOURCE AND PURITY OF MATERIALS:

- 1, 2. Purity approximately 99 mole per cent.
- 3. Mixture of C12to C16 aliphatic alcohols (industrial product).

# ESTIMATED ERROR:

 $\delta T/K = \pm 1.0; \quad \delta p/p = \pm 0.01;$  $\delta\alpha$  = ±3% (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon Monoxide; CO; [630-08-0]
- 3. Alcohols

# ORIGINAL MEASUREMENTS:

Loktev, S. M.; Androsov, D. I.; Zuev, A. A. Zh. Prikl. Khim. 1978, 51, 2023-2027; J. Appl. Chem. USSR 1978, 51, 1914-1917.

# EXPERIMENTAL VALUES:

m /12	Mole fraction of hydrogen in gas		pressure	Bunsen coes	
T/K	before saturation	p/atm	p/MPa	α _{H₂}	^α co
371	0.485	20	2.03	0.80	1.25
		40	4.05	1.60	2.30
		60	6.08	2.38	3.42
		80	8.11	2.91	4.54
		100	10.13	3.49	5.45
	0.57	20	2.03	0.68	1.43
		40	4.05	1.34	2.74
		60	6.08	2.02	4.06
		80	8.11	2.60	5.16
		100	10.13	3.35	6.20
457	0.69	40	4.05	3.10	1.74
		60	6.08	4.59	2.47
		80	8.11	5.82	3.07
		100	10.13	7.00	4.07
	0.515	20	2.03	1.15	1.52
		40	4.05	2.12	2.81
		60	6.08	3.16	4.19
		80	8.11	4.14	5.60
		100	10.13	4.86	6.70
	0.43	20	2.03	0.97	1.78
		40	4.05	1.82	3.30
		60	6.08	2.78	4.82
		80	8.11	3.58	6.30
		100	10.13	4.51	7.70

315  0.56  0.435  0.0061  20  2.03  0.59  0.95  40  4.05  1.23  1.91  60  6.08  1.75  2.68  80  8.11  2.37  3.60  100  10.13  3.04  4.40  100  10.13  3.04  4.40  100  10.13  3.04  4.40  100  10.13  3.04  4.40  100  10.13  3.04  4.40  100  10.13  3.04  4.40  100  10.13  3.04  4.40  100  10.13  3.04  4.20  1.86  100  10.13  4.20  1.86  1.80  8.11  3.25  1.54  100  10.13  4.20  1.86  100  10.13  4.20  1.86  100  10.13  4.20  1.86  100  10.13  1.41  7.20  100  10.13  1.41  7.20  100  10.13  1.41  7.20  100  10.13  1.41  7.20  100  10.13  1.41  7.20  100  10.13  1.41  7.20  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  10.13  1.41  7.12  100  1	
Temperature, pressure, gaseous composition  C. L. Young  Charlet  A H2  C. Co  Aliphatic allowland  A H2  C. Co  Aliphatic allowland  C. L. Young  Call  A L. Mixture of C12to C.  C. Aliphatic allowland  (industrial production)  C. L. Young  Call  C. L. Young  A L. Mixture of C12to C.  C. Aliphatic allowland  (industrial production)  C. L. Young  Call  C. L. Young  Call  C. L. Young  Call  C. L. Young  Call  C. C. C.  C. C. C. S.  C. L. Young  Call  C. C. C. C.  C. C. C. S.  C. L. Young  Call  Call  C. C. C.  C. C. C. C.  Call  Ca	23-
Composition    Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   Composition   C	
Mole fractions in gaseous phase before saturation	
T/K before saturation	
315  0.56  0.435  0.0061  20  2.03  0.59  0.95  40  4.05  1.23  1.91  60  6.08  1.75  2.68  80  8.11  2.37  3.60  100  10.13  3.04  4.40  0.80  0.190  0.0078  20  2.03  0.86  0.41  60  6.08  2.56  1.18  80  8.11  3.25  1.54  100  10.13  4.20  1.86  0.245  0.745  0.0075  20  2.03  0.29  1.63  40  4.05  0.56  3.21  60  6.08  0.88  4.80  80  8.11  1.08  6.06  6.08  0.88  4.80  80  8.11  1.08  6.06  6.08  0.88  4.80  80  8.11  1.08  6.06  6.08  0.88  4.80  80  8.11  1.08  6.06  6.08  0.88  4.80  80  8.11  1.08  6.06  6.08  0.88  4.71  80  8.11  1.10  5.92  100  10.13  1.41  7.12  (cont.)  AUXILIARY INFORMATION  AUXIL	ents
40	α _{C₂H₂}
0.80 0.190 0.0078 20 2.03 0.86 0.41 40 4.05 1.70 0.81 60 6.08 2.56 1.18 80 8.11 3.25 1.54 100 10.13 4.20 1.86 0.245 0.745 0.0075 20 2.03 0.29 1.63 40 4.05 0.56 3.21 60 6.08 0.88 4.80 80 8.11 1.08 6.06 60 6.08 0.88 4.80 80 8.11 1.08 6.06 100 10.13 1.41 7.20 0.25 0.74 0.0103 20 2.03 0.31 1.55 40 4.05 0.56 3.20 60 6.08 0.86 4.71 80 8.11 1.10 5.92 100 10.13 1.41 7.12 (cont.)  AUXILIARY INFORMATION  AUXILIARY INFOR	0.36 0.68 0.91 1.00
0.245 0.745 0.0075 20 2.03 0.29 1.63 40 4.05 0.56 3.21 60 6.08 0.88 4.80 80 8.11 1.08 6.06 100 10.13 1.41 7.20 0.25 0.74 0.0103 20 2.03 0.31 1.55 40 4.05 0.56 3.20 60 6.08 0.86 4.71 80 8.11 1.10 5.92 100 10.13 1.41 7.12 (cont.)  AUXILIARY INFORMATION  AUXILIARY INFORMATION  AUXILIARY INFORMATION  AUXILIARY INFORMATION  AUXILIARY INFORMATION  4. Mixture by bubbling gas through liquid in a stirred vessel.  Samples of liquid analysed by volumetric technique and gas  (industrial production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the production of the	1.15 0.56 1.00 1.28 1.44 1.60
0.25 0.74 0.0103 20 2.03 0.31 1.55 40 4.05 0.56 3.20 60 6.08 0.86 4.71 80 8.11 1.10 5.92 100 10.13 1.41 7.12 (cont.)  AUXILIARY INFORMATION  ETHOD/APPARATUS/PROCEDURE:  Liquid saturated with gaseous inixture by bubbling gas through liquid in a stirred vessel.  Samples of liquid analysed by volumetric technique and gas  (industrial productions)	0.43 0.81 1.05 1.33
AUXILIARY INFORMATION  AUXILIARY INFORMATION  SOURCE AND PURITY OF MATERIALS:  1, 2, 3. Purity approximate  99 mole per cent.  Iquid in a stirred vessel.  Samples of liquid analysed by  Volumetric technique and gas  AUXILIARY INFORMATION  1, 2, 3. Purity approximate  99 mole per cent.  4. Mixture of C ₁₂ to C  aliphatic alcohols	0.60 1.10 1.46 1.74 1.99
ETHOD/APPARATUS/PROCEDURE:  Liquid saturated with gaseous  mixture by bubbling gas through liquid in a stirred vessel.  Samples of liquid analysed by  Volumetric technique and gas  SOURCE AND PURITY OF MATERIALS:  1, 2, 3. Purity approximate 99 mole per cent.  4. Mixture of C ₁₂ to C aliphatic alcohols	_
Liquid saturated with gaseous  mixture by bubbling gas through liquid in a stirred vessel.  Samples of liquid analysed by  Volumetric technique and gas  1, 2, 3. Purity approximate 99 mole per cent.  4. Mixture of C ₁₂ to C aliphatic alcohols	
mixture by bubbling gas through  liquid in a stirred vessel.  Samples of liquid analysed by  Volumetric technique and gas  99 mole per cent.  4. Mixture of C ₁₂ to C aliphatic alcohols	
Samples of liquid analysed by  Volumetric technique and gas  (industrial production)	ly
chromatography.	
ESTIMATED ERROR: $\delta T/K = \pm 1.0$ ; $\delta p/p = \pm 0.01$ ; $\delta \alpha = \pm 3\%$ (estimated by compile	er).
REFERENCES:	

- Hydrogen; H₂; [1333-74-0]
   Carbon monoxide; CO; [630-08-0]
   Ethyne (acetylene); C₂H₂; [74-86-2]
- 4. Alcohols

# ORIGINAL MEASUREMENTS:

Loktev, S. M.; Androsov, D. I.; Zuev, A. A. Zh. Prikl. Khim. 1978, 51, 2023-2027; J. Appl. Chem. USSR 1978, 51, 1914-1917.

# **EXPERIMENTAL VALUES:**

m /v	Mole fractions gaseous phase	!		Dungo		
T/K	before saturati		l pressure		n coeffi	
	y' _{H2} y'CO y'C	2H ₂ p/atm	n <i>p/</i> MPa	α _{H 2}	αco	α _{C₂H₂}
315	0.516 0.485 0.0		2.03	0.54	1.13	0.52
ļ		40 60	4.05 6.08	1.16 1.73	2.23 3.11	0.89 1.21
		80	8.11	2.21	3.86	1.45
		100	10.13	2.70	4.57	1.65
371	0.56 0.435 0.0	061 20	2.03	0.83	1.01	0.17
		40	4.05	1.72	2.05	0.32
		60	6.08	2.45	3.11	0.45
1		80	8.11	3.30	4.00	0.56
ŀ	0.80 0.19 0.0	100 078 20	10.13 2.03	3.85 1.16	5.22 0.45	0.66 0.25
	0.00 0.19 0.0	40	4.05	2.26	0.90	0.47
		60	6.08	3.37	1.45	0.64
ł		80	8.11	4.24	1.95	0.79
		100	10.13	5.20	2.31	0.85
	0.245 0.745 0.0		2.03	0.43	1.75	0.20
		40	4.05	0.72	3.75	0.37
		60	6.08	1.05	5.04	0.50
		80 100	8.11 10.13	1.45 1.86	6.81 7.90	0.614 0.73
	0.250 0.740 1.0		4.05	0.79	3.55	0.73
	0.230 0.740 1.0	60	6.08	1.17	5.10	0.63
		80	8.11	1.54	6.86	0.80
		100	10.13	1.75	7.70	0.87
į	0.516 0.485 0.9		2.03	0.84	1.15	0.27
		40	4.05	1.59	2.31	0.50
1		60	6.08	2.25	3.39	0.67
		80 100	8.11 10.13	2.82 3.50	4.08 5.40	0.79 0.87
457	0.56 0.435 0.0		2.03	1.17	1.37	0.09
337	0.30 0.433 0.0	40	4.05	2.32	2.73	0.18
		60	6.08	3.25	4.02	0.25
ĺ		80	8.11	4.48	5.12	0.32
		100	10.13	5.20	6.15	0.37
1	0.80 0.19 0.0		2.03	1.76	0.65	0.18
		40	4.05	3.30	1.21	0.32
1		60	6.08 8.11	4.91 6.22	1.68 2.28	0.42 0.52
		80 100	10.13	7.36	2.20	0.52
	0.245 0.745 0.0		2.03	0.57	2.31	0.14
		40	4.05	1.12	4.48	0.26
İ		60	6.08	1.57	6.28	0.35
		80	8.11	2.07	8.18	0.45
		100	10.13	2.50	9.75	0.50
	0.25 0.74 0.0		2.03	0.61	2.25	0.21
]		40 60	4.05 6.08	1.05	4.30 6.37	0.38 0.52
		80	8.11	1.50 1.96	7.85	0.65
		100	10.13	2.43	9.60	0.72
Ì	0.516 0.485 0.0		2.03	1.13	1.43	0.18
		40	4.05	2.21	2.84	0.35
		60	6.08	3.27	4.00	0.46
l		80	8.11	4.04	5.50	0.54
		100	10.13	4.75	6.75	0.64
					<del></del>	

# COMPONENTS: ORIGINAL MEASUREMENTS: Simnick, J.J.; Sebastian, H.M., Lin, H.M.; Chao, K.C. J. Chem. Thermodyn., 1979, 11, 531-7. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

PERIMENTAL V	ALUES:			
		Mole fraction		
T/K	p/MPa	in liquid, $x_{ m H_2}$	in vapour, y _{H2}	
462.1	0.07046* 2.037 3.04 5.05 10.13 15.34 20.16 25.40	0 0.0076 0.0115 0.0188 0.0370 0.0546 0.0698	0 0.9643 0.9752 0.9847 0.9916 0.9939 0.9949 0.9955	
502.9	0.1842* 2.037 3.03 5.06 10.16 15.10 20.27 25.30	0 0.0089 0.0136 0.0225 0.0442 0.0649 0.0846 0.1090	0 0.9001 0.9303 0.9578 0.9772 0.9828 0.9859 0.9879	
541.8	0.4283* 2.047 3.04 5.09 10.15 15.13 20.31 25.26	0 0.0094 0.0154 0.0266 0.0538 0.0800 0.1039 0.1255	0 0.7756 0.8420 0.8992 0.9439 0.9602 0.9671	

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Details in ref. (1).

# SOURCE AND PURITY OF MATERIALS:

- 1. Air Products sample, purity 99.95 mole per cent.
- Aldrich Chemical Co., gold label grade, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.6; \quad \delta p/MPa = \pm 0.02$   $\delta x_{\rm H_2}, \quad \delta y_{\rm H_2} = \pm 1 \text{% (estimated by compiler)}$ 

# REFERENCES:

 Sebastian, H.M.; Simnick, J.J.; Lin, H-M.; Chao, K-C.
 J. Chem. Engng. Data, 1978, 23, 305-8.

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. m-Cresol; C₇H₈O; [108-39-4] Simnick, J.J.; Sebastian, H.M., Lin, H.M.; Chao, K.C. J. Chem. Thermodyn. 1979, 11, 531-7.

T/K	p/MPa		n of hydrogen
	p/rira	in liquid, $x_{\rm H_2}$	in vapour, $y_{\rm H_2}$
582.1	0.8759*  2.027 3.02 5.07 10.14 15.20 20.27 25.33	0 0.0081 0.0156 0.0295 0.0624 0.0939 0.1227 0.1509	0 0.5161 0.6671 0.7900 0.8846 0.9163 0.9318 0.9421
624.5	1.577* 2.027 3.06 5.06 10.11 15.17 20.23 25.26	0 0.0043 0.0137 0.0314 0.0751 0.1141 0.1522 0.1833	0 0.1840 0.4003 0.5960 0.7668 0.8298 0.8633 0.8849
662.0	2.681* 3.05 5.07 10.12 15.22 20.25 25.37	0 0.0046 0.0296 0.0875 0.1413 0.1935 0.2354	0 0.0734 0.3259 0.5742 0.6812 0.7374 0.7733

^{*} Vapor pressure of m-cresol.

- (1) Hydrogen; H₂; [1333-74-0]
- (2) 4-Methyl-1,3-dioxolan-2-one or propylene carbonate; C4H6O3; [108-32-7]

# ORIGINAL MEASUREMENTS:

Schmack, P; Bittrich, H.-J.

Wiss. Z. Tech. Hochsch. Chem. Leuna-Merseburg 1966, 8 (2-3), 182 - 186.

Chem. Abstr. 1967, 66, 6095u.

VARIABLES:

T/K: 278.15 - 333.15 P/kPa: 101.325, 892 - 1034 (1, 8.8 - 10.2 atm)

PREPARED BY:

H. L. Clever

# EXPERIMENTAL VALUES:

T/K	P/atm	Bunsen Coefficient $\alpha/\text{cm}^3$ (STP) cm ⁻³ atm ⁻¹	P/atm	Bunsen Coefficient $\alpha/\text{cm}^3$ (STP) cm ⁻³ atm ⁻¹
278.15	1.0	0.0258	9.3	0.0295
283.15	1.0	0.0290	9.3	0.0312
288.15	1.0	0.0308	9.5	0.0319
293.15	1.0	0.0284	8.8	0.0340
298.15	1.0	0.0320	9.6	0.0342
303.15	1.0	0.0314	9.1	0.0367
308.15	1.0	0.0314	10.1	0.0378
313.15	1.0	0.0341	10.2	0.0388
318.15	1.0	0.0405	9.3	0.0425
323.15	1.0	0.0368	9.0	0.0427
328.15	1.0	0.0382	9.1	0.0438
333.15	1.0	0.0431	9.2	0.0472

The authors give the enthalpy of solution of hydrogen in propylene carbonate as (  $6200 \pm 2500)$  J mol  $^{-1}$ .

At 298.15 K and 1 atm partial pressure hydrogen the mole fraction solubility is 1.2 x 10

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Two methods were used. The apparatus used for the solubility measurements at one atm is modeled after the apparatus of Schay et al. (1). It consists of an absorption flask with magnetic stirrer that is connected to a Hg manometer, a gas buret with Hg leveling bulb, and a water jet vacuum pump. Gas volume changes in the apparatus are calibrated with res-Pect to pressure and temperature. The solubility can be determined at several temperature with one charging ESTIMATED ERROR: of gas and solvent.

For the measurements near 10 atm a rocking autoclave apparatus similar to that of Dean and Tooke (2) is used The saturated liquid is transferred to a buret system at one atm for analysis.

# SOURCE AND PURITY OF MATERIALS:

- (1) Hydrogen. No information.
- (2) Propylene carbonate. Prepared from propylene glycol and phosgene at VEB Leuna-Werke "Walter Ulbricht". Boiling point/ ${}^{0}C = 235$ ,  $n_{D}^{25} = 1.4196$ ,  $\rho_{4}^{25}/g \text{ cm}^{-3} = 1.206$ , and  $\epsilon^{25} = 65$ .

 $\delta T/K = \pm 0.2$  $\delta\alpha/\alpha$  = 0.12 at 1 atm 0.08 at 10 atm

- Schay, G.; Székely, Gy.;
   Rácz, Gy.; Traply, G.
   Periodica Polytech. (Budapest) 1958, 2, 1 - 24.
- 2. Dean, A. R.; Tooke, J. W. Ind. Eng. Chem. 1946, 38, 389.

- Hydrogen;  $H_2$ ; [1333-74-0]
- 4-Methyl-1,3-dioxolan-2-one, (Propylene carbonate); C4H6O3; [108-32-7]

# ORIGINAL MEASUREMENTS:

Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. Khim. Prom. 1973, 49, 108-110.

# VARIABLES:

Temperature, pressure

# PREPARED BY:

C. L. Young

EXPERIMENTAL V	ALUES:
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EXPERIMENTAL	VALUES:		
T/K	P/bar	Mole fraction of hydrogen in liquid, ${}^{x}{}_{ m H_{2}}$	α [†] vol/vol
283.15	83.4	0.00661	1.75
	95.1	0.00808	2.14
	98.9	0.00800	2.12
	99.6	0.00796	2.11
	112.9	0.00897	2.38
	120.2	0.00965	2.56
298.15	75.6	0.00673	1.78
	87.3	0.00789	2.09
	95.1	0.00912	2.42
	109.3	0.01043	2.77
	113.8	0.01021	2.71
	126.6	0.01154	3.07
323.15	76.0	0.00852	2.26
	89.3	0.00961	2.55
	95.1	0.01073	2.85
	100.1	0.01084	2.88
	112.6	0.01203	3.20
	121.6	0.01351	3.60
	141.8	0.01532	4.09

quoted in original paper, appears to be volume of gas at T/K = 273.15and P = 1 atmosphere adsorbed by unit volume of liquid at room temperature.

# AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

Mixture stirred by ball in rocking autoclave. Sample of liquid analysed by a volumetric method. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- Dried and oxygen removed; purity 99.8 mole per cent.
- 2. Distilled; purity 99.9 mole per cent determined by gas chromatography.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/bar = \pm 0.1;$  $\delta x_{\rm H_2} = \pm 5\%$  (estimated by compiler).

		Organic Compound	S Containing Oxygen		4/-
COMPONE	NTS:		ORIGINAL MEASUREMENTS:		
1. H ₃	ydrogen; H ₂	; [1333-74-0]	Shakova, S. F.; Zul Kaplan, L. K. Khii		
2. Pe	entanedioic	acid, dimethyl ester	, 108-110.		
	(Dimethyl [1119-40-0	glutarate); C ₇ H ₁₂ O ₄	;		
VARIABL			PREPARED BY:		
Pressu	ıre		C. L. Young		
EXPERIM	ENTAL VALUES:			<del></del>	
T/K	P/bar	Mole fraction of hydrogen in liquid, ^x H ₂	α [†] vol/vol		
313.15	5 43.7 71.4 98.6 126.3 128.5	0.0123 0.0194 0.0264 0.0339 0.0354	1.89 3.01 4.12 5.33 5.59		

quoted in original paper, appears to be the volume of gas T/K = 273.15 and P = 1 atmosphere adsorbed by unit volume of liquid at room temperature.

HAD - FF

# AUXILIARY INFORMATION

	INFORMATION
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixture stirred by ball in rocking autoclave. Sample of liquid analysed by a volumetric method. Details in source.	<ol> <li>Dried and oxygen removed, purity 99.8 mole per cent.</li> <li>Analytical grade sample.</li> </ol>
1	
	ESTIMATED ERROR:
	$\delta T/K = \pm 0.1;  \delta P/bar = \pm 0.1;$
	$\delta x_{\rm H_2} = \pm 5\%$ (estimated by compiler).
	REFERENCES:
_	1

# COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. Ahim. Prom. 1973, 1,2,3-Propanetriol, triacetate, 49, 108-110. (Glycerol triacetate); C9H14O6; [102-76-1] VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

EXPERIMENT.	AL VALUES:		
т/к	P/bar	Mole fraction of hydrogen in liquid, "H ₂	α [†] vol/vol
298.15	70.1	0.0177	2.14
	85.8	0.0214	2.59
	87.3	0.0218	2.64
	104.0	0.0268	3.26
	118.1	0.0291	3.55
	139.7	0.0340	4.17
323.15	85.3	0.0259	3.15
	106.9	0.0320	3.91
	115.7	0.0345	4.23
	140.2	0.0412	5.09
	141.8	0.0427	5.28
343.15	89.8	0.0311	3.80
	111.8	0.0383	4.72
	145.2	0.0500	6.23
	155.9	0.0527	6.59

[†] quoted in original paper, appears to be volume of gas at T/K = 273.15 and P = 1 atmosphere adsorbed by unit volume of liquid at room temperature.

# AUXILIARY INFORMATION

# METHOD / APPARATUS / PROCEDURE:

Mixture stirred by ball in rocking autoclave. Sample of liquid analysed by a volumetric method. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. Dried and oxygen removed; purity 99.8 mole per cent.
- 2. Distilled and dried; purity 99.4 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$ ;  $\delta x_{\mbox{\scriptsize H}_{2}}$  = ±5% (estimated by compiler).

COMPONENTS:	EVALUATOR:		
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Amines</li> </ol>	Colin L. Young Department of Chemistry, University of Melbourne, Parkville, 3052, Victoria, Australia: June, 1980		

# CRITICAL EVALUATION:

The solubility of hydrogen in amines at elevate pressures has been studied by Moore and Otto (1) and by Brunner (2). The former workers (1) only worked up to 2 MPa and found that, within experimental error, mole fraction solubility was linear with pressure and quoted equations for Henry's law constants. Brunner (2) on the other hand studied solubilities up to 10 MPa and found a slightly non-linear relationship between pressure and mole fraction solubility. He evaluated the limiting slope of pressure-mole fraction solubility graphs as pressure tends to zero to obtain Henry's law constants which can be compared with those of Moore and Otto (1). There is only fair agreement between the two groups for the systems studied by both i.e. ethanamine, 1,2-ethanediamine and 1- propanamine. The Henry's law values of Moore and Otto (1) are 5-10% larger than those of Brunner (2). This could be partly due to Moore and Otto's assumption that there is a linear relationship between pressure and mole fraction solubility. From Brunners data it appears that this assumption could lead to Henry's law constant being 2-5% larger than when estimated allowing for the small non-linearity of mole fraction solubility as a function of pressure.

Brunner (2) also quoted partial molar volumes of hydrogen at infinite dilution,  $V^{\infty}$  and partial molar heats of solution  $\Delta h$  where these were calculated from the equations.

$$\ln p_{\rm H_2}/x_{\rm H_2} = \ln H + V^{\infty} p_{\rm H_2}/RT$$
 (1)

$$\frac{\partial \ln x_{\rm H_2}}{\partial (1/T)} \bigg|_{p} = -\frac{\Delta h}{R} \tag{2}$$

where H is Henry's law constant at zero partial pressure of hydrogen.

Values of  $H/10^5$  Pa,  $V^{\infty}/cm^3mol^{-1}$  and  $\Delta h/J$  mol⁻¹ are given below for hydrogen in amines. The values calculated from the data of Moore and Otto (1) are given in parentheses.

Amine	T/K	<i>H</i> /10 ⁵ Pa	$V^{\infty}/cm^3mol^{-1}$	Δh/J mol-1
Methanamine	203.2 213.2 223.2 233.2 243.2 253.2 263.2 273.2 283.2 293.2 303.2	(13647) (12028) (10609) (9373) (8305) (7380) (6580) (5891) (5294) (4775) (4322)		
Ethanamine	203.2 213.2 223.2 233.2 243.2 253.2 263.2	( 9063) ( 8191) ( 7348) ( 6499) ( 5751) ( 5151) ( 4676)		

Amine	T/K	<i>H</i> /10 ⁵ Pa	$V^{\infty}/cm^3mol^{-1}$	$\Delta h/J \text{ mol}^{-1}$
Ethanamine	273.2 283.2 293.2 303.2 298.15 323.15 373.15	( 4293) ( 3946) ( 3585) ( 3174) 3020 2420 1540	35 41 50	8140
1,2-Ethanediamine	293.2 303.2 298.15 323.15 373.15	(15430) (13500) 13820 10540 6280	17 22 33	9770
1-Propanamine	203.2 213.2 223.2 233.2 243.2 253.2 263.2 273.2 283.2 293.2 303.2 298.15 323.15 373.15	( 7800) ( 6931) ( 6193) ( 5561) ( 5016) ( 4548) ( 4142) ( 3788) ( 3480) ( 3209) ( 2970) 2930 2400 1680	22 26 34	8860
2-Propanamine	298.15 323.15 373.15	2585 2117 1368	20 21 24	
1,2-Propanediamine	243.2 253.2 263.2 273.2 283.2 293.2 303.2	(13539) (10267) (10658) (9577) (8675) (7916) (7263)		
1,3-Propanediamine	298.15 323.15 373.15	9400 9370 4680	35 39 47	8650
Pyrrolidine	298.15 323.15 373.15	4616 3815 2585	31 35 42	7200
Piperidine	298.15 323.15 373.15	3890 3170 2280	38 42 50	6580
1-Methylpyrrolidine	298.15 323.15 373.15	2400 2080 1555	36 39 45	5390
N,N-dimethy1-1,3- propanediamine	298.15 323.15 373.15	3120 2600 1840	32 37 48	6520
l-Methylpiperidine	298.15 323.15 373.15	2390 2090 1590	40 42 47	5080
N,N-Diethylethan- amine	298.15 323.15 373.15	1675 1370 1085	28 33 42	5285

Amine	T/K	<i>H</i> /10 ⁵ Pa	V [∞] /cm³mol-¹	Δh/J mol-1
1,6-Hexanediamine	298.15 323.15 373.15	4027 3354 2860	23 25 27	6860
N-(3-aminopropyl)- 1,3-propanediamine	298.15 323.15 373.15	6530 5010 3357	28 34 46	8180
N,N-Dimethylcyclo- hexanamine	298.15 323.15 373.15	2413 2090 1605	39 44 52	5055
N-Butyl-1-butan- amine	298.15 323.15 373.15	1763 1463 1120	34 40 51	5555
N-(2-aminoethyl)- N-(3-aminopropyl)- 1,3- propane- diamine	298.15 323.15 373.15	5715 4520 3060	19 22 29	7720
N-N-dibutyl-1- Butanamine	298.15 323.15 373.15	1360 1170 933	31 36 46	4615

The data of Moore and Otto (1) are classified as doubtful whereas those of Brunner (2) are classified as tentative.

- 1. Moore, R.G.; Otto, F.D. Can. J. Chem. Eng. 1972, 50, 355.
- 2. Brunner, E. Ber. Bunsenges. Phys. Chem. <u>1978</u>, 82, 798.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Moore, R.G.; Otto, F.D.
2. Methanamine; CH ₅ N; [74-89-5]	Can. J. Chem. Engng. <u>1972</u> , 50, 355-60.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES:	
T/K	Mole fraction of hydrogen * in liquid, $x_{ m H_{2}}$
203.2 213.2 223.2 233.2 243.2 253.2 263.2 273.2 283.2 293.2 303.2	0.00007425 0.00008424 0.00009551 0.0001081 0.0001220 0.0001373 0.0001540 0.0001720 0.0001914 0.0002122 0.0002344
* at a partial pressu	re of 101.3 kPa cont.

# AUXILIARY INFORMATION

# METHOD APPARATUS/PROCEDURE:

Recirculating flow apparatus fitted with magnetic pump. Amine saturated with hydrogen for a minimum of 8 hr. Samples of liquid withdrawn and amine frozen out, hydrogen released collected in calibrated gas buret.

Matheson sample, purity 98.0 mole per cent. Dried.
Fractionally distilled under ected in calibrated gas buret.

Amount of amine determined gravimetrically.

# SOURCE AND PURITY OF MATERIALS:

- Matheson sample, purity 99.999 mole per cent. Dried.
- vacuum.

# **ESTIMATED ERROR:**

 $\delta T/K = \pm 0.1; \ \delta x_{H_2} = \pm 4\%.$ (estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- Methanamine; CH₅N; [74-89-5]

ORIGINAL MEASUREMENTS:

Moore, R.G.; Otto, F.D.

Can. J. Chem. Engng. 1972, 50 355-60.

# DATA taken from deposited document

		DATA taken from deposited document				
		Total Pressure	Partial of hydro	pressure ogen	Solub- ility +	Mole fract- ion of hydrogen
T/ ^O C	T/K	P/atm	P/atm	P/MPa		x _{H2}
-24.67 -24.73	248.48 248.42	4.17 9.42	3.77 9.01	0.382	0.3473	0.004811
-24.73	248.42	9.42	9.01	0.913	0.8548	0.01183
-24.95	248.20	9.41	9.01	0.913 0.913	0.8533	0.01181
-24.70	248.45	17.43	17.02	1.725	0.8332	0.01153
-24.70	248.45	17.45	17.02	1.727	1.5722	0.02174
-24.95	248.20	17.41	17.01	1.724	1.5826	0.02188
-24.95	248.20	17.40	17.00	1.723	1.5985	0.02210
-24.81	248.34	17.40	17.00	1.723	1.6226	0.02243
-24.95	248.20	10.29	9.89	1.002	1.5960 0.9435	0.02207
-60.49	212.66	7.84	7.80	0.790	0.4824	0.01306
~60.49	212.66	7.87	7.83	0.793		0.006680
~61.30	211.85	13.93	13.89	1.407	0.4787 0.8289	0.006629
~61.52	211.63	13.93	13.89	1.407	0.8265	0.01147
-61.67	211.48	20.07	20.03	2.030	1.1671	0.01144 0.01615
-61.61	211.54	20.07	20.03	2.030	1.1766	0.01628
-62.16	210.99	16.70	16.67	1.689	0.9767	0.01352
-62.16	210.99	16.70	16.67	1.689	0.9734	0.01332
62.35	210.80	15.99	15.95	1.616	0.9652	0.01336
36.51	236.64	10.79	10.58	1.072	0.8773	0.01330
36.51	236.64	10.79	10.58	1.072	0.8502	0.01177
35.12	238.03	11.50	11.27	1.188	0.9534	0.01319
35.24	237.91	8.82	8.60	0.871	0.7149	0.009896
35.24	237.91	8.82	8.60	0.871	0.7154	0.009904
34.60	238.55	14.40	14.17	1.436	1.1894	0.01645
34.66	238.49	14.40	14.17	1.436	1.1782	0.01630
34.02	239.13	19.03	18.79	1.904	1.5744	0.02177
34.02	239.13	19.03	18.79	1.904	1.5712	0.02173
-0.21	272.94	14.04	12.72	1.289	1.5700	0.02171
-0.21 -0.37	272.94	14.04	12.72	1.289	1.5758	0.02179
-0.37	272.78	20.96	19.65	1.991	2.4257	0.03350
20.14	272.78	20.96	19.65	1.991	2.4373	0.03366
22.75	253.01	17.65	14.69	1.488	2.2523	0.03111
22.75	250.40	21.07	17.81	1.805	2.8261	0.03901
~4./5	250.40	21.07	17.81	1.805	2.8058	0.03873
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Volume of hydrogen (cm³) reduced to 101.31Pa and 273.15k dissolved by 1 gm of methanamine

486	Hydrogen and Deuterium Solubilities above 200kPa				
COMPC	ONENTS:	ORIGINAL MEASUREMENTS:			
1.	Hydrogen; H ₂ ; [1333-74-0]	Moore, R.G.; Otto, F.D.			
2.	Ethanamine; C ₂ H ₇ N; [74-04-7]	Can. J. Chem. Engng. 1972, 50, 355-60.			
VARI/	ABLES:	PREPARED BY:			
	Temperature	C.L. Young			
EXPE	RIMENTAL VALUES:				
	T/K	$10^4 \times$ Mole fraction of hydrogen * in liquid, $10^4 x_{ m H_2}$			
	203.2 213.2 223.2 233.2 243.2 253.2 263.2 273.2 283.2 293.2 303.2 *at a partial pressure	1.118 1.237 1.379 1.559 1.762 1.967 2.167 2.360 2.568 2.826 3.192			

# AUXILIARY INFORMATION

# METHOD APPARATUS / PROCEDURE:

Recirculating flow apparatus fitted with magnetic pump. Amine saturated with hydrogen for a minimum of 8 hr. Samples of liquid withdrawn and amine frozen out, hydrogen released collected in calibrated gas burst collected in calibrated gas buret. Amount of amine determined gravimetrically.

# SOURCE AND PURITY OF MATERIALS:

- 1. Matheson sample, purity 99.999 mole per cent. Dried.
- Matheson sample, purity 98.5 mole per cent. Dried. Fractionally distilled under vacuum.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \delta x_{H_2} = \pm 4%.$ (estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ethanamine;  $C_2H_7N$ ; [74-04-7]

# ORIGINAL MEASUREMENTS:

Moore, R.G.; Otto, F.D.

Can. J. Chem. Engng. 1972, 50, 355-60.

# DATA taken from deposited document

			Total pressure	Partial p		Solubil- ity +	Mole fract-
١	T/ ^O C	T/K	P/atm	P/atm	P/MPa		
	T/°C -24.11 -24.53 -24.53 -24.28 -24.28 -24.00 -24.11 -61.39 -61.76 -68.01 -68.17 -68.17 -68.17 -68.17 -68.17 -68.17 -61.03 -61.03 -60.84 -61.06 -60.62 -60.62 -35.64 -35.12	T/K 249.04 249.04 248.62 248.62 248.87 249.15 249.15 249.15 249.15 249.15 249.16 211.39 211.39 201.39 201.39 212.31 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98 204.98	P/atm 11.34 11.34 11.34 14.76 14.75 17.84 10.56 10.56 14.30 11.44 13.68 13.68 13.68 17.26 17.26 17.67 17.67 17.67 17.69 15.14 18.08 18.08 17.33 17.33 17.33 15.90 15.90	P/atm 11.21 11.21 14.63 14.61 17.70 10.42 10.42 14.16 11.43 13.67 13.68 18.34 17.25 17.67 17.67 17.67 17.67 17.27 17.68 15.13 18.06 17.26 17.26 17.26 17.26 15.83 15.83	P/MPa  1.136 1.136 1.482 1.480 1.793 1.793 1.056 1.056 1.435 1.158 1.385 1.386 1.858 1.748 1.748 1.790 1.750 1.750 1.750 1.751 1.533 1.533 1.830 1.830 1.749 1.749 1.604	1.0720 1.0561 1.3688 1.3563 1.6553 1.6502 0.9911 0.9748 1.3388 0.7063 0.8347 0.8083 1.0480 0.9882 0.9906 1.0112 0.9806 1.0112 0.9806 1.0728 1.0359 1.0887 1.0887 1.08895 0.9393 0.9242 1.1250 1.0991 1.4336 1.4207 1.3062 1.3169	hydrogen  **H ₂ 0.02152 0.02120 0.02746 0.02721 0.03319 0.03309 0.01997 0.02686 0.01419 0.01676 0.01623 0.02104 0.01984 0.01989 0.02030 0.01969 0.02153 0.02187 0.01887 0.01887 0.01887 0.01887 0.01856 0.02258 0.02206 0.02850 0.02621 0.02642
	-36.54 0.11	236.61 273.29	13.99 20.66	13.83 20.17	1.401 2.044	1.1307 2.3784	0.02269 0.04762
Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Married Marrie	-0.29 -0.29 22.42 22.65 22.65	272.86 272.86 295.57 295.80 295.80	17.93 17.93 16.37 20.82 20.82	17.45 17.45 15.10 19.55 19.55	1.768 1.768 1.530 1.981	2.0514 2.0601 2.1873 2.8407 2.8538	0.04110 0.04127 0.04381 0.05682 0.05708
	22.90	296.05	18.21	16.92	1.714	2.4654	0.04935

⁺ Volume of hydrogen (cm³), reduced to 101.31Pa and 273.15K, dissolved by 1 gram of ethanamine.

### Hydrogen and Deuterium Solubilities above 200kPa 488 COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. Ethanamine (Aminoethane) Ber. Bunsenges. Phys. Chem. 1978, 82, $C_2H_7N$ ; [75-04-7]. 798-805. VARIABLES: PREPARED BY: Temperature, pressure. C.L. Young. EXPERIMENTAL VALUES: $p^{*}/10^{5}Pa$ p⁺/10⁵Pa 10 x Mole fraction T/K of hydrogen, 10 4xH2 1.42 0 0 298.15 53.0 87.7 51.6 164 86.3 267 323.15 3.41 0 0 193 52.8 49.5 88.4 85.1 319 373.15 13.3 0 0 58.6 45.6 283 98.5 85.8 510 total pressure * partial pressure

# AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static cell fitted with stirrer. 1. No details given After equilibrium established liquid sample withdrawn and analysed Fluka AG sample, purity 99 per by stripping out hydrogen. Details cent. in source. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \delta p/MPa = \pm 0.01;$ $\delta x_{\rm H_2} = \pm 2.0\%$ . (estimated by compiler) REFERENCES:

# COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Moore, R.G.; Otto, F.D. 1. Can. J. Chem. Engng. 1972, 50, 355-1, 2-Ethanediamine; C2H8N2; [107-15-3] VARIABLES: PREPARED BY: Temperature C.L. Young EXPERIMENTAL VALUES: 10 4x Mole fraction of T/K

hydrogen in liquid,  $10^4 x_{\rm H_2}$ 

293.2 0.6567 303.2 0.7506

* at a partial pressure of 101.3kPa

### DATA taken from deposited document

		Total pressure	Partial proof		Solubil- ity +	Mole fract- ion of hydrogen
T/°C	T/K	P/atm	P/atm	P/MPa		$x_{\rm H_2}$
26.38	299.53	14.46	14.44	1.463	0.3849	0.01031
26.38	299.53	14.46	14.44	1.463	0.3845	0.01030
25.43	298.58	18.01	17.99	1.823	0.4735	0.01268
25.88	299.03	21.20	21.18	2.146	0.5613	0.01503
25.88	299.03	21.20	21.18	2.146	0.5670	0.01518
33.13	306.28	21.69	21.65	2.194	0.6355	0.01701
33.13	306.28	21.69	21.65	2.194	0.6338	0.01697
33.61	306.76	18.11	18.08	1.832	0.5250	0.01406
33.61	306.76	18.11	18.08	1.832	0.5263	0.01409

Volume of hydrogen (cm 3 ), reduced to 101.3kPa and 273.15k, dissolved by 1 gram of 1,2-ethanediamine

### AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Recirculating flow apparatus fitted with magnetic pump. Amine saturated with hydrogen for a minimum of 8 hr. Samples of liquid withdrawn and amine frozen out, hydrogen released collected in calibrated gas buret. Amount of amine determined gravimetrically.

### SOURCE AND PURITY OF MATERIALS:

- 1. Matheson sample, purity 99.999 mole per cent. Dried.
- 2. Fischer Scientific sample purity 98.0 mole per cent. Dried. Fractionally distilled under vacuum.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta x_{H_2} = \pm 4\%.$ 

(estimated by compiler)

### 490 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Brunner, E. 1,2-Ethanediamine, (1,2-Ber. Bunsenges. Phys. Chem. 1978, 82, Diaminoethane); C2H8N2; 798-805. [107-15-3] VARIABLES: PREPARED BY: C.L. Young. Temperature, pressure EXPERIMENTAL VALUES: p⁺/10⁵Pa p*/10⁵Pa 10 x Mole fraction T/K of hydrogen, 10 4 x H 2 0.02 0 Λ 298.15 53.4 73.7 38.51 53.3 52.8 73.7 0.07 22.5 323.15 22.21 22.5 30.5 30.5 28.65 50.2 50.1 47.00 85.1 79.1 85.2 0.56 0 0 373.15 30.3 29.7 46.36 87.5 57.1 57.6 120.8 80.7 80.2 + total pressure * partial pressure. AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. BASF Aktiengesellschaft sample, purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/MPa = \pm 0.01;$  $\delta x_{\rm H_2} = \pm 2.0\%.$ (estimated by compiler)

ORIGINAL MEASUREMENTS: Moore, R.G.; Otto, F.D.
Can. J. Chem. Engng. <u>1972</u> , 50, 355-60.
PREPARED BY: C.L. Young
$^{+}$ x Mole fraction of * drogen in liquid, $10^{+}x_{ m H_{2}}$
1.299 1.462 1.636 1.822 2.020 2.228 2.446 2.675 2.912 3.158 3.412
uoted in original partial pressure of 101.31Pa. cont.
INFORMATION
SOURCE AND PURITY OF MATERIALS:
<ol> <li>Matheson sample, purity 99.999     mole per cent. Dried.</li> <li>Eastman Organic Chemicals sample,     purity 98.0 mole per cent. Dried.     Fractionally distilled under     vacuum.</li> </ol>

 $\delta T/K = \pm 0.1; \delta x_{H_2} = \pm 4\%.$ (estimated by compiler)

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. 1-Propanamine; C₃H₉N; [107-10-8] ORIGINAL MEASUREMENTS: Moore, R.G.; Otto, F.D. Can. J. Chem. Engng. 1972, 50, 355-60.

### DATA taken from deposited document

		Total pressure	Partial of hydro	pressure gen	Solubil- ity +	Mole fract- ion of
T/°C	T/K	P/atm	P/atm	P/MPa		hydrogen $x_{ m H_2}$
-24.61	248.54	4.20	4.17	0.423	0.3374	0.008891
-24.67	248.48	11.14	11.11	1.126	0.9211	0.02423
-24.67	248.48	11.14	11.11	1.126	0.9171	0.02413
-24.67	248.48	11.09	11.06	1.121	0.8955	0.02356
-27.34	245.81	13.94	13.92	1.410	1.1345	0.02983
-24.67	248.48	17.26	17.23	1.746	1.3981	0.03673
-24.67	248.48	17.26	17.23	1.746	1.3923	0.03658
-23.29	249.66	10.58	10.54	1.068	0.8584	0.02259
-23.29	249.66	10.58	10.54	1.068	0.8498	0.02236
-23.34	249.81	14.11	14.08	1.427	1.1386	0.02994
-23.34	249.81	14.11	14.08	1.427	1.1281	0.02966
-24.67	248.48	17.18	17.15	1.738	1.3885	0.03648
-24.67	248.48	17.18	17.15	1.738	1.3796	0.03625
-61.79	211.36	16.65	16.65	1.687	0.8949	0.02354
-61.79	211.36	16.65	16.65	1.687	0.9170	0.02412
-61.42	211.73	18.42	18.42	1.866	1.0095	0.02655
-61.42	211.73	18.42	18.42	1.866	1.0031	0.02638
-62.01	211.14	15.89	15.89	1.610	0.8717	0.02293
-62.73	210.42	17.41	17.41	1.764	0.9430	0.02481
-67.92	205.23	18.44	18.44	1.868	0.9300	0.02447
-67.28	205.87	17.59	17.59	1.782	0.8904	0.02343
-67.28	205.87	17.49	17.49	1.772	0.8841	0.02326
-36.28	236.87	18.86	18.84	1.909	1.3766	0.03617
-36.28	236.87	18.86	18.84	1.909	1.3811	0.03629
-36.16	236.99	12.29	12.28	1.244	0.8778	0.02309
-36.16	236.99	12.29	12.28	1.244	0.8791	0.02313
-36.22	236.93	12.29	12.27	1.243	0.8801	0.02316
-27.20	245.95	16.91	16.88	1.710	1.3431	0.03529
-27.20	245.95	16.91	16.88	1.710	1.3196	0.03468
0.11	273.04	13.93	13.80	1.398	1.4063	0.03695
0.11	273.04	13.93	13.80	1.398	1.4091	0.03702
0.03	273.12	20.73	20.60	2.087	2.0965	0.05498
0.03	273.12	20.73	20.60	2.087	2.1044	0.05519
21.87	251.28	15.27	14.92	1.512	1.8117	0.04755
21.87	251.28	15.27	14.92	1.512	1.8227	0.04784

Volume of hydrogen (cm³), reduced to 101.3kPa and 273.15K, dissolved by 1 gram of 1-propanamine

### ORIGINAL MEASUREMENTS: COMPONENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. 2. 1-Propanamine (Aminopropane) Ber. Bunsenges. Phys. Chem. 1978, 82, 798-805. $C_3H_9N$ ; [107-10-8] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young. EXPERIMENTAL VALUES: $p^*/10^5$ Pa p⁺/10⁵Pa 10 4x Mole fraction T/K of hydrogen, 10 x_{H2} 298.15 0.41 0 28.7 28.3 95.3 49.1 49.5 167 86.7 86.3 287 1.10 0 323.15 27.6 26.5 109 54.3 53.2 217 75.1 74.0 298 373.15 4.91 0 19.3 84.8 14.4 51.5 73.7 46.7 270 69.0 394 total pressure partial pressure

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample, purity 99.9 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{H_2} = \pm 2.0$ % (estimated by compiler)

494		Hydrogen and Deuteriun	n Solubilities abo	ve 200kPa
COMPO	NENTS:		ORIGINAL MEAS	SUREMENTS:
1.		; [1333-74-0]	Brunner,	
2.	2-Propanamir C₃H ₉ N; [75-3	e (2-Amino propane); 1-0]	Ber. Buns 82, 798-8	enges. Phys. Chem. <u>1978</u> , 805.
VARIA	ABLES: Temperatu	re, pressure	PREPARED BY:	C.L. Young
EXPER	RIMENTAL VALUES:			
	T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	10 $^{\circ}$ x Mole fraction of hydrogen, 10 $^{\circ}x_{\rm H_2}$
	298.15	0.78 10.1 19.0 43.7 73.7	0 9.32 18.3 43.1 72.9	0 35.9 70.9 163 278
 	323.15	1.92 30.8 51.4 70.4 79.6	0 28.9 49.5 68.5 77.8	0 136 232 318 364
	373.15	7.54 40.7 55.6 73.0	0 34.4 48.3 65.8	0 247 350 469
	+ total p	ressure,		
	* partial	pressure.		
		AUXILIAR	INFORMATION	
METHO	OD/APPARATUS/PRO	CEDURE:	SOURCE AND P	URITY OF MATERIALS:
Aft liq ana	er equilibrio quid sample w	ipping out hydrogen.	1. No de	tails given. Aktiengesellschaft sample, y 99.5 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/MPa = \pm 0.01; \\ \delta x_{H_2} = \pm 2.0 \%.$  (estimated by compiler)

3 77-3	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Moore, R.G.; Otto, F.D.
2. 1, 2-Propanediamine; C ₃ H ₁₀ N ₂ ; [78-90-0]	Can. J. Chem. Engng. <u>1972</u> , 50, 355-60.
VARIABLES:	PREPARED BY:
Temperature	C.L. Young
EXPERIMENTAL VALUES:	
T/K	10 ⁴ x Mole fraction of * hydrogen in liquid, 10 ⁴ x _{H2}
243.2 253.2 263.2 273.2 283.2 293.2 303.2	0.7484 0.8475 0.9507 1.058 1.168 1.280
* at a partial pressur	e of 101.3 kPa cont.
	INFORMATION
	SOURCE AND PURITY OF MATERIALS:
AUXILIAR	SOURCE AND PURITY OF MATERIALS:  1. Matheson sample, purity 99.999 mole per cent. Dried.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 1, 2-Propanediamine;  $C_3H_{10}N_2$ ;

# ORIGINAL MEASUREMENTS:

Moore, R.G.; Otto, F.D.

Can. J. Chem. Engng. 1972, 50 355-60.

# DATA taken from deposited document

ļ				-		
		Total pressure	Partial of hydro	pressure gen	Solub- ility +	Mole fract- of hydrogen
τ∕°c	T/K	P/atm	P/atm	P/MPa		$x_{ m H_2}$
-23.89	249.26	7.54	7.54	0.754	0.1811	0.005987
-24.14	249.01	10.44	10.44	1.058	0.2566	0.008479
-24.45	248.70	13.85	13.85	1.465	0.3456	0.01142
-24.78	248.37	13.79	13.79	1.397	0.3400	0.01123
-24.45	248.70	18.82	18.82	1.907	0.4610	0,01522
-17.06	256.09	17.56	17.56	1.779	0.4590	0.01516
-17.06	256.09	17.56	17.56	1.779	0.4585	0.01514
-18.41	254.74	16.00	16.00	1.621	0.4160	0.01374
-18.41	254.74	16.00	16.00	1.621	0.4189	0.01384
-12.08	261.07	13.17	13.17	1.334	0.3701	0.01222
0.11	273.26	16.65	16.65	1.687	0.5286	0.01745
0.11	273.26	16.65	16.65	1.687	0.5296	0.01748
- 0.43	272.72	18.16	18.15	1.839	0.5735	0.01893
- 0.43	272.72	18.16	18.15	1.839	0.5724	0.01889
10.74	290.89	13.27	13.27	1.345	0.4755	0.01570
10.74	290.89	13.27	13.27	1.345	0.4670	0.01542
10.41	290.56	17.18	17.18	1.741	0.6131	0.02024
10.41	290.56	17.18	17.18	1.741	0.6110	0.02017
10.56	290.71	18.48	18.48	1.872	0.6640	0.02191
10.56	290.71	18.48	18.48	1.872	0.6634	0.02189
10.36	290.51	17.71	17.70	1.793	0.6378	0.02105

⁺ Volume of hydrogen (cm³) reduced to 101.3kPa and 273.15k, dissolved by 1 gram of amine

COMPONENTS:		ORIGINAL ME	ASUREMENTS:
1. Hydrogen; H	H ₂ ; [1333-74-0]	Brunner,	E.
2. 1,3-Diamino [109-76-2]	opropane, C ₃ H ₁₀ N ₂ ;	Ber. Bun 798-805.	nsenges. Phys. Chem. <u>1978</u> , 82
VARIABLES:		PREPARED BY	······································
Temperatu	are, pressure		C.L. Young.
EXPERIMENTAL VALUES	S:		
T/K	p ⁺ /10 ⁵ Pa	p [*] 10 ⁵ Pa	$10^4$ x Mole fraction of hydrogen, $10^4x_{ m H_2}$
298.15	0.006 38.9 97.2	0 38.0 97.2	0 39.8 94.9
323.15	0.03 50.0 94.2	0 50.0 94.2	0 65.3 118.2
373.15	0.27 54.8 76.9	0 54.5 76.6	0 109.5 150.4
+ total	pressure		•
* partia	l pressure		
	AUXILIAI	RY INFORMATION	
METHOD/APPARATUS/PF	ROCEDURE:	SOURCE AND	PURITY OF MATERIALS:
	tted with stirrer.	1. No d	etails given.
			Aktiengesellschaft sample ty 98 mole per cent.
		$\delta x_{\rm H_2}$	ERROR: = $\pm 0.1$ ; $\delta p / MPa = \pm 0.01$ ; = $\pm 2.0$ %. Imated by compiler)
		REFERENCES:	

COMPONENTS:		ORIGINAL MEA	ORIGINAL MEASUREMENTS:		
1. Hydrogen; H	2; [1333-74-0]	Brunner, B	Brunner, E.		
2. l-Methylpyrrolidine; C ₅ H ₁₁ N; [120-94-5].		Ber. Bunse 798-805.	Ber. Bunsenges. Phys. Chem. 1978, 82, 798-805.  PREPARED BY:		
		PREPARED BY:			
Temperature, pressure			C.L. Young		
EXPERIMENTAL VALUES		<del>_</del>			
т/к	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4 \mathrm{x}$ Mole fraction of hydrogen, $10^4 x_{\mathrm{H}_2}$		
298.15	0.15 31.7 65.6 98.0	0 31.6 65.5 97.9	0 128.5 256 374		
323.15	0.40 30.3 59.7 99.2	0 29.9 59.3 98.8	0 141.5 269 439		
373.15	1.95 32.6 84.9	0 30.7 83.1	0 193.2 485		
+ total	pressure				
* partia	l pressure				
		· · · · · · · · · · · · · · · · · · ·			

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. BASF Aktiengesellschaft sample, purity 99 per cent 0.4 weight per cent water.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \delta p/MPa = \pm 0.01; \\ \delta x_{H_2} = \pm 2.0%.$ 

(estimated by compiler)

### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. 2. Pyrrolidine; C4H9N; [123-75-1] Ber. Bunsenges. Phys. Chem. 1978, 82, 798-805. VARIABLES: PREPARED BY: C.L. Young. Temperature, pressure EXPERIMENTAL VALUES: p*/10⁵Pa p⁺/10⁵Pa 10 x Mole fraction T/K of hydrogen, $10^4x_{\rm H_2}$ 298.15 0.08 0 0 45.3 102.7 45.2 95.5 102.6 207.4 323.15 0.27 0 36.4 93.3 36.7 88.5 88.2 216.8 0 373.15 1.53 151.5 42.0 40.5 93.4 91.9 327 + total pressure partial pressure

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer.
After equilibrium established
liquid sample withdrawn and analysed
by stripping out hydrogen.
Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{H_2} = \pm 2.0$ %.

(estimated by compiler)

COMPONENTS:		ORIGINAL MEAS	UREMENTS:		
1. Hydrogen; H	1. Hydrogen; H ₂ ; [1333-74-0]		Brunner, E.		
2. Piperidine,	C ₅ H ₁₁ N; [100-89-	Ber Bunse 798-805	nges. Phys. Chem. <u>1978</u> , 82		
VARIABLES:	V	PREPARED BY:			
Tempera	ture, pressure		C.L. Young.		
EXPERIMENTAL VALUES:					
т/к	P ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	10 $^{\circ}$ x Mole fraction of hydrogen, 10 $^{\circ}$ $_{\rm H_2}$		
298.15	0.04 40.2 87.0	0 40.2 87.0	0 99.2 204		
323.15	0.14 45.4 98.2	0 45.3 98.1	0 136.7 283		
373.15	0.85 28.1 51.1	0 27.3 50.5	0 116.7 210.7		
+ total p	essure.				
* partial	pressure.				
		· · · · · · · · · · · · · · · · · · ·			

# AUXILIARY INFORMATION

# ${\tt METHOD/APPARATUS/PROCEDURE:}$

Static cell fitted with stirrer.
After equilibrium established
liquid sample withdrawn and analysed
by stripping out hydrogen. Details
in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Merck AG sample, purity 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/MPa = \pm 0.01; \\ \delta x_{\rm H_2} = \pm 2.0 \%. \\ ({\rm estimated \ by \ compiler.})$ 

PEPPENCEC.

- 1. Hydrogen; H₂; [1333-74-0]
- N,N-dimethyl-1,3-propanediamine, (1-Dimethylamino-3-propylamine); C₅H₁4N₂; [109-55-7].

### ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. <u>1978</u>, 82, 798-805.

VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

### EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	10 4 x Mole fraction of hydrogen, 10 4 x $_{\rm H_2}$
298.15	0.008	0	0
	44.2	44.2	137.9
	69.6	69.6	210
	105.1	105.1	313
323.15	0.04	0	0
	56.5	56.5	208
	82.9	82.9	299
373.15	0.34	0	0
	67.3	67.0	337
	93.6	93.3	457
	95.9	95.6	464
+ total p	pressure		

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

* partial pressure.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample, purity 98 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{\rm H_2} = \pm 2.0$ %. (estimated by compiler)

### 502 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; $H_2$ ; [1333-74-0] Brunner, E. 1-Methylpiperidine; $C_6H_{14}N_2$ ; [109-55-7] 2. Ber. Bunsenges. Phys. Chem. 1978, 82, 798-805. **VARIABLES:** PREPARED BY: C.L. Young. Temperature, pressure EXPERIMENTAL VALUES: $10^4 \times Mole fraction$ of hydrogen, $10^4 x_{\rm H_2}$ $p^{+}/10^{5}$ Pa $p^{*}/10^{5}$ Pa T/K 298.15 0.05 0 0 27.8 27.8 113 50.1 50.1 197 103.0 103.0 385 323.15 0.17 0 29.6 29.4 136 53.4 53.2 240 98.9 98.7 422 0 1.03 373.15 50.6 49.6 298 98.0 97.0 557 + total pressure. * partial pressure

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer.
After equilibrium established
liquid sample withdrawn and
analysed by stripping out hydrogen.
Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. Merck AG sample, purity 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{H_2} = \pm 2.0$ %.

(estimated by compiler)

### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Brunner, E. Ber. Bunsenges. Phys. Chem. 1978, N, N-Diethylethanamine, (Triethylamine); C6H15N; 82, 798-805. [121-44-8] VARIABLES: PREPARED BY: Temperature, pressure. C.L. Young. EXPERIMENTAL VALUES: $10^4 \mathrm{x}$ Mole fraction of hydrogen, $10^4 x_{\mathrm{H}_2}$ $p^{*}/10^{5}$ Pa $p^{+}/10^{5}$ Pa T/K 293.15 0.09 0 34.0 199.5 34.1 52.7 308.0 52.8 93.8 93.7 535 323.15 0.37 0 0 20.7 149.1 21.1 349.6 49.7 50.1 81.9 82.2 560 373.15 1.40 0 0 25.5 230.9 26.9 93.2 94.5 798 97.5 98.8 836 total pressure. partial pressure AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static cell fitted with stirrer. No details given. After equilibrium established liquid sample withdrawn and BASF Aktiengesellschaft sample 2. analysed by stripping out hydrogen. purity 99.5 mole per cent. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta p/MPa = \pm 0.01$ ; $\delta x_{\rm H_2} = \pm 2.0\%$ . (estimated by compiler). REFERENCES:

### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; $H_2$ ; [1333-74-0] Brunner, E. 1,6-Hexanediamine, (1,6-Ber Bunsenges. Phys. Chem. 1978, 82, 2. Diaminohexane); C6H16N2; 798-805 [124-09-4] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young. EXPERIMENTAL VALUES: p⁺/10⁵Pa p*/10⁵Pa T/K 10 4x Mole fraction of hydrogen, 10 xH 2 298.15 0.002 0 0 95.3 232.0 95.3 147.9 147.9 348.7 202.7 202.6 469.6 301.9 672 301.9 0.009 0 323.15 0 144.1 49.4 49.4 425.8 147.9 147.9 301.9 301.9 810 373.15 0.03 0 0 49.4 169.7 49.4 171.2 49.4 49.4 490.9 147.9 147.9 147.9 147.9 488.6 300.9 300.9 948 total pressure. partial pressure. AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

- No details given.
- 2. BASF Aktiengesellschaft sample purity 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/MPa = \pm 0.01;$  $\delta x_{\rm H_2} = \pm 2.0\%.$ 

(estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. N-(3-aminopropyl)- 1,3-propane diamine), (Bis-(3-aminopropyl)- amine);  $C_6H_{1.7}N_3$ ; [56-18-8]

### ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. <u>1978</u>, 82, 798-805.

### VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

### EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	10 $^{\circ}$ x Mole fraction of hydrogen, 10 $^{\circ}$ $x_{\rm H_2}$
298.15	0.0004	0	0
	61.0	61.0	91.0
	97.4	97.4	143
323.15	0.003	0	0
	47.4	47.4	91.6
	85.5	85.5	161
373.15	0.008	0	0
	42.1	42.1	120
	99.5	99.5	267

- + total pressure
- partial pressure.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample, purity 99.2 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/MPa = \pm 0.01; \ \delta x_{H_2} = \pm 2.0$ 

(estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- N,N-Dimethylcyclohexanamine, (Dimethylaminocyclohexane); C₈H₁₇N; [98-94-2]

### ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. <u>1978</u>, 82, 798-805.

### VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young.

### EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4$ x Mole fraction of hydrogen, $10^4x_{ m H_2}$
298.15	0.003	0	0
	50.4	50.4	198
	83.0	83.0	315
323.15	0.01	0	0
	41.6	41.6	190
	79.4	79.4	351
373.15	0.14	0	0
	48.9	48.8	288
	89.0	48.9	506

* partial pressure.

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample, purity 98 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta p/\text{MPa} = \pm 0.01; \\ \delta x_{\text{H}_2} = \pm 2.0 \text{\$}. \\ \text{(estimated by compiler)}$ 

COMPONENTS:		ORIGINAL MEAS	SUREMENTS:
1. Hydrogen; H ₂	. Hydrogen; H ₂ ; [1333-74-0]		Ε.
2. N-Butyl-1-butanamine, (Dibutylamine); C ₀ H ₁₉ N; [111-92-2]		Ber. Buns 82, 798-8	enges. Phys. Chem. <u>1978</u> ,
VARIABLES:		PREPARED BY:	
Temperatur	e, pressure		C.L. Young.
EXPERIMENTAL VALUES:			······································
T/K	p ⁺ /10 ⁵ Pa	p [*] /10 ⁵ Pa	$10^4  imes  ext{Mole fraction}$ of hydrogen, $10^4  imes_{ ext{H}_2}$
298.15	0.004 39.9 72.7 92.3	0 39.9 72.7 92.3	0 219 388 487
323.15	0.02 23.8 54.7 75.7	0 23.8 54.7 75.7	0 159 354 482
373.15	0.19 20.7 50.2 83.9	0 20.5 50.0 83.8	0 179 421 681
+ total p	ressure		
* partial	pressure		

### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample, purity 98 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{H_2} = \pm 2.0$ %

(estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- N-(2-aminoethy1)-N(3-aminopropy1)-1,3-propanediamine, (N,N-Bis-(3-aminopropy1)-ethylenediamine;C₈H₂2N₄;
  [41240-13-5]

### ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges. Phys. Chem. <u>1978</u>, 82, 798-805.

### VARIABLES:

Temperature, pressure.

### PREPARED BY:

C.L. Young.

### EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4 x$ Mole fraction of hydrogen, $10^4 x_{ m H_2}$
298.15	0.0001	0	0
	31.5	31.5	55.0
	60.9	60.9	106
	91.5	91.5	157
323.15	0.0001	0	0
	44.8	44.8	98
	87.3	87.3	189
373.15	0.0007	0	0
2.0120	44.3	44.3	142
	83.9	83.9	264

- + total pressure.
- partial pressure.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- BASF Aktiengesellschaft sample, purity 98.2 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{\rm H_2} = \pm 2.0$ %. (estimated by compiler)

# COMPONENTS: 1. Hydr 2. N,N-

. Hydrogen; H₂; [1333-74-0]

N,N-Dibutyl-1-butanamine, (Tri-n-butylamine); C₁₂H₂₇N; [102-82-9] ORIGINAL MEASUREMENTS:

Brunner, E.

Ber. Bunsenges, Phys. Chem. <u>1978</u>, 82, 798-805.

### VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young.

### EXPERIMENTAL VALUES:

T/K	p ⁺ /10 ⁵ Pa	p*/10 ⁵ Pa	$10^4 x$ Mole fraction of hydrogen, $10^4 x_{ m H_2}$
298.15	0.0004	0	0
	43.8	43.8	315
	75.5	75.5	522
	90.6	90.6	630
323.15	0.002	0	0
	44.0	44.0	363
	75.0	75.0	607
373.15	0.03	0	0
	44.1	44.1	453
	76.8	76.8	759

- total pressure,
- partial pressure.

# AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static cell fitted with stirrer. After equilibrium established liquid sample withdrawn and analysed by stripping out hydrogen. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2. BASF Aktiengesellschaft sample purity 98 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x_{H_2} = \pm 2.0$ %. (estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Quinoline; C₉H₇N; [91-22-5]

### ORIGINAL MEASUREMENTS:

Sebastian, H.M., Simnick, J.J.; Lin, H-M.; Chao, K.-C.

J. Chem. Engng. Data. 1978, 23,305-8

### **VARIABLES:**

Temperature, pressure

PREPARED BY:

C.L. Young

XPERIME:	NTAL VALUES:	Mole frac	tion of			Mole frac	ction of
т/к	P/bar	hydroge liquid, ^x H ₂	n in gas, ^y H ₂	т/к	P/bar	hydroge liquid, ^x H ₂	en in gas, ^y H ₂
462.45	0.3156 20.14 30.46 50.65 101.3 152.4 202.7 253.0	0.0000 0.0072 0.0110 0.0180 0.0359 0.0527 0.0700 0.0857	0.0000 0.9845 0.9893 0.9930 0.9963 0.9972 0.9977	621.75	7.397 20.32 30.52 50.65 101.7 151.7 201.9 253.0	0.0000 0.0097 0.0169 0.0308 0.0652 0.0965 0.1290 0.1532	0.0000 0.6029 0.7282 0.8278 0.9040 0.9345 0.9465 0.9539
541.85	1.943 20.27 30.39 50.72 100.99 152.4 202.7 253.0	0.0000 0.0095 0.0147 0.0252 0.0495 0.0730 0.0946 0.1160	0.0000 0.8959 0.9277 0.9558 0.9757 0.9821 0.9861 0.9878	701.65	19.81 30.66 50.65 102.0 151.3 201.6 252.7	0.0000 0.0118 0.0332 0.0837 0.1294 0.1708 0.2071	0.0000 0.2607 0.5107 0.7143 0.7939 0.8333 0.8634

### AUXILIARY INFORMATION

### METHOD: /APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure with Bourdon gauge.

### SOURCE AND PURITY OF MATERIALS:

- 1. Air products sample, minimum purity 99.95 mole per cent.
- 2. Fisher Scientific Co. sample, distilled over zinc under helium, purity better than 99 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.5$ %;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 0.001$ .

(estimated by compiler)

- 1. Hydrogen;  $H_2$ ; [1333-74-0]
- 2. l-Methyl-2-pyrrolidinone, (N-methylpyrrolidinone); C₅H₉NO; [872-50-4]

ORIGINAL MEASUREMENTS:

Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. *Khim. Prom.* 1973, 49, 108-110.

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMENTAL	VALUES:	Walls Greation of hydrogen	.1.
т/к	P/bar	Mole fraction of hydrogen in liquid, ${}^x_{ m H_2}$	α [†] vol/vol
283.15	66.2	0.0079	1.84
	74.6	0.0088	2.06
	78.4	0.0092	2.16
	87.2	0.0103	2.42
	96.2	0.0114	2.67
	122.6	0.0142	3.35
298.15	60.3	0.0082	1.92
	69.6	0.0095	2.22
	83.9	0.0108	2.52
	98.1	0.0129	3.02
	107.1	0.0144	3.38
	118.1	0.0156	3.67
323.15	130.4	0.0172	4.05
	72.1	0.0117	2.74
	77.5	0.0122	2.87
	96.7	0.0152	3.59
	105.0	0.0162	3.82
	112.8	0.0174	4.10
	116.7	0.0181	4.28
	137.3	0.0214	5.07

quoted in original paper, appears to be volume of gas at T/K = 273.15 and P = 1 atmosphere adsorbed by unit volume of liquid at room temperature.

### AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

Mixture stirred by ball in rocking autoclave. Sample of liquid analysed by a volumetric method. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Dried and oxygen removed; purity 99.8 mole per cent.
- Distilled; purity 99.9 mole per cent determined by gas chromatography.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$ ;

 $\delta x_{\rm H_2} = \pm 5$ % (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 1,5-Dimethyl-2-pyrrolidinone,
   (5-methyl-N-methylpyrrolidinone);
   C₆H₁₁NO; [5075-92-3]

### ORIGINAL MEASUREMENTS:

Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. Khim. Prom. 1973, 49, 108-110.

### VARIABLES:

Temperature, pressure

### PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

т/к	P/bar	Mole fraction of hydrogen in liquid, $^{x}{ m H}_{2}$	α [†] vol/vol
283.15	80.5	0.0128	2.65
	94.1	0.0149	3.09
	113.8	0.0178	3.70
298.15	76.5	0.0135	2.80
	99.1	0.0169	3.51
	127.5	0.0223	4.66
323.15	76.5	0.0158	3.28
	95.7	0.0194	4.04
	122.6	0.0257	5.37

 $^{^\}dagger$  quoted in original paper, appears to be volume of gas at T/K = 273.15 and  p  = 1 atmosphere adsorbed by unit volume of liquid at room temperature.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Mixture stirred by ball in rocking autoclave. Sample of liquid analysed by a volumetric method. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Dried and oxygen removed; purity 99.8 mole per cent.
- Distilled; purity 99.3 mole per cent determined by gas chromatography.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/\text{bar} = \pm 0.1;$  $\delta x_{\text{H}_2} = \pm 5\% \text{ (estimated by compiler)}.$ 

- 1. Hydrogen; H₂; [1333-74-0]
- Tetrafluoromethane, (Perfluoromethane); CF₄; [75-73-0]

### ORIGINAL MEASUREMENTS:

Shiau, J.F.; Ziegler, W.T.

J. Chem. Engng. Data. 1980, 25, 239-246.

### VARIABLES:

Temperature, pressure

### PREPARED BY:

C.L. Young

XPERIMENTAL VALUI	ES:		Mole fraction	of hydrogen
T/K	P/atm	P/MPa	in liquid	in vapor
			$x_{ m H_{2}}$	$y_{ m H_2}$
164.99	20.13	2.0397	0.01644	-
	40.30	4.083	0.03545	0.8780
	40.30	4.083	0.03511	0.8788
	40.30	4.083	0.03517	0.8784
	59.91	6.070	0.05437	0.9059
	80.19	8.125	0.07115	0.91434
	100.06	10.139	0.08965	0.91985
	100.04	10.137	0.0998	0.92016
	119.99	12.158	-	0.92332
149.98	20.05	2.0316	0.01433	0.91299
	40.30	4.083	0.02923	0.94665
	59.76	6.055	0.04377	0.95667
	80.04	8.110	0.05886	0.96057
	100.06	10.139	0.07011	0.96259
	120.06	12.165	0.08446	0.96305
135.01	20.19	2.046	0.01198	0.96946
	40.30	4.083	0.02355	0.98018
	60.17	6.097	0.03399	0.98324
	80.11	8.117	0.04475	0.98441
	100.11	10.144	0.05578	0.98466
	120.05	12.164	0.06287	0.98441

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Single pass flow apparatus with two compartment equilibrium cell. Temperature measured with platinum resistance thermometer; pressure measured with Bourdon gauge. Pure hydrogen bubbled through liquid fluorocarbon. Samples analysed by gas chromatography. Details in source and ref. 1.

### SOURCE AND PURITY OF MATERIALS:

- Airco sample, purity 99.97 mole per cent.
- Du Pont de Nemours Inc. sample, purity 99.9 mole per cent.

### ESTIMATED ERROR:

 $\begin{array}{lll} \delta {\rm T/K} &=& \pm 0.03; & \delta P/{\rm MPa} &=& \pm 0.5 \\ \delta x_{\rm H_2} &=& \pm 2.0 \\ \ast; & \delta (1 - y_{\rm H_2}) &=& \pm 2.5 \\ \end{array}$ 

### REFERENCES:

1. Kirk, B.S.; Ziegler, W.T.

Adv. Cryogen. Eng. 1965, 10, 160

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Tetrafluoromethane, (Perfluoromethane); CF₄; [75-73-0]

# ORIGINAL MEASUREMENTS:

Shiau, J.F.; Ziegler, W.T.

J. Chem. Engng. Data. 1980, 25, 239-246.

EXPERIMENTAL	VALUES:
11371 111/11/11/11/11/11/11/11/11/11/11/11/1	ATTORD.

T/K	P/atm	P/MPa	Mole fraction in liquid	in vapor
-/	1,400	171114	x _{H₂}	y _{H₂}
119.94	20.06	2.033	0.008981	0.991922
	40.01	4.054	0.01793	0.994517
	60.38	6.118	0.02576	0.995034
	79.91	8.097	0.03216	0.995020
	100.08	10.141	0.03970	0.994854
	119.98	12.157	0.04657	0.994569
L05.01	20.07	2.034	0.006356	0.998655
	40.19	4.072	0.01201	0.998904
	60.18	6,098	0.01704	0.998905
	79.93	8,099	0.02179	0.998907
	99.99	10.131	0.02629	0,998716
	120.00	12.159	0.03048	0.998537
94.94	20.14	2.041	0.004676	0.9996676
	20.21	2,048	0.004692	0.9996570
	20.09	2.036	0.004682	0.9996722
	40.37	4.090	0.008833	0.9997177
	60.17	6.097	0.01262	0.9996845
	80.04	8.110	0.01572	0.9996921
	100.06	10.139	0.01846	0.9995534
	119.94	12.153	0.02136	0.9994568
	119.38	12.096	0.02114	0.9994667
	119.38	12.096	0.02123	0.9994664

### Miscellaneous Organic Fluids 515 ORIGINAL MEASUREMENTS: COMPONENTS: Hydrogen; H₃; [1333-74-0] Shiau, J.F.; Ziegler, W.T. Chlorotrifluoromethane; CClF3; J. Chem. Engng. Data. 1980, 25, 239-246. [75-72-9] VARIABLES: PREPARED BY: C.L. Young. Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen P/MPa in liquid, in vapor, T/K P/atm $x_{\rm H_2}$ $y_{\rm H_2}$ 0.01630 219.99 20.20 2.047 0.7883 2.094 0.01620 0.7850 20.67 2.033 0.01616 0.7811 20.06 0.03481 4.043 0.8758 39.90 6.060 0.05340 0.90199 59.90 0.07213 0.91845 79.91 8.097 99.98 10.130 0.08984 0.92646 0.10487 0.93239 12.158 119.99 0.10585 0.93267 119.99 12.158 0.01544 205.03 2.047 0.8872 20.20 40.10 4.063 0.02213 0.93180 6.069 0.04773 0.94861 59.90 79.91 8.097 0.06412 0.95539 . 10.148 0.07869 0.95898 100.15 120.02 12.161 0.09365 0.96117 0.01407 189.97 20.09 2.036 0.94449 0.96707 0.02920 40.16 4.069 59.76 6.055 0.04201 0.97460 0.97710 8.096 79.90 80.25 8.131 0.05480 0.97724 0.97898 0.06890 99.91 10.123 119.98 12.157 0.08200 0.97976 AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Single pass flow apparatus with two Airco sample, purity 99.97 mole compartment equilibrium cell. per cent. Temperature measured with platinum 2. Du Pont de Nemours inc. sample resistance thermometer; pressure measured with Bourdon gauge. Pure purity 99.9 mole per cent. hydrogen bubbled through liquid fluorocarbon. Samples analysed by gas chromatography. Details in source and ref. (1).

### ESTIMATED ERROR:

$$\delta T/K = \pm 0.03$$
;  $\delta P/MPa = \pm 0.5$ %  $\delta x_{\rm H_2} = \pm 2.0$ %;  $\delta (1-y_{\rm H_2}) = \pm 3$ %

### REFERENCES:

Kirk, B.S.; Ziegler, W.T.
 Adv. Cryogen. Eng. 1965, 10, 160.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Chlorotrifluoromethane; CClF3;
  [75-72-9]

# ORIGINAL MEASUREMENTS:

Shiau, J.F.; Ziegler, W.T.

J. Chem. Engng. Data. <u>1980</u>, 25, 239-246.

EXPERIMENTAL	VALUES:			
m /**	D /- 1	D /44D	Mole fraction	3 3
T/K	P/atm	P/MPa	in liquid,	in vapor,
			x _{H2}	^у н ₂
175.02	20.06	2.036	0.01212	0.97632
	40.37	4.090	0.02448	0.98622
	59.97	6.076	0.03647	0.98858
	79.70	8.076	0.04673	0.98972
	99.91	10.123	0.05716	0.99026
	119.88	12.157	0.06864	0.990397
160.02	20.13	2.040	0.01055	0.992078
	40.17	4.070	0.02018	0.994890
	59.77	6.056	0.03090	0.995764
	79.63	8.069	0.03909	0.996097
	100.05	10.138	0.04790	0.996199
	119.99	12.158	0.05681	0.996087
145.02	20.26	2.053	0.008783	0.997836
	40.23	4.076	0.01667	0.998583
	59.97	6.076	0.02446	0.998700
	79.50	8.055	0.03182	0.998746
	99.84	10.116	0.03889	0.998704
	119.92	12.151	0.04553	0.998637
134.97	20.09	2.036	0.007477	0.999263
	20.06	2.033	0.007453	0.999251
	20.06	2.033	0.007382	0.999252
	40.17	4.070	0.01419	0.999473
	59.83	6.062	0.02051	0.999511
	79.63	8.069	0.02674	0.999497
	99.84	10.116	0.03311	0.999463
	119.91	12.150	0.03894	0.999408
	120.02	12.161	0.03894	0.999413

- 1. Hydrogen, H₂; [1333-74-0]
- Benzo [b] thiophene, (Thianaphthene); C₀H₆S; [95-15-8]

# ORIGINAL MEASUREMENTS:

Sebastian, H.M.; Simnick, J.J.; Lin, H.M.; Chao, K.C.

Can. J. Chem. Engng. 1978, 56,743-6

### VARIABLES:

Temperature, pressure

PREPARED BY:

C.L. Young

ion of budueses
ion of hydrogen in gas
——————————————————————————————————————
у _{Н 2}
0.9768
0.9836
0.9904
0.9944
0.9958
0.9965
0.9970
0.0000
0.8626
0.9070
0.9384
0.9653
0.9750
0.9801
0.9835
0.0000
0.5045
0.6635
0.7923
0.8839
0.9156

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell. Composition of samples found by stripping out gas and estimating volumetrically and solvent gravimetrically. Temperature measured with thermocouple and pressure measured with Bourdon gauge. Details in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Air Products sample, minimum purity 99.95 mole per cent.
- Aldrich sample, zone refined and colourless sections used combined with fraction obtained by distillation.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 1$ %.

### REFERENCES:

1. Simnick, J.J. Lawson, C.C.; Lin, H.M.; Chao, K.C.

Am. Inst. Chem. Engnrs. J. <u>1977</u>, 23, 469.

- 1. Hydrogen, H₂; [1333-74-0]
- 2. Benzo [b] thiophene,
   (Thianaphthene); C₈H₆S;
   [95-15-8]

# ORIGINAL MEASUREMENTS

Sebastian, H.M.; Simnick, J.J. Lin, H.M.; Chao, K.C.

Can. J. Chem. Engng. 1978, 56, 743-6.

### EXPERIMENTAL VALUES:

T/K	P/MPa	Mole fraction of in liquid, $^{x}{ m H}_{2}$	f hydrogen in gas, ^y H ₂	
621.2	20.31	0.1307	0.9330	
	25.30	0.1585	0.9425	
702.7	3.071	0.0087	0.1834	
	5.049	0.0315	0.4148	
	10.062	0.0861	0.6565	
	15.13	0.1431	0.7601	
	20.19	0.1836	0.8060	
	25.33	0.2260	0.8437	

^{*} vapor pressure of pure thianaphthene.

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. Khim. Prom. 1973, 49, 108-110. 2. Tributyl phosphate; C12H27PO4; [126-73-8] VARIABLES: PREPARED BY: C. L. Young Pressure **EXPERIMENTAL VALUES:** Mole fraction $\alpha^{\,\dagger}$ of hydrogen T/K P/bar vol/vol in liquid, $x_{\rm H_2}$ 1.50 313.15 22.8 0.0171 2.59 42.3 0.0292 0.0403 59.4 3.62 5.08 83.1 0.0557

5.98

6.29

7.17

0.0649

0.0681

0.0769

### AUXILIARY INFORMATION

### METHOD / APPARATUS / PROCEDURE:

98.6

104.8

116.7

Mixture stirred with ball in rocking autoclave. Sample of liquid analysed by a volumetric method. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Dried and oxygen removed, purity 99.8 mole per cent.
- 2. Analytical grade sample.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$ ;  $\delta x_{\rm H_2} = \pm 5$ % (estimated by compiler).

[†] quoted in original paper, appears to be volume of gas at T/K = 273.15 and P = 1 atmosphere adsorbed by unit volume of liquid at room temperature.

# COMPONENTS: ORIGINAL MEASUREMENTS: Cannon, P.; St. Pierre, L.E.; Miller, A.A. Hydrogen; H₂; [1333-74-0] 2. Octamethylcyclotetrasiloxane; J. Chem. Engng. Data. 1960, 5, 236. $C_8H_2 + O_4Si_4$ ; [556-67-2] VARIABLES: PREPARED BY: Pressure C.L. Young EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K p/MPa in liquid 0.77 0.058 303.5 1.55 0.115 2.14 0.161

### AUXILIARY INFORMATION

### METHOD APPARATUS / PROCEDURE:

Automatic gravimetric sorption balance. Mass of hydrogen determined directly. Correction for buoyancy made. Pressure measured with Bourdon gauge.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Purified by distillation, no other details given.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.01$ ;  $\delta x = \pm 0.001$ 

(estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hydrocarbon Blend (Heavy naphtha)

ORIGINAL MEASUREMENTS:

Frolich, P. K.; Tauch, E. J.; Hogan, J. J.; Peer, A. A.

Ind. Eng. Chem. 1931, 23, 548-550.

VARIABLES:

PREPARED BY:

Pressure

C. L. Young

### EXPERIMENTAL VALUES:

T/K	P/atm	P/MPa	Solubility, $s^*$
298.15	10	1.0	0.75
	20	2.0	1.5
	30	3.0	2.25
	40	4.1	3.0
	50	5.1	3.7
	60	6.1	4.4
	70	7.1	5.1
	80	8.1	5.8
	90	9.1	6.5
	100	10.1	7.2
	110	11.1	7.9
	120	12.2	8.6
	130	13.2	9.3
	140	14.2	10.0
	150	15.2	10.7
	160	16.2	11.4
	170	17.3	12.1
	180	18.3	12.8

Volume of gas measured at 101.325 kPa pressure and 298.15 K dissolved by unit volume of liquid measured under the same conditions.

### AUXILIARY INFORMATION

# METHOD APPARATUS / PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric method. Allowance was made for vapor pressure of liquid and the solubility of the gas at atmospheric pressure. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen was of the highest purity available.
- Density 0.8003 g cm⁻³, vapor pressure 80 mmHg at 298.15 K.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S = \pm 5\%.$ 

# COMPONENTS: ORIGINAL MEASUREMENTS: Frolich, P. K.; Tauch, E. J.; 1. Hydrogen; H₂; [1333-74-0] Hogan, J. J.; Peer, A. A. Ind. Eng. Chem. 1931, 23, 548-550. 2. Hydrocarbon Blend (Gas oil) VARIABLES: PREPARED BY: C. L. Young

1		
EVDE	RIMENTAL	WAT IICC.
CAFE	KILENIAL	VALUES:

Pressure

T/K	P/atm	P/MPa	Solubility, $s^{*}$
298.15	10	1.0	0.67
	20	2.0	1.34
	30	3.0	2.01
	40	4.1	2.68
	50	5.1	3.35
	60	6.1	4.02
	70	7.1	4.69
	80	8.1	5.36
	90	9.1	6.03
	100	10.1	6.70
	110	11.1	7.37
	120	12.2	8.04
	130	13.2	8.71
	140	14.2	9.38
	150	15.2	10.35
	160	16.2	10.72
	170	17.3	11.39
	180	18.3	12.06

Volume of gas measured at 101.325 kPa pressure and 298.15 K dissolved by unit volume of liquid measured under the same conditions.

### AUXILIARY INFORMATION

# METHOD APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid saturated with gas and after equilibrium established samples removed and analysed by volumetric Allowance was made for vapor pressure of liquid and the solubility of the gas at atmospheric pressure. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Hydrogen was of the highest purity available.
- 2. Density 0.8319 g  $cm^{-3}$ , vapor pressure 2 mmHg at 298.15 K.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta S = \pm 5\%.$ 

### Miscellaneous Organic Fluids COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Prather, J. W.; Ahangar, A. M.; Pitts, W. S.; Henley, J. P.; 2. Solvent Refined Coal Recycle Oil Tarrer, A. R.; Guln, J. A. Ind. Eng. Chem. Process. Des. Dev. 1977, 16, 267-270. VARIABLES: PREPARED BY: C. L. Young Temperature, pressure EXPERIMENTAL VALUES: Solubility, S (g of $H_2/10^4$ g $^{P}_{\rm H_{2}}$ $P_{\rm H_2}$ Solubility, S $P_{\rm H_2}$ $^{P}_{\rm H_{2}}$ $(g \text{ of } H_2/10^4g)$ of oil) T/K /MPa T/K /psia /MPa /psia of oil) 473.15 573.15 1289 8.89 1104 7.61 11.59 12.29 1089 7.51 10.74 1974 13.61 20.57 1994 7.25 13.75 1051 10.88 19.44 2124 14.64 19.72 1979 13.64 19.46 19.29 2891 19.93 30.50 2084 14.37

20.68

29.73

26.33

24.93

5.58

6.38

6.28

12.47

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

2043

3130

2959

2845

639

614

599

1204

573.15

14.09

21.58

20.40

19.62

4.41

4.23

4.13

8.30

Stirred equilibrium cell of 1 U.S. gallon capacity. Pressure measured with Bourdon gauge and temperature with thermocouple. Samples of liquid and vapor analysed by volumetric methods and gas chromatography, respectively.

# SOURCE AND PURITY OF MATERIALS:

2899

2882

3170

1105

1048

1820

1758

2291

2267

673.15

19.99

19.87

21.86

7.62

7.23

12.55

12.12

15.80

15.63

27.78

28.90

34.23

15.86

16.50

26.30

26.51

35.36

33.22

- 1. Linde sample, purity 99.995 mole per cent.
- 2. Wilsonville recycle solvent. Detailed description given in ref. (1).

### ESTIMATED ERROR:

 $\delta T/K = \pm 1$ %;  $\delta S = \pm 4-6$ %.

### REFERENCES:

1. S.R.C. Tech. Report No. 7. Analysis of Operations, Solvent Refined Coal Pilot Plant, Southern Services Inc. Wilsonville 1975.

## COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Prather, J. W.; Ahangar, A. M.; Pitts, W. S.; Henley, J. P.; 2. Creosote Oil Tarrer, A. R.; Guln, J. A. Ind. Eng. Chem. Process. Des. Dev. 1977, 16, 267-270. VARIABLES: PREPARED BY:

Temperature, pressure

C. L. Young

EXPERIMENT	AL VALUES			***			
Ì	$P_{}$	PH ₂	Solubility, S		P _{H2}	P _{H2}	Solubility, S
	H ₂	H 2	$(g \text{ of } H_2/10^4g)$		,H ₂	H ₂	$(g \text{ of } H_2/10^4g$
T/K	/psia	/MPa	of oil)	T/K	/psia	/MPa	of oil)
373.15	510	3.52	2.95	473.15	2003	13.81	13.05
3,0120	515	3.55	3.00		2007	13.84	14.08
<b>\</b>	1015	7.00	5.97		2009	13.85	13.66
į	1015	7.00	5.92		2507	17.29	17.20
	1515	10.45	7.78		2946	20.31	19.54
i	1513	10.43	8.27		2999	20.68	19.80
	2015	13.89	11.66	573.15	506	3.49	3.7
1	2013	13.88	11.62		526	3.63	3.95
ł	2015	13.89	12.00		986	6.80	8.06
	2515	17.34	15.48		1005	6.93	7.42
	2512	17.32	15.56		1025	7.07	7.62
	2512	17.32	14.79		1487	10.25	11.14
ì	2765	19.06	17.57		1504	10.37	11.73
	2961	20.42	17.16		1528	10.54	10.38
l	3015	20.79	19.00		1987	13.70	15.83
1	3015	20.79	17.30		2002	13.80	16.37
473.15	507	3.50	4.26		2496	17.21	19.74
1	534	3.68	4.76		2497	17.22	19.73
	600	4.14	5.03		2945	20.31	23.21
1	1008	6.95	7.16		2986	20.59	23.88
	1009	6.96	6.95		3060	21.10	22.25
	1011	6.97	6.60	673.15	385	2.65	4.32
1	1509	10.40	12.65		390	2.69	3.60
1	1509	10.40	11.29		448	3.09	3.68
	1567	10.80	12.54				(cont.)

### AUXILIARY INFORMATION

### METHOD 'APPARATUS / PROCEDURE:

Stirred equilibrium cell of 1 U.S. gallon capacity. Pressure measured with Bourdon gauge and temperature with thermocouple. Samples of liquid and vapor analysed by volumetric methods and gas chromatography, respectively.

### SOURCE AND PURITY OF MATERIALS:

- 1. Linde sample, purity 99.995 mole per cent.
- 2. Allied Chemical Co. sample 24-CB; boiling range 175 to 350 °C. Density at 293.15 K = 1.096 g cm⁻³. Detailed analysis in source.

ESTIMATED ERROR:

 $\delta T/K = \pm 1\%; \quad \delta S = \pm 4-6\%.$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Creosote Oil

## ORIGINAL MEASUREMENTS:

Prather, J. W.; Ahangar, A. M.;
Pitts, W. S.; Henley, J. P.;
Tarrer, A. R.; Guln, J. A.

Ind. Eng. Chem. Process. Des. Dev.
1977, 16, 267-270.

### EXPERIMENTAL VALUES:

T/K	P _{H2} /psia	P _{H2} /MPa	Solubility, S (g of H ₂ /10 g of oil)	T/K	P _{H2} /psia	P _{H₂} /MPa	Solubility, S (g of H ₂ /10 ⁴ g of oil)
673.15	850 864 865 1380 1388 1858	5.86 5.96 5.96 9.51 9.57 12.81	8.45 8.24 7.55 13.08 14.22 18.61 17.23	673.15	1899 2387 2403 2420 2875 2892 2979	13.09 16.46 16.57 16.69 19.82 19.94 20.54	17.63 21.81 22.98 23.93 26.96 29.16 28.99

.

- 1. Hydrogen; H₂; [1333-74-0]

### ORIGINAL MEASUREMENTS:

Grove, N.H.; Whiteley, F.J.; Woolmer, R.N.

J. Appl. Chem. 1960, 10, 101-109.

Santowax R;

### VARIABLES:

Temperature, pressure

### PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

T/K	P/bar	Solubility*	Ostwald coefficient
505	1.81	8.4	0.183
508	4.66	16.0	0.136
511	2.48	9.7	0.156
514	1.89	8.7	0.184
521	1.72	8.2	0.192
595	2.04	16.3	0.346
598	5.12	35.3	0.298
602	1.91	13.4	0.305
604	1.99	17.2	0.377
604	2.70	22.3	0.358
677	5.33	55.0	0.466
680	2.77	31.7	0.517
680	2.00	20.5	0.464
681	2.04	27.0	0.600
684	1.97	26.6	0.611

moles of hydrogen per mg of Santowax R.

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static cell with null pressure transducer. Pressure measured with Bourdon gauge. Temperature measured with thermocouple. Sample placed in cell and gas added at room temperature. Cell then heated to experimental temperature. Pressure on both sides of transducer kept approximately equal. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- Analysis by infrared method showed sample to be 11.8% o-terphenyl, 56.3% m-terphenyl, 29.3% p-terphenyl, 2.6% diphenyl and higher polyphenyls. Obtained from Monsanto Chemicals Limited.

### ESTIMATED ERROR:

 $\delta T/K = \pm 1$ ;  $\delta P/bar = \pm 0.01$ ;

 $\delta x_{\rm H_2} = \pm 10\%.$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
<ol> <li>Hydrogen; H₂; [1333-74-0]</li> <li>Jojoba Oil</li> </ol>	Wisniak, J.; Stein, S.  J. Amer. Oil Chem. Soc. 1974, 51, 482.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young
EXPERIMENTAL VALUES: †Mole frac	tion [†] Mole fraction

L							
EXPERIME	NTAL VAL	M	ole fraction				Mole fraction
T/K	P/bar	Kuenen coefficient,	of hydrogen	T/K	P/bar	Kuenen	of hydrogen $x_{\rm H_2}$
323.15	7.6	0.44	0.0118	423.15	34.5	3.11	0.0776
	13.8	0.84	0.0222		41.4	3.70	0.0910
1	20.7	1.21	0.0324		48.3	4.32	0.105
l	27.6	1.61	0.0417		55.2	4.90	0.116
	34.5	2.00	0.0513	473.15	7.6	0.80	0.0212
	41.4	2.41	0.0611		13.8	1.49	0.0387
ì	48.3	2.78	0.0700		20.7	2.20	0.0562
ĺ	55.2	3.18	0.0792		27.6	2.83	0.0711
373.15	7.6	0.56	0.0150		34.5	3.58	0.0882
ĺ	13.8	1.06	0.0280		41.4	4.29	0.104
l	20.7	1.50	0.0400		48.3	4.98	0.119
1	27.6	2.00	0.0513		55.2	5.64	0.132
	34.5	2.51	0.0635	523.15	7.6	0.91	0.0240
1	41.4	3.00	0.0750		13.8	1.69	0.0437
	48.3	3.49	0.0863		20.7	2.46	0.0624
}	55.2	3.97	0.0970		27.6	3.23	0.0803
423.15	7.6	0.68	0.0181		34.5	4.01	0.0979
	13.8	1.28	0.0333		41.4	4.80	0.115
	20.7	1.88	0.0484		48.3	5.58	0.131
	27.6	2.50	0.0634		55.2	6.37	0.147
<u>L</u>							

[†] Reported in source, calculated assuming a molecular weight of 606 for the jojoba oil.

### AUXILIARY INFORMATION

### METHOD /APPARATUS/PROCEDURE:

Static equilibrium cell. Liquid phase sample analysed by allowing hydrogen to bubble out at atmospheric pressure in a gas buret system.

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.9 mole per cent.
- Prepared by crushing jojoba seeds. Details of composition in source.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.5$ ;  $\delta P/bar = \pm 0.2$ ;  $\delta S = \pm 1-2\%$ ;  $\delta x_{\rm H_2} = \pm 1-2\%$ .

### 528 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; $H_2$ , [1333-74-0] Trust, D.B.; Kurata, F. 1. 2. Carbon Monoxide; CO; [630-08-0] Am. Inst. Chem. Engnrs. J. 1971, 17, 86-91. 3. Propane; $C_3H_8$ ; [74-98-6] VARIABLES: PREPARED BY: Temperature, pressure C.L. Young. EXPERIMENTAL VALUES: Liquid composition Vapor composition Mole fractions Mole fractions T/K p/MPa $x_{ m H_2}$ $x_{CO}$ x C $_{3}$ H $_{8}$ $y_{\rm H_2}$ $y_{CO}$ $y_{C_3H_8}$ 0.7830 223.15 3.447 0.0051 0.0724 0.9225 0.1933 0.0237 0.0092 0.0533 0.9375 0.3752 0.0153 0.6095 0.7607 0.0164 0.0191 0.9645 0.2253 0.0140 0.0115 0.0180 0.9705 0.8474 0.1414 0.0112 0.0311 6.895 0.0051 0.1683 0.8266 0.0702 0.8987 0.0107 0.1421 0.8472 0.1642 0.8087 0.0271 0.0180 0.1052 0.8768 0.3628 0.6132 0.0240 0.0300 0.0540 0.9160 0.6625 0.3176 0.0199 13.790 0.0080 0.3384 0.6536 0.0422 0.9083 0.0495 0.0081 0.3316 0.6603 0.0436 0.9077 0.0487 0.0325 0.2186 0.7489 0.3000 0.6674 0.0326 0.8403 0.5877 0.3927 0.0525 0.1072 0.0196 0.0672 0.0411 0.8917 0.8378 0.1477 0.0145 0.0043 0.1001 0.6797 273.15 0.0670 0.2202 3.447 0.9287 0.0134 0.0405 0.9461 0.3701 0.4258 0.2041 0.0178 0.9546 0.1924 0.0276 0.5157 0.2919 0.9613 0.6188 0.1878 0.1934 0.0222 0.0165 6.895 0.8766 0.2916 0.5702 0.1382 0.0226 0.1008 0.4295 0.0297 0.0774 0.8929 0.4455 0.1250 0.0509 0.9057 0.0434 0.6610 0.2280 0.1110 13.790 0.0530 0.1976 0.7494 0.3204 0.5754 0.1042 0.0546 0.1862 0.7592 0.3279 0.5548 0.1173 0.0834 0.0634 0.1632 0.7734 0.4246 0.4920

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Static equilibrium cell (0.1 dm3 capacity) fitted with magnetic Temperature measured stirrer. with platinum resistance thermometer. Pressure measured with Bourdon gauge. Contents charged into cell, equilibriated, samples withdrawn and analysed by gas chromatography. Details in source and ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- Purity 99.93 mole per cent.
- Purity 99.79 mole per cent. Purity 99.91 mole per cent. 2.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ ;  $\delta p/MPa = \pm 0.02$ ;  $\delta x, \ \delta y = \pm 1 - 2 \%.$ 

(estimated by compiler).

### REFERENCES:

Sinor, J.E.; Schindler, D.L.; Kurata, F.

> Am. Inst. Chem. Engnrs. J. 1966, 12, 353.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon Monoxide; CO; [630-08-0]
- 3. Propane; C₃H₈; [74-98-6]

ORIGINAL MEASUREMENTS:

Trust, D.B.; Kurata, F.

Am. Inst. Chem. Engnrs. J.

<u>1971</u>, *17*, 86-91.

		Йo	le fract:	ion	Mole	e fraction	ns
T/K	p/MPa	$x_{ m H_{2}}$	^x co	x C $_{3}$ H $_{8}$	$y_{\rm H_2}$	^у со	$y_{C_3H_8}$
73.15	13.790	0.0670	0.1595	0.7735	0.4608	0.4709	0.0683
		0.0864	0.0952	0.8184	0.6366	0.3004	0.0630
	•	0.0918	0.0952	0.8130	0.6372	0.2920	0.0708
23.15	3.447	0.0047	0.0366	0.9587	0.0339	0.3363	0.6298
		0.0085	0.0266	0.9649	0.1595	0.2609	0.5796
		0.0094	0.0259	0.9647	0.1652	0.2389	0.5959
		0.0161	0.0100	0.9739	0.3152	0.1063	0.5785
	6.895	0.0110	0.1225	0.8665	0.0685	0.5072	0.4243
		0.0260	0.0867	0.8873	0.2298	0.4111	0.3591
		0.0430	0.0493	0.9077	0.4053	0.2389	0.3558
	13.790	0.0697	0.2491	0.6812	0.1589	0.4203	0.4208
		0.1069	0.1208	0.7723	0.3807	0.2655	0.3538

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Cosway, H. F.; Katz, D. L. 2. Nitrogen; N₂; [7727-37-9] Am. Inst. Chem. Engnrs. J. 3. Methane; CH₄; [74-82-8] 1959, 5, 46-50. VARIABLES: PREPARED BY: Temperature, pressure, composition C. L. Young

EXPERIMENTAL VALUES:

Mole fractions in liquid Mole fractions in gas

1.010	Tractions in	++qu-u	1101	c fractions in	gus
ж _{Н 2}	$x_{N_2}$	^x CH₄	$^{y}_{\mathrm{H}_{2}}$	$y_{N_2}$	$^{\mathcal{Y}}$ CH $_{4}$
	T/K = 199.8	P/psia =	500	P/MPa = 3.	45
0.0343 0.0286 0.0155 0.00302 0.0000	0.0000 0.0998 0.2739 0.4176 0.4900 0.5090	0.9657 0.8716 0.7106 0.5794 0.5100 0.4910	0.6392 0.4337 0.1677 0.0236 0.0000	0.0000 0.2191 0.5080 0.6793 0.7300 0.7520	0.3608 [†] 0.3472 0.3243 0.2971 _* 0.2700 _{\$} 0.2480 [§]
	T/K = 144.3	P/psia =	1000	P/MPa = 6.	89
0.0781 0.0832 0.0826 0.0849 0.0915 0.0932 0.0926 0.1157	0.0000 0.0000 0.0617 0.1791 0.3733 0.3912 0.4137 0.5354	0.9219 0.9168 0.8557 0.7360 0.5352 0.5156 0.4937 0.3489	0.7618 0.7601 0.6735 0.5002 0.3130 0.3005 0.2758	0.0000 0.0000 0.0838 0.2377 0.4291 0.4413	0.2382 [†] 0.2399 0.2427 0.2621 0.2579 0.2582 0.2605

[†] Data quoted in original but taken from Benham, A. L.; Katz, D. L. Am. Inst. Chem. Engnrs. J. 1957, 3, 33.

(cont.)

### AUXILIARY INFORMATION

### METHOD 'APPARATUS / PROCEDURE:

Recirculating vapor flow system based on that described in ref. (1).

Details of present apparatus in source and ref. (2). Temperature measured with thermocouple. Pressure measured with Bourdon gauge.

High pressure magnetic circulating pumo employed.

Cell charged under pressure. Samples of each phase expanded to room temperature and pressure; analysed by mass spectrometry.

### SOURCE AND PURITY OF MATERIALS:

- 1 and 2. No details given.
- Phillips Petroleum Co. sample.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/MPa = \pm 0.03$ ;  $\delta x$ ,  $\delta y = \pm 2\%$  (estimated by compiler).

- Dodge, B. F.; Dunbar, A. K.
   J. Am. Chem. Soc. 1927, 49, 591.
- Aroyan, H. J.; Katz, D. L.
   Ind. Eng. Chem. <u>1951</u>, 43, 185.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]
- 3. Methane; CH4; [74-82-8]

### ORIGINAL MEASUREMENTS:

Cosway, H. F.; Katz, D. L.

Am. Inst. Chem. Engnrs. J.

1959, 5, 46-50.

### EXPERIMENTAL VALUES:

* Data quoted in original but taken from Bloomer, O. T.; Parent, J. D. Chem. Eng. Progr. Symposium Ser. 1953, No. 6, 49, 11.

Data quoted in original but taken from
Cines, M. R.; Roach, J. T.; Hogan, R. J.; Roland, C. H.
Chem. Eng. Progr. Symposium Ser. 1953, No. 6, 49, 1.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hydrogen; H ₂ ; [1333-74-0]	Cosway, H. F.; Katz, D. L.
2. Methane; CH4; [74-82-8]	Am. Inst. Chem. Engnrs. J.
3. Ethane; C ₂ H ₆ ; [74-84-0]	<u>1959</u> , 5, 46-50.
VARIABLES:	PREPARED BY:
Temperature, pressure, composition	C. L. Young

### EXPERIMENTAL VALUES:

Mole	fractions in	liquid		Mole	fractions i	n gas
$x_{ m H_{2}}$	x CH $_4$	x C ₂ H ₆		$y_{ m H_{2}}$	$^{\mathcal{Y}}$ CH ₄	y C ₂ H ₆
	T/K = 199.8		P/psia	= 500	P/MPa =	3.45
0.0187 0.0133 0.0134 0.0120 0.0101 0.0000	0.0000 0.2942 0.3255 0.3859 0.4325 0.6600	0.9813 0.6925 0.6611 0.6021 0.5575 0.3400		0.9166 0.4623 0.3940 0.3062 0.2308 0.0000	0.0000 0.4586 0.5230 0.6153 0.6913 0.9300	0.0834 [†] 0.0791 0.0830 0.0786 0.0779 _* 0.0700
	T/K = 199.8		P/psia	= 1000	P/MPa =	
0.0390 0.0382 0.0351 0.0400 0.0376	0.0000 0.0000 0.0441 0.1153 0.4957	0.9610 0.9618 0.9208 0.8447 0.4667		0.9476 0.9483 0.9325 0.8372 0.4579	0.0000 0.0000 0.0324 0.1102 0.4862	0.0524 [†] 0.0517 0.0351 0.0526 0.0559
	T/K = 144.3		P/psia	= 500	P/MPa =	3.45
0.0120 0.0167 0.0175 0.0327 0.0343	0.0000 0.5224 0.7608 0.9203 0.9637	0.9880 0.4609 0.2217 0.0470 0.0000		0.9969 0.8154 0.7412 0.6915 0.6392	0.0000 0.1819 0.2572 0.3080 0.3608	0.0031 [†] 0.00272 0.00164 0.0051 _§
					(con	it.)

### AUXILIARY INFORMATION

### METHOD APPARATUS/PROCEDURE:

Recirculating vapor flow system based on that described in ref. (1).

Details of present apparatus in source and ref. (2). Temperature measured with thermocouple. Pressure measured with Bourdon gauge.

High pressure magnetic circulating pump employed.

Cell charged under pressure.

Samples of each phase expanded to room temperature and pressure; analysed by mass spectrometry.

### SOURCE AND PURITY OF MATERIALS:

- 1. No details given.
- 2 and 3. Phillips Petroleum Co. sample.

## ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/MPa = \pm 0.03$ ;  $\delta x$ ,  $\delta y = \pm 2\%$  (estimated by compiler).

- Dodge, B. F.; Dunbar, A. K.
   J. Am. Chem. Soc. 1927, 49, 591.
- Aroyan, H. J.; Katz, D. L.
   Ind. Eng. Chem. 1951, 43, 185.

1. Hydrogen; H₂; [1333-74-0]

2. Methane; CH₄; [74-82-8]

3. Ethane;  $C_2H_6$ ; [74-84-0]

ORIGINAL MEASUREMENTS:

Cosway, H. F.; Katz, D. L.

Am. Inst. Chem. Engnrs. J.

1959, 5, 46-50.

### EXPERIMENTAL VALUES:

Mole fractions in liquid

Mole fractions in gas

$x_{ m H_2}$	x CH $_4$	x C ₂ H ₆	${y_{\mathtt{H}}}_{\mathtt{2}}$	y CH $_{4}$	y C ₂ H ₆
	T/K = 144.3		P/psia = 500	P/MPa	= 6.89
0.0225 0.0242 0.0296 0.0313 0.0487 0.0643 0.0832	0.0000 0.1115 0.3504 0.4081 0.7571 0.8732 0.9168	0.9775 0.8643 0.6200 0.5607 0.1942 0.0625 0.0000	0.9974 0.9710 0.9115 0.9009 0.8233 0.7929 0.7601	0.0000 0.0266 0.0856 0.0968 0.1754 0.2065 0.2399	0.0026 [†] 0.00231 0.00290 0.00230 0.00136 0.00061 0.0000

[†] Data quoted in original but taken from Williams, R. B.; Katz, D. L. Ind. Eng. Chem. 1954, 46, 2512.

^{*} Data quoted in original but taken from
Bloomer, O. T.; Gami, D. C.; Parent, J. D. Inst. Gas Tech. Res.
Bull. 1953, 22, 1.

Data quoted in original but taken from Benham, A. L.; Katz, D. L. Am. Inst. Chem. Engnrs. J. 1957, 3, 33.

- Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. Ethane;  $C_2H_6$ ; [74-84-0]

ORIGINAL MEASUREMENTS:

Cohen, A.E.; Hipkin, H.G.; Koppany, C.R.

Chem. Eng. Prog. Symp. Ser. No. 81. 1967, 63, 10-17.

### VARIABLES:

Temperature, pressure, composition

PREPARED BY:

C.L. Young

EXPERIMEN'	TAL VALUES:		composit fraction			compositi e fraction	
T/K	<i>p</i> /10 ⁵ Pa	æ _{H₂}	^x CH₄	^x C₂H ₆	^у н ₂	^y ch₄	^у С ₂ Н ₂
115.3	137.2	0.0754	0.597	0.328	0.964	0.0357	0.00016
116.3	103.4	0.0819	0.611	0.307	0.963	0.0367	0.00023
116.3	69.77	0.0379	0.638	0.324	0.963	0.0368	0.00031
116.3	53.31	0.0301	0.640	0.330	0.962	0.0384	0.00017
116.3	34.65	0.0192	0.628	0.353	0.954	0.0461	0.00006
116.1	14.12	0.00793	0.648	0.344	0.905	0.0947	0.00026
116.2	13.49	0.00462	0.275	0.720	0.957	0.0431	0.00020
116.2	35.38	0.00584	0.278	0.716	0.980	0.0206	0.00048
116.2	51.57	0.0116	0.248	0.740	0.983	0.0171	0.00030
116.2	68.95	0.0129	0.250	0.737	0.985	0.0154	0.00021
116.2	101.7	0.0204	0.240	0.740	0.986	0.0140	0.00032
116.2	136.9	0.0362	0.211	0.753	0.986	0.0137	0.00035
116.5	13.93	0.00389	0.0960	0.900	0.985	0.0153	0.00029
116.4	34.01	0.00958	0.0890	0.901	0.992	0.0077	0.00019
116.4	51.41	0.0117	0.0803	0.908	0.994	0.0063	0.00019
116.5	67.70	0.0168	0.0788	0.904	0.995	0.0054	0.00022
116.5	103.4	0.0258	0.0717	0.902	0.995	0.0048	0.00018
116.4	135.5	0.0312	0.0637	0.905	0.996	0.0044	0.00026
142.3	14.45	0.0100	0.412	0.578	0.673	0.324	0.0025
144.0	36.00	0.0188	0.516	0.465	0.817	0.181	0.0016
144.0	51.68	0.0313	0.518	0.451	0.862	0.136	0.0017
144.1	68.86	0.0416	0.491	0.467	0.883	0.115	0.00166
144.1	102.7	0.0573	0.438	0.505	0.907	0.0910	0.00161
144.0	137.2	0.0574	0.440	0.503	0.944	0.0535	0.00206
144.1	103.4	0.0473	0.280	0.673	0.944	0.0540	0.00201

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Equilibrium established in cell by recirculating vapor through external flow line at room temperature. Pressure measured with dead weight gauge. Temperature measured with platinum resistance thermometer. Liquid and vapor samples analysed by gas chromatography using thermal conductivity and flame ionisation detectors. Details in source and ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- Air Reduction Corp. bone dry sample, purity 99.8 mole per cent or better. Dried.
- 2. High purity sample. Dried.
- Matheson CP grade purity 99.0 mole per cent. Dried.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.05$ ;  $\delta P/MPa = \pm 0.007$  or 1% whichever greater;  $\delta x, \delta y \approx 3\%$  (greater when x or y less than 0.01)

### REFERENCES:

Hipkin, H.G.
 Am. Inst. Chem. Eng. J. 1966,
 12, 484.

- Hydrogen; H₂; [1333-74-0]
   Methane; CH₆; [74-82-8]
   Ethane; C₂H₆; [74-84-0]

### ORIGINAL MEASUREMENTS:

Cohen, A.E.; Hipkin, H.G.; Koppany, C.R.

Chem. Eng. Prog. Symp. Ser. No. 81. 1967, 63, 10-17.

EXPERIMENTAL V	ALUES: Liquid	composi	tions ns		composit	
T/K p/10		$x_{\mathrm{CH}_4}$	x _{C2H6}	$y_{\rm H_2}$	y _{CH4}	^у С ₂ Н ₂
144.0 51. 144.1 34. 144.1 15. 143.8 13. 144.2 34. 144.1 136. 172.2 13. 172.2 51. 172.2 69. 172.2 103. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 136. 172.1 137. 172.1 34. 172.1 35. 172.1 34. 172.1 35. 172.1 36. 172.1 102. 172.1 36. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 172.1 102. 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172.1 103. 172.1 103. 172.1 103. 172.1 103. 172	.87       0.00604         .14       0.00777         .38       0.0118         .2       0.00620         .28       0.0180         .62       0.0291         .94       0.0584         .6       0.0630         .5       0.0712         .4       0.0641         .78       0.0388         .64       0.0266         .52       0.0180         .89       0.0140         .67       0.0222         .65       0.0194         .63       0.0448         .4       0.0660         .9       0.0122         .74       0.0208         .74       0.0208         .72       0.116         .40       0.0827         .47       0.0475         .73       0.0388         .21       0.0241         .99       0.0191         .5       0.104         .74       0.0590         .44       0.0415         .50       0.0405         .74       0.0590         .74       0.0405         .53       0.0766	0.264 0.264 0.237 0.0842 0.08806 0.07449 0.2103 0.1623 0.1098325 0.0163 0.08325 0.0524 0.163 0.098325 0.0471 0.471 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- Hydrogen; H₂; [1333-74-0]
   Methane; CH₄; [74-82-8]
   Ethane; C₂H₆; [74-84-0]

### ORIGINAL MEASUREMENTS:

Cohen, A.E. Hipkin, H.G. Koppany, C.R.

Chem. Eng. Prog. Symp. Ser. No. 81, 1967, 63, 10-17.

	NTAL VALUE		fraction			r composi le fracti	
T/K	P/10 ⁵ Pa	$x_{ m H_{2}}$	^x CH₄	^x C₂H ₆	$y_{\rm H_2}$	^y CH₄	y _{C2H6}
255.4	54.30	0.0088	0.250	0.741	0.066	0.559	0.375
255.4	70.39	0.0280	0.288	0.684	0.177	0.469	0.354
255.4	83.90	0.0595	0.300	0.640	0.248	0.406	0.346
255.4	98.94	0.1180	0.315	0.567	0.327	0.362	0.311
255.4	111.01	0.1020	0.266	0.632	0.342	0.339	0.319

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. Ethene;  $C_2H_4$ ; [74-85-1]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Arai, Y.; Saito, S. J. Chem. Engng. Japan 1972, 5,

339-348.

### VARIABLES:

Temperature, pressure, composition

### PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

T/K	P/bar	$x_{ m H_{2}}$	x CH $_4$	^ж С ₂ Н ₄	$y_{ m H_{2}}$	$^{\mathcal{Y}}$ CH $_{4}$	$y_{C_2H_4}$
123.15	20.3	0.00698	0.189	0.804	0.934	0.0633	0.00243
		0.00756	0.321	0.672	0.908	0.0898	0.00258
		0.00930	0.476	0.515	0.877	0.122	0.00111
		0.0118	0.625	0.363	0.856	0.143	0.00088
		0.0177	0.826	0.157	0.842	0.157	0.00061
	40.5	0.0113	0.194	0.795	0.959	0.0386	0.00202
		0.0131	0.309	0.678	0.944	0.0541	0.00207
		0.0187	0.493	0.489	0.923	0.0756	0.00104
		0.0254	0.631	0.344	0.914	<b>0.</b> 0850	0.00056
		0.0346	0.814	0.152	0.896	0.104	0.00051
	60.8	0.0171	0.193	0.790	0.965	0.0327	0.00193
		0.0170	0.326	0.657	0.954	0.0450	0.00141
		0.0263	0.501	0.473	0.937	0.0622	0.00051
		0.0328	0.631	0.337	0.931	0.0687	0.00044
		0.0504	0.803	0.147	0.911	0.0887	0.00060
	81.1	0.0251	0.193	0.782	0.970	0.0283	0.00183
		0.0321	0.384	0.584	0.953	0.0457	0.00083
		0.0388	0.491	0.470	0.943	0.0559	0.00083
		0.0527	0.617	0.331	0.937	0.0628	0.00032
		0.0678	0.782	0.150	0.922	0.0774	0.00030
148.15	20.3	0.00828	0.178	0.814	0.799	0.180	0.0217
		0.00717	0.280	0.713	0.725	0.254	0.0212
		0.00722	0.382	0.611	0.657	0.325	0.0176
		0.0107	0.518	0.471	0.570	0.415	0.0147
		0.0124	0.668	0.319	0.493	0.495	0.0123
		0.0149	0.856	0.129	0.400	0.594	0.00655
						(c	cont.)

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static stainless steel cell of capacity  $5 \times 10^5$  mm³ fitted with magnetic stirrer and sampling valves. Cell enclosed in cryostat. Temperature measured with thermocouple. Pressure measured using Bourdon gauge. Gases added to cell and equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- Nippon Sanso Co. Ltd. sample, purity 99.99 mole per cent.
- Takachiho Chemical Industry Co. Ltd. sample, purity 99.9 mole per cent.
- Takachiho Chemical Industry Co. Ltd. sample, purity 99.5 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/bar = \pm 0.1; \quad \delta x_{H_2}, \\ \delta x_{CH_4}, \quad \delta x_{C_2H_4}, \quad \delta y_{H_2}, \quad \delta y_{CH_4}, \quad \delta y_{C_2H_4}, \\ = \pm 1 *.$ 

```
COMPONENTS:
                                          ORIGINAL MEASUREMENTS:
                                          Sagara, H.; Arai, Y.;
                                                                     Saito, S.
1.
    Hydrogen;
                H<sub>2</sub>;
                       [1333-74-0]
                                          J. Chem. Engng. Japan 1972, 5,
                       [74 - 82 - 8]
2.
    Methane;
               CH 4;
                       [74-85-1]
                                          339-348.
    Ethene; C2H4;
EXPERIMENTAL VALUES:
T/K
          P/bar
                        x_{\rm H_2}
                                  ^xCH _4
                                            x<sub>C2H4</sub>
                                                         y_{\rm H_2}
                                                                   y_{CH_4}
                                                                             y<sub>C2H4</sub>
                                                                 0.102
                                                                           0.0155
                                0.174
                                          0.809
                                                       0.883
148.15
          40.5
                     0.0165
                                0.282
                                                       0.841
                                                                 0.145
                                                                           0.0148
                     0.0168
                                          0.701
                                                                           0.0143
                                                       0.801
                                                                 0.185
                     0.0212
                                0.373
                                          0.606
                     0.0249
                                                      0.747 \\ 0.708
                                                                 0.241
                                0.511
                                          0.464
                                                                           0.0119
                                                                 0.283
                                                                           0.00915
                                          0.317
                     0.0304
                                0.653
                     0.0386
                                                                           0.00479
                                0.835
                                          0.126
                                                       0.651
                                                                 0.344
          60.8
                     0.0260
                                0.177
                                          0.797
                                                       0.911
                                                                 0.0767
                                                                           0.0123
                                          0.692
                                                                           0.0100
                     0.0278
                                0.280
                                                       0.877
                                                                 0.133
                     0.0333
                                0.368
                                          0.599
                                                       0.847
                                                                 0.142
                                                                           0.0110
                     0.0369
                                0.508
                                          0.456
                                                       0.810
                                                                 0.181
                                                                           0.00846
                     0.0436
                                0.649
                                          0.307
                                                       0.772
                                                                 0.221
                                                                           0.00712
                                                      0.729
                                                                           0.00320
                                                                 0.268
                     0.0641
                                0.815
                                          0.121
                                0.169
          81.1
                                          0.798
                                                       0.926
                                                                 0.0647
                                                                           0.00905
                     0.0332
                                                       0.894
                                                                 0.0957
                                                                           0.00985
                     0.0376
                                0.274
                                          0.688
                                          0.589
                                                       0.871
                                                                 0.121
                                                                           0.00863
                     0.0437
                                0.368
                                                                           0.00754
                                                                 0.151
                     0.0502
                                          0.452
                                                       0.842
                                0.498
                                                       0.804
                                                                 0.189
                                                                           0.00688
                     0.0638
                                0.631
                                          0.305
                                                                 0.232
                                                       0.746
                                                                           0.00443
                     0.0924
                                0.789
                                          0.118
                                0.0886
                                          0.903
                                                       0.752
                                                                 0.168
                                                                           0.0807
173.15
          20.3
                     0.00875
                                                                           0.0800
                     0.00856
                                0.260
                                          0.731
                                                       0.491
                                                                 0.429
                                                      0.329
0.317
                     0.00808
                                0.400
                                          0.592
                                                                 0.600
                                                                           0.0712
                                                                           0.0724
                     0.00811
                                0.403
                                          0.589
                                                                 0.611
                     0.00439
                                0.599
                                          0.397
                                                       0.131
                                                                 0.808
                                                                           0.0609
                                                                           0.0488
          40.5
                     0.0188
                                0.0902
                                          0.891
                                                       0.857
                                                                 0.0941
                     0.0197
                                0.251
                                                       0.711
                                                                 0.243
                                                                           0.0453
                                          0.729
                     0.0237
                                0.389
                                          0.587
                                                       0.607
                                                                 0.346
                                                                           0.0479
                                                       0.449
                                                                 0.514
                                                                           0.0374
                     0.0271
                                0.602
                                          0.371
                     0.0278
                                0.712
                                          0.260
                                                       0.386
                                                                 0.585
                                                                           0.0286
                                                                 0.0696
                                0.0898
                                                                           0.0376
          60.8
                                                      0.893
                     0.0314
                                          0.879
                     0.0328
                                          0.718
0.585
                                                                 0.178
                                0.250
                                                       0.787
                                                                           0.0352
                                                                 0.263
                                                                           0.0380
                                                       0.699
                     0.0391
                                0.376
                                                                 0.384
                     0.0482
                                0.581
                                          0.371
                                                       0.585
                                                                           0.0314
                     0.0522
                                0.687
                                                                 0.452
                                                                           0.0279
                                          0.260
                                                       0.520
                                0.0938
                                                                 0.0579
                                                                           0.0325
          81.1
                     0.0418
                                          0.864
                                                       0.910
                     0.0465
                                0.243
                                          0.710
                                                       0.820
                                                                 0.147
                                                                           0.0329
                                0.365
                                          0.580
                                                       0.748
                                                                 0.219
                                                                           0.0334
                     0.0557
                     0.0693
                                0.566
                                          0.365
                                                       0.639
                                                                 0.330
                                                                           0.0306
                                                       0.591
                                                                 0.383
                                                                           0.0269
                                0.665
                     0.0781
                                          0.257
                                0.0327
                                                                 0.101
                                                                           0.254
198.15
          20.3
                     0.00988
                                          0.957
                                                       0.644
                                                                           0.251
                                          0.903
                                                      0.494
                                                                 0.255
                     0.00843
                                0.0882
                               0.155
                                                                           0.248
                     0.00589
                                          0.839
                                                       0.314
                                                                 0.437
                     0.00374
                                0.226
                                          0.770
                                                       0.170
                                                                 0.592
                                                                           0.239
                                          0.761
                                                      0.141
0.700
                               0.236
                                                                 0.626
                                                                           0.233
                     0.00318
          40.5
                     0.0238
                                0.0912
                                          0.885
                                                                 0.160
                                                                           0.140
                                0.0916
                                          0.886
                                                       0.705
                                                                 0.147
                                                                           0.149
                     0.0221
                     0.0227
                                0.139
                                          0.838
                                                       0.629
                                                                 0.226
                                                                           0.145
                                                       0.400
                     0.0198
                                          0.669
                                                                 0.468
                                                                           0.132
                                0.312
                               0.392
0.576
                                          0.589
0.413
                                                       0.330
                                                                 0.541
                                                                           0.129
                     0.0186
                                                      0.145
                                                                 0.741
                                                                           0.114
                     0.0116
                                0.116
                                          0.846
                                                       0.743
                                                                 0.144
                                                                           0.114
          60.8
                     0.0375
                     0.0379
                                0.286
                                          0.676
                                                       0.569
                                                                 0.320
                                                                           0.111
                                                       0.492
                                                                 0.409
                                                                           0.0999
                                0.384
                                          0.577
                     0.0393
                     0.0383
                                0.561
                                          0.401
                                                       0.328
                                                                 0.577
                                                                           0.0956
                                0.686
                                          0.276
                                                       0.216
                                                                 0.698
                                                                           0.0861
                     0.0380
                                0.212
                                          0.734
                                                       0.714
                                                                 0.193
                                                                           0.0932
          81.1
                     0.0537
                                                                           0.0951
                     0.0564
                                0.284
                                          0.660
                                                       0.642
                                                                 0.263
                                          0.426 \\ 0.260
                                0.509
                                                       0.445
                                                                 0.462
                                                                           0.0934
                     0.0651
                                                                           0.0874
                                                       0.296
                     0.0743
                                0.666
                                                                 0.617
                                0.0329
                                                       0.309
                                                                 0.136
                                                                           0.555
223.15
                                          0.961
          20.3
                     0.00632
                                                                           0.565
                     0.00497
                                0.0519
                                          0.943
                                                       0.227
                                                                 0.208
                                0.0745
                                          0.922
                                                       0.153
                                                                 0.282
                                                                           0.565
                     0.00378
```

(cont.)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH₄; [74-82-8]
- 3. Ethene;  $C_2H_4$ ; [74-85-1]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Arai, Y.; Saito, S.

J. Chem. Engng. Japan 1972, 5,

339-348.

### EXPERIMENTAL VALUES:

T/K	P/bar	$x_{ m H_{2}}$	^x CH ₄	^ж С ₂ Н ₄	$y_{ m H_{2}}$	$^{\mathcal{Y}}$ CH 4	^у С ₂ Н ₄
223.15	40.5	0.0241	0.0914	0.885	0.482	0.190	0.328
ł		0.0204	0.122	0.858	0.428	0.258	0.314
ł		0.0172	0.192	0.791	0.302	0.386	0.311
		0.0131	0.259	0.728	0.200	0.499	0.301
248.15	30.4	0.00554	0.0332	0.961	0.115	0.106	0.780
l		0.00392	0.0532	0.943	0.0708	0.166	0.763
İ		0.00389	0.0498	0.946	0.0775	0.157	0.766
ł		0.00179	0.0689	0.929	0.0333	0.219	0.748
ļ	40.5	0.0168	0.0498	0.933	0.233	0.123	0.644
		0.0135	0.0806	0.906	0.174	0.191	0.635
ļ		0.00600	0.143	0.851	0.0629	0.315	0.623

 $x_{\rm H_2}$ ,  $x_{\rm CH_4}$  and  $x_{\rm C_2H_4}$  mole fraction of hydrogen, methane and ethene in liquid phase, respectively.

 $y_{\rm H_2}$ ,  $y_{\rm CH_4}$  and  $y_{\rm C_2H_4}$  mole fraction of hydrogen, methane and ethene in gas phase, respectively.

ORIGINAL MEASUREMENTS:

, H ₂ ; [13	337-74-0]		Benham, A.L.; Katz, D.L.					
•	_				. Engnrs.e	J. <u>1957</u> ,3,		
Compositi	ion		PREPARED BY: C.L. Young					
ALUES:								
) /h o w								
/par	<i>x</i> _{H₂}	x _{CH} ,	^ж С ₃ Н ₆	у _{Н2}	^y CH₄	^у С ₃ Н ₆		
(	.00986		0.5786	0.2933	0.8337 0.6909 0.00			
			<b></b>					
	CH ₄ ; [74 C ₃ H ₆ ; [2 Composit: ALUES: P/bar	CH ₄ ; [74-82-8]  C ₃ H ₆ ; [115-07-1]  Composition  ALUES:  Liquid  Mole f  P/bar  x H ₂	C ₃ H ₆ ; [115-07-1]  Composition  ALUES:  Liquid composition  Mole fractions.  P/bar  **H ₂ **CH ₄ 44.47  0.00728  0.5126  0.00986  0.4115	CH4; [74-82-8]  C3H6; [115-07-1]  PREPARED  Composition  ALUES:  Liquid composition  Mole fractions.  P/bar  xH2  xCH4  C3H6  44.47  0.00728  0.5126  0.4801  0.00986  0.4115  0.5786	CH4; [74-82-8]  C3H6; [115-07-1]  PREPARED BY:  Composition  C.L  Am. Inst. Chem. 33-36.  PREPARED BY:  Composition  C.L  Auues:  Liquid composition  Mole fractions.  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapor of Mole  Wapo	CH4; [74-82-8]  C3H6; [115-07-1]  PREPARED BY:  Composition  C.L. Young  ALUES:  Liquid composition  Mole fractions.  Wapor composition  Mole fractions  Wapor composition  Mole fractions  Wapor composition  Mole fractions  Wapor composition  Mole fractions  Wapor composition  Mole fractions  Wapor composition  Mole fractions  O'bar  **A***  C3H6  **YH2  **CH4  **C3H6  O.00728  O.00728  O.00728  O.00986  O.4801  O.1493  O.8337  O.00986  O.4115  O.5786  O.2933  O.6909		

### AUXILIARY INFORMATION

### METHOD:/APPARATUS/PROCEDURE:

Recirculating vapor flow system described in ref. 1. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Vapor recirculated by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room pressure and analysed by mass spectrometer.

### SOURCE AND PURITY OF MATERIALS:

- Purity better than 99.5 mole per cent; further purified to remove water.
- Purity better than 99.0 mole per cent; further purified to remove water and higher hydrocarbons.
   Purity better than 99.0 mole per cent; further purified to remove water and higher hydrocarbons.
- ESTIMATED ERROR:  $\delta T/K = \pm 0.6$ ;  $\delta P/bar = \pm 0.5$ ;  $\delta x_{H_2}$ ;  $\delta x_{CH_4}$ ,  $\delta x_{C_3H_6}$ ,  $\delta y_{H_2}$ ,  $\delta y_{CH_4}$ ,  $\delta y_{C_3H_6}$ =  $\pm 0.5$ %

### REFERENCES:

Aroyan, H.J.; Katz, D.L.
 Ind. Eng. Chem. <u>1951</u>, 43,185.

## Miscellaneous Organic Fluids 541 ORIGINAL MEASUREMENTS: COMPONENTS: Hydrogen; H₂; [1333-74-0] Benham, A.L.; Katz, D.L. 2. Methane; CH4; [74-82-8] Am. Inst. Chem. Engnrs. J. 1957,3, 33-36. 3. Propane, C₃H₈; [74-98-6] VARIABLES: PREPARED BY: Temperature, pressure, composition C.L. Young EXPERIMENTAL VALUES:

EAFERIMENTAL	vanues:	Liquid composition Mole fraction			Vapor composition Mole fraction			
T/K	P/bar	x _{H2}	xCH4	xC3H6	у _{Н2}	^y CH₄	^у С ₃ Н ₈	
255.37	34.47	0.0015 0.00329 0.00717 0.00907 0.0113 0.0131 0.0100 0.0230	0.2583 0.2357 0.2098 0.1613 0.1367 0.1172 0.0797	0.7402 0.7610 0.7830 0.8296 0.8520 0.8698 0.9103 0.9770	0.0398 0.0831 0.1396 0.2790 0.3726 0.4576 0.5875 0.9070	0.8408 0.8026 0.7329 0.6070 0.5208 0.4337 0.3166 0.0000	0.1194 0.1143 0.1275 0.1140 0.1066 0.1087 0.0959 0.0930	
199.82	34.47	0.0000 0.00452 0.00645 0.00683 0.0109 0.0122 0.0116 0.0155	0.620 0.4958 0.4499 0.4238 0.2493 0.2140 0.1607 0.0000	0.380 0.4997 0.5436 0.5694 0.7398 0.7738 0.8277 0.9845	0.0000 0.1436 0.2213 0.2457 0.5980 0.6872 0.6783 0.9902	0.9870 0.8443 0.7673 0.7421 0.3925 0.3046 0.3104 0.0000	0.0130 0.0121 0.0114 0.0122 0.0095 0.0082 0.0113 0.00976	
144.26	34.47	0.0086 0.00789 0.0179 0.0285 0.0343	0.0000 0.0859 0.4367 0.8707 0.9657	0.9914 0.9062 0.5454 0.1008 0.0000	0.999+ 0.9573 0.8340 - 0.6392	0.0000 0.0379 0.1592 - 0.3608	0.0000 0.0048 0.0068 -	

### AUXILIARY INFORMATION

### METHOD:/APPARATUS/PROCEDURE:

Recirculating vapor flow system described in ref. 1. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Vapor recirculated by high pressure magnetic pump. Cell charged under pressure. Samples of each phase expanded to room pressure and analysed by mass spectrometer.

- SOURCE AND PURITY OF MATERIALS:
  1. Purity better than 99.5 mole per cent; further purified to remove water and higher hydrocarbons.
- 2. Purity better than 99.0 mole per cent; further purified to remove water vapor.
- 3. Purity better than 99.0 mole per cent; further purified to remove water vapor.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.06$ ;  $\delta P/bar = \pm 0.5$ %;  $\delta x_{\text{H}_2}$ ,  $\delta x_{\text{CH}_4}$ ,  $\delta x_{\text{C}_3 \text{H}_8}$ ,  $\delta y_{\text{H}_2}$ ,  $\delta y_{\text{CH}_4}$ ,  $\delta y_{\text{C}_3 \text{H}_8}$ , = ±0.5%.

### REFERENCES:

1. Aroyan, H.J.; Katz, D.L. Ind. Eng. Chem. 1951, 43,185

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH₄; [74-82-8]
- 3. Propane; C₃H₈; [74-98-6]

### ORIGINAL MEASUREMENTS

Benham, A.L.; Katz, D.L.;

Am. Inst. Chem. Engnrs. J., <u>1957</u>, 3, 33-36

EXPERIMENT	EXPERIMENTAL VALUES: Liquid composition Vapor composition  Mole fractions Mole fractions										
т/к	P/bar	<i>x</i> _{H2}	x _{CH4}	^ж С ₃ Н ₈	^у н ₂	y _{CF4}	y _{C3H8}				
255.37	68.95	0.0000 0.0202 0.0267 0.0275 0.0309 0.0379 0.0475	0.5300 0.3277 0.2570 0.2430 0.1790 0.1303 0.0000	0.4700 0.6521 0.7163 0.7295 0.7901 0.8318 0.9525	0.0000 0.2554 0.4549 0.4689 0.5895 0.6657	0.9030 0.6609 0.4777 0.4578 0.3457 0.2657	0.0970 0.0837 0.0674 0.0733 0.0648 0.0686 0.0592				
199.82	68.95	0.0302 0.0276 0.0327 0.0327 0.0366	0.0000 0.1470 0.3428 0.4637 0.5844	0.9698 0.8254 0.6245 0.5036 0.3790	0.9931 0.8562 0.6182 - 0.4323	0.0000 0.1339 0.3681 - 0.5301	0.0069 0.0099 0.0137 - 0.0376				
144.26	68.95	0.0163 0.0179 0.0300 0.0296 0.0312 0.0597 0.0781	0.0000 0.1014 0.5593 0.5784 0.5914 0.8122 0.9219	0.9837 0.8807 0.4107 0.3920 0.3774 0.1281 0.0000	0.999+ 0.9900 0.8770 0.8770 0.8666 0.8008 0.7618	0.0000 0.0037 0.1204 0.1204 0.1307 0.1961 0.2382	0.0000 0.0063 0.0026 0.0026 0.0027 0.0031 0.0000				

### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sagara, H.; Arai, Y.; Saito, S. J. Chem. Engng. Japan 1972, 5, 2. Ethene; $C_2H_4$ ; [74-85-1] 339-348. 3. Ethane; $C_2H_6$ ; [74-84-0] VARIABLES: PREPARED BY: Temperature, pressure, composition C. L. Young EXPERIMENTAL VALUES: T/K P/bar $y_{\rm H_2}$ x C₂H₆ $x_{\rm H_2}$ $x_{C_2H_4}$ y_{C2H4} yC2H6 0.983 0.00640 0.220 0.774 0.0104 148.15 20.3 0.00621 0.00675 0.423 0.570 0.981 0.0112 0.00802 0.980 0.0126 0.562 0.00782 0.00597 0.432 0.00587 0.977 0.0174 0.636 0.358 0.00576 0.288 0.975 0.00736 0.704 0.0195 0.00510 0.00642 0.977 0.0191 0.704 0.290 0.00396 0.990 40.5 0.0123 0.220 0.768 0.00393 0.00651 0.222 0.766 0.990 0.00394 0.00625 0.0123 0.549 0.988 0.00752 0.0121 0.439 0.00455 0.424 0.564 0.987 0.00785 0.00472 0.0129 0.986 0.0132 0.637 0.350 0.0107 0.00332 0.296 0.693 0.985 0.0115 0.00318 0.0116 0.765 60.8 0.219 0.993 0.00310 0.00425 0.0162 0.434 0.550 0.990 0.00606 0.0160 0.00408 0.639 0.345 0.990 0.00819 0.0163 0.00232 0.989 0.00848 0.693 0.291 0.0162 0.00227 0.759 81.1 0.0229 0.218 0.994 0.00266 0.00355 0.993 0.00445 0.0269 0.426 0.547 0.00266 0.630 0.350 0.990 0.00778 0.0205 0.00252 0.288 0.991 0.00785 0.686 0.00159 0.0256 173.15 20.3 0.224 0.768 0.954 0.0218 0.00816 0.0240 0.536 0.455 0.943 0.0394 0.00922 0.0179 0.383 0.933 0.0526 0.00919 0.608 0.0143 0.00896 0.281 0.710 0.932 0.0577 0.0108 0.00800 0.764 0.229 0.931 0.0604 0.00904 (cont.) AUXILIARY INFORMATION METHOD/APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static stainless steel cell of capacity 5 $\times$ $10^5~\text{mm}^3$ fitted with magnetic 1. Nippon Sanso Co. Ltd. sample, purity 99.99 nole per cent. stirrer and sampling valves. Cell 2. Takachiho Chemical Co. Ltd. enclosed in cryostat. Temperature sample, purity 99.5 mole per cent. measured with thermocouple. Pressure 3. Takachiho Chemical Co. Ltd. measured with Bourdon gauge. Gases added to cell and equilibrated. sample, purity 99.7 mole per cent. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity Details in source. detector. ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta P/bar = \pm 0.1$ ; $\delta x_{H_2}$ $\delta x_{C_2H_4}$ , $\delta x_{C_2H_6}$ , $\delta y_{H_2}$ , $\delta y_{C_2H_4}$ , $\delta y_{C_2H_6}^{112}$ = ±1%. REFERENCES:

### 544 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H2; [1333-74-0] Sagara, H.; Arai, Y.; Saito, S. 1. 2. Ethene; C2H4; [74-85-1]J. Chem. Engng. Japan 1972, 5, Ethane; C2H6; [74-84-0] 339-348. EXPERIMENTAL VALUES: T/K P/bar $x_{ m H_2}$ ^жС 2 Н 4 $x_{C_2H_6}$ $y_{\rm H_2}$ ^уС 2 Н ц $y_{C_2H_6}$ 173.15 40.5 0.0148 0.219 0.767 0.972 0.0120 0.0159 0.526 0.965 0.0163 0.457 0.0230 0.0117 0.0158 0.606 0.378 0.960 0.0310 0.00950 0.0315 0.0155 0.705 0.280 0.962 0.00676 0.0154 0.753 0.231 0.960 0.0344 0.00579 60.8 0.0256 0.215 0.759 0.978 0.00934 0.0123 0.0241 0.454 0.522 0.00969 0.972 0.0180 0.0265 0.600 0.374 0.970 0.0231 0.00695 0.969 0.0257 0.00525 0.0253 0.702 0.273 0.0281 0.741 0.231 0.968 0.0272 0.00519 0.750 0.00806 81.1 0.217 0.0330 0.980 0.0116 0.0352 0.516 0.975 0.00848 0.449 0.0161 0.0200 0.0341 0.597 0.369 0.974 0.00624 0.973 0.0334 0.694 0.273 0.0222 0.00467 0.0231 0.0350 0.732 0.233 0.973 0.00398 198.15 20.3 0.0106 0.852 0.161 0.829 0.0480 0.100 0.0102 0.265 0.725 0.843 0.0717 0.0852 0.00970 0.497 0.124 0.0604 0.494 0.816 0.0104 0.501 0.482 0.805 0.132 0.0631 0.0517 0.0104 0.375 0.787 0.161 0.615 0.191 0.0100 0.703 0.287 0.764 0.0453 40.5 0.0221 0.818 0.913 0.0274 0.0592 0.160 0.718 0.0214 0.261 0.902 0.0428 0.0557 0.0205 0.501 0.478 0.888 0.0734 0.0388 0.0742 0.0217 0.501 0.477 0.888 0.0376 0.0910 0.0210 0.608 0.371 0.879 0.0303 0.0215 0.691 0.288 0.872 0.103 0.0256 60.8 0.0320 0.158 0.810 0.935 0.0201 0.0453 0.0320 0.704 0.0302 0.264 0.930 0.0395 0.0349 0.487 0.479 0.914 0.0559 0.0303 0.480 0.0544 0.488 0.917 0.0318 0.0286 0.0351 0.603 0.362 0.0677 0.0240 0.908 0.284 0.0332 0.683 0.898 0.0811 0.0210 81.1 0.0449 0.160 0.795 0.944 0.0164 0.0397 0.697 0.0347 0.0437 0.260 0.940 0.0250 0.0449 0.479 0.476 0.928 0.0469 0.0251 0.0457 0.479 0.474 0.932 0.0455 0.0226 0.592 0.0208 0.0488 0.0573 0.359 0.922 0.0472 0,671 0.282 0.917 0.0648 0.0179 0.150 223.15 0.767 20.3 0.0105 0.223 0.575 0.275

0.0103

0.00947

0.00879

0.0258

0.0256

0.0255

0.0273

0.0411

0.0427

0.0421

0.0423

0.0558

0.0573

0.0587

0.0585

40.5

60.8

81.1

0.328

0.524

0.713

0.223

0.327

0.522

0.685

0.221

0.317

0.507

0.670

0.216

0.316

0.502

0.661

0.662

0.466

0.278

0.752

0.647

0.453

0.288

0.738

0.640

0.451

0.288

0.728

0.627

0.439

0.280

0.542

0.520

0.428

0.762

0.737

0.706

0.656

0.807

0.806

0.780

0.737

0.850

0.837

0.813

0.778

0.221

0.315

0.456

0.125

0.193

0.272

0.0651

0.0920

0.143

0.208

0.0508

0.0746

0.121

0.173

0.0818

0.238

0.165

0.116

0.156

0.138

0.101

0.0730

0.128

0.101

0.0767

0.0549

0.0991

0.0880

0.0657

0.0487

 $y_{\rm H_2}$ ,  $y_{\rm C_2H_4}$  and  $y_{\rm C_2H_6}$  mole fractions of hydrogen, ethene and ethane in vapor phase, respectively.

 $x_{\rm H_2}$ ,  $x_{\rm C_2H_4}$  and  $x_{\rm C_2H_6}$  mole fractions of hydrogen, ethene and ethane in liquid phase, respectively.

## ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Sagara, H; Mihara, S.; Arai, Y.; 2. Ethene (Ethylene); C₂H₄; Saito, S. [74-85-1] J. Chem. Engng. Japan 1975, 8, 98-104. VARIABLES: Temperature, pressure, composition C. L. Young

EXPERIMEN	TAL VALUES	<b>:</b>					
		Mole fr	actions in	liquid	Mole	fractions in	n vapor
T/K	P/MPa	$x_{ m H_{2}}$	$x_{C_2H_4}$	$x_{{ m C}_3H_8}$	$y_{ m H_{2}}$	y C ₂ H ₄	y C $_{3}$ H $_{8}$
173.2	2.03	0.00782 0.00845	0.454 0.519	0.538 0.473	0.962 0.955	0.0371 0.0430	0.00108 0.00147
	4.05	0.00845 0.0171	0.681 0.473 0.681	0.311 0.510 0.303	0.947 0.976 0.970	0.0525 0.0231 0.0292	0.00059 0.00090 0.00048
	6.08	0.0162 0.0244 0.0249	0.465 0.672	0.510 0.303	0.982 0.977	0.0292 0.0173 0.0221	0.00044
	8.11	0.0314	0.453 0.666	0.516 0.301	0.985 0.980	0.0145 0.0194	0.00060
198.2	2.03	0.00823 0.00813 0.00976	0.332 0.412 0.705	0.659 0.580 0.285	0.910 0.894 0.821	0.0835 0.101 0.175	0.00652 0.00565 0.00348
	4.05	0.0181 0.0185	0.703 0.399 0.700	0.583 0.281	0.939 0.907	0.0570 0.0912	0.00392
	6.08	0.0288 0.0323	0.392 0.678	0.579 0.290	0.955 0.933	0.0420 0.0658	0.00326 0.00159
	8.11	0.0378 0.0427	0.388 0.667	0.574 0.290	0.962 0.942	0.0352 0.0564	0.00291 0.00164
223.2	2.03	0.00916 0.0104	0.434 0.804	0.557 0.185	0.705 0.542	0.269 0.446	0.0259 0.0117
	4.05	0.0222 0.0261	0.414 0.787	0.564 0.186	0.853 0.742	0.132 0.251	0.0152 0.00613
	6.08	0.0360 0.0397	0.372 0.743	0.592 0.217	0.896 0.815	0.0917 0.179 (cont.)	0.0122 0.00539
						(COIIL.)	

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static stainless steel cell of capacity  $5 \times 10^5$  mm³ fitted with magnetic stirrer and sampling valves. Cell enclosed in cryostat. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Gases added to cell and equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.99 mole per cent.
- 2. Purity 99.5 mole per cent.
- 3. Purity 99.7 mole per cent.

## ESTIMATED ERROR:

 $\begin{array}{lll} \delta T/K = \pm 0.1; & \delta P/MPa = \pm 0.01; \\ \delta x_{\rm H_2}, & \delta x_{\rm C_2H_4}, & \delta x_{\rm C_3H_8}, & \delta y_{\rm H_2}, & \delta y_{\rm C_2H_4}, \\ \delta y_{\rm C_3H_8} = \pm 1 \text{\$}. \end{array}$ 

### REFERENCES:

Sagara, H.; Arai, Y.; Saito, S.
 J. Chem. Engng. Japan 1972, 5,
 339.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ethene (Ethylene);  $C_2H_4$ ; [74-85-1]
- 3. Propane; C₃H₈; [74-98-6]

## ORIGINAL MEASUREMENTS:

Sagara, H; Mihara, S.; Arai, Y.;

Saito, S.

J. Chem. Engng. Japan <u>1975</u>, 8,
 98-104.

### EXPERIMENTAL VALUES:

		Mole fr	actions in	liquid	Mole :	fractions in	n vapor
T/K	P/MPa	$x_{ m H_{2}}$	^x C ₂ H ₄	^ж С 3 Н 8	$y_{ m H_2}$	^у С ₂ Н ₄	^у С ₃ Н ₈
223.2	8.11	0.0474 0.0531	0.364 0.691	0.588 0.256	0.915 0.856	0.0742 0.138	0.0108 0.00588
248.2	2.03	0.0101 0.00780	0.334	0.656 0.451	0.541 0.363	0.138 0.370 0.568	0.00388 0.0891 0.0693
	4.05	0.00583 0.0246	0.704 0.318	0.290 0.657	0.226 0.748	0.723 0.202	0.0504 0.0502
	6.08	0.0250 0.0223 0.0419	0.519 0.705 0.312	0.456 0.273 0.646	0.640 0.517 0.821	0.318 0.452 0.140	0.0420 0.0310 0.0386
	0.00	0.0419	0.503	0.454 0.270	0.733	0.235	0.0324
	8.11	0.0562 0.0586	0.298 0.656	0.646 0.285	0.854 0.713	0.114 0.264	0.0325 0.0231
		0.0435 0.0414 0.0562	0.503 0.689 0.298	0.454 0.270 0.646	0.733 0.639 0.854	0.235 0.336 0.114	0.0324 0.0248 0.0325

1

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Propene (Propylene); C₃H₆; [115-07-1]
- 3. Propane; C₃H₈; [74-98-6]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Mihara, S.; Arai, Y.;

Saito, S.

J. Chem. Engng. Japan 1975, 8,

98-104.

### VARIABLES:

Temperature, pressure, composition

PREPARED BY:

C. L. Young

### EXPERIMENTAL VALUES:

		Mole fra	actions in	liquid	Mole	fractions in	vapor
T/K	P/MPa	$x_{ m H_2}$	$x_{C_3H_6}$	^x C₃H8	у _{н2}	$y_{C_3H_6}$	^у С 3 Н 8
173.2	2.03	0.00705 0.00828	0.246 0.492	0.747 0.499	0.998 0.998	0.00066 0.00116	0.00132 0.00098
	4.05	0.00625 0.0134 0.0139	0.749 0.237 0.490	0.244 0.749 0.496	0.998 0.998 0.998	0.00175 0.00047 0.00089	0.00068 0.00117 0.00086
	6.08	0.0135 0.0196 0.0204	0.750 0.246 0.489	0.237 0.734 0.491	0.998 0.999 0.998	0.00135 0.00039 0.00082	0.00048 0.00099 0.00075
	8.11	0.0198 0.0317 0.0255	0.739 0.241 0.476	0.241 0.727 0.498	0.998 0.999 0.999	0.00116 0.00041 0.00074	0.00042 0.00100 0.00066
198.2	2.03	0.0253 0.00907 0.00909	0.737 0.252 0.523	0.237 0.739 0.468	0.999 0.990 0.989	0.00096 0.00329 0.00616	0.00037 0.00664 0.00445
	4.05	0.00890 0.0175 0.0193	0.746 0.241 0.521	0.245 0.741 0.459	0.989 0.994 0.994	0.00849 0.00188 0.00362	0.00244 0.00401 0.00267
	6.08	0.0172 0.0257 0.0253	0.736 0.235 0.514	0.246 0.739 0.461	0.993 0.995 0.995	0.00520 0.00150 0.00290	0.00174 0.00346 0.00222
	8.11	0.0221 0.0305 0.0337 0.0319	0.728 0.244 0.502 0.726	0.250 0.725 0.464 0.242	0.994 0.996 0.995 0.995	0.00437 0.00143 0.00271 0.00411	0.00136 0.00320 0.00212 0.00132

### AUXILIARY INFORMATION.

### METHOD/APPARATUS/PROCEDURE:

Static stainless steel cell of capacity  $5 \times 10^5$  mm³ fitted with magnetic stirrer and sampling valves. Cell enclosed in cryostat. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Gases added to cell and equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.99 mole per cent.
- 2. Purity 99.5 mole per cent.
- 3. Purity 99.7 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \quad \delta P/MPa = \pm 0.01; \\ \delta x_{H_2}, \quad \delta x_{C_3H_6}, \quad \delta x_{C_3H_8}, \quad \delta y_{H_2}, \quad \delta y_{C_3H_6}, \\ \delta y_{C_3H_8} = \pm 1 .$ 

### REFERENCES .

1. Sagara, H.; Arai, Y.; Saito, S.

J. Chem. Engng. Japan 1972, 5,

339.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Propene (Propylene);  $C_3H_6$ ; [115-07-1]
- 3. Propane; C₃H₈; [74-98-6]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Mihara, S.; Arai, Y.; Saito, S.

J. Chem. Engng. Japan 1975, 8, 98-104.

### EXPERIMENTAL VALUES:

		Mole fra	actions in	liquid	Mole fractions in vapor			
T/K	P/MPa	$x_{ m H_{2}}$	^x C₃H ₆	^x C₃H ₈	$y_{ m H_{2}}$	^у С ₃ Н ₆	^у С ₃ Н ₈	
223.2	2.03	0.0108	0.280	0.709	0.964	0.0128	0.0230	
		0.0106	0.480	0.509	0.958	0.0229	0.0186	
		0.00976	0.697	0.293	0.958	0.0307	0.0109	
	4.05	0.0206	0.281	0.699	0.978	0.00742	0.0141	
		0.0210	0.465	0.514	0.976	0.0125	0.0110	
		0.0198	0.686	0.294	0.976	0.0173	0.00626	
	6.08	0.0319	0.272	0.696	0.984	0.00527	0.0103	
		0.0307	0.466	0.504	0.981	0.0101	0.00877	
		0.0295	0.683	0.288	0.982	0.0133	0.00480	
	8.11	0.0414	0.265	0.694	0.985	0.00494	0.00966	
		0.0386	0.459	0.503	0.984	0.00833	0.00736	
		0.0396	0.668	0.293	0.984	0.0115	0.00434	
248.2	2.03	0.0115	0.323	0.665	0.876	0.0478	0.0761	
		0.0119	0.479	0.509	0.871	0.0701	0.0590	
		0.0109	0.642	0.347	0.864	0.0931	0.0426	
	4.05	0.0250	0.320	0.655	0.930	0.0269	0.0430	
		0.0256	0.465	0.509	0.930	0.0369	0.0328	
		0.0247	0.631	0.345 .	0.928	0.0495	0.0229	
	6.08	0.0403	0.317	0.642	0.950	0.0189	0.0309	
		0.0392	0.465	0.496	0.946	0.0284	0.0255	
		0.0399	0.624	0.336	0.946	0.0366	0.0174	
	8.11	0.0536	0.304	0.642	0.957	0.0160	0.0270	
		0.0549	0.457	0.488	0.957	0.0220	0.0210	
		0.0537	0.612	0.335	0.953	0.0318	0.0150	

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. Propene (Propylene);  $C_3H_6$ ; [115-07-1]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Mihara, S.; Arai, Y.;

Saito, S.

J. Chem. Engng. Japan 1975, 8,

98-104.

### VARIABLES:

Temperature, pressure, composition

PREPARED BY:

C. L. Young

### **EXPERIMENTAL VALUES:**

			actions in	-		fractions i	
т/к	P/MPa	ж _{Н 2}	^x CH₄	^ж С ₃ Н ₆	у _{Н2}	^у СН ₄	^у С ₃ Н ₆ *
173.2	2.03	0.0	0.848	0.152	0.0	1.0	
		0.00360	0.500	0.497	0.236	0.764	
		0.00493	0.246	0.749	0.504	0.496	
		0.00375	0.155	0.841	0.662	0.338	
		0.00427	0.116	0.880	0.734	0.266	
		0.00436	0.0	0.996	1.0	0.0	
	4.05	0.0154	0.690	0.294	0.459	0.541	
		0.0145	0.524	0.462	0.528	0.472	
		0.0109	0.309	0.680	0.679	0.321	
		0.0108	0.107	0.882	0.861	0.139	
		0.00944	0.0	0.991	1.0	0.0	
	6.08	0.0303	0.633	0.337	0.585	0.415	
		0.0253	0.500	0.475	0.640	0.360	
		0.0201	0.291	0.689	0.765	0.235	
		0.0163	0.0994	0.884	0.906	0.0935	
		0.0143	0.0	0.986	1.0	0.0	
	8.11	0.0770	0.842	0.0805	0.518	0.482	
		0.0622	0.788	0.150	0.566	0.434	
		0.0622	0.772	0.165	0.574	0.426	
		0.0352	0.566	0.399	0.660	0.340	
		0.0251	0.234	0.741	0.823	0.177	
						(con	t.)

The mole fraction of propylene in the gas phase at 173.15 K was too small for accurate estimation.

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Static stainless steel cell of capacity  $5 \times 10^5$  mm³ fitted with magnetic stirrer and sampling valves. Cell enclosed in cryostat. Temperature measured with thermocouple. Pressure measured with Bourdon gauge. Gases added to cell and equilibrated. Samples of liquid and gas withdrawn and analysed using a gas chromatograph with thermal conductivity detector. Details in ref. (1).

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.99 mole per cent.
- 2. Purity 99.9 mole per cent.
- 3. Purity 99.5 mole per cent.

### ESTIMATED ERROR: $\delta T/K = \pm 0.1$ ; $\delta P/MPa = \pm 0.01$ ; $\delta x_{H_2}$ , $\delta x_{CH_4}$ , $\delta x_{C_3H_6}$ , $\delta y_{H_2}$ , $\delta y_{CH_4}$ , $\delta y_{C_3H_6} = \pm 1\%$ .

### REFERENCES:

Sagara, H.; Arai, Y.; Saito, S.
 J. Chem. Engng. Japan 1972, 5,
 339.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. Propene (Propylene);  $C_3H_6$ ; [115-07-1]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Mihara, S.; Arai, Y.;

Saito, S.

J. Chem. Engng. Japan 1975, 8,

98-104.

### EXPERIMENTAL VALUES:

	_ /	Mole fr	actions in			fractions	
T/K	P/MPa	^x H ₂	^ж сн ₄	^ж С ₃ Н ₆	у _{Н2}	y _{CH} 4	^у С ₃ Н ₆ *
173.2	8.11	0.0229	0.126	0.851	0.897	0.103	
100 0	2 22	0.0200	0.0	0.980	1.0	0.0	
198.2	2.03	0.0	0.384	0.616	0.0	0.991	0.00942
		0.00244 0.00355	0.259 0.178	0.739 0.818	0.197 0.389	0.794 0.601	0.00854 0.00969
		0.00475	0.116	0.879	0.573	0.418	0.00858
		0.00600	0.0672	0.927	0.754	0.238	0.00808
		0.00599	0.0	0.994	0.992	0.0	0.00768
	4.05	0.0	0.851	0.149	0.0	0.993	0.00707
		0.00984	0.516	0.474	0.257	0.735	0.00776
		0.0101 0.0104	0.386 0.245	0.604 0.744	0.386 0.558	0.610 0.435	0.00457 0.00678
		0.0104	0.124	0.866	0.758	0.238	0.00421
		0.0108	0.0	0.989	0.996	0.0	0.00423
	6.08	0.0230	0.622	0.355	0.335	0.660	0.00434
		0.0199	0.381	0.600	0.533	0.462	0.00521
		0.0197	0.219	0.761	0.694	0.301	0.00458
		0.0209 0.0166	0.163 0.0	0.816 0.983	0.775 0.996	0.219 0.0	0.00521
	8.11	0.0359	0.587	0.377	0.453	0.543	0.00388 0.00304
	0.11	0.0329	0.438	0.529	0.563	0.433	0.00385
		0.0286	0.227	0.744	0.743	0.253	0.00374
		0.0263	0.161	0.813	0.811	0.185	0.00449
		0.0239	0.0	0.976	0.997	0.0	0.00327
223.2	2.03	0.0	0.226	0.774	0.0	0.960	0.0401
		0.00162 0.00424	0.180 0.110	0.818 0.885	0.123 0.389	0.828 0.567	0.0488 0.0439
		0.00589	0.0693	0.925	0.597	0.364	0.0392
		0.00741	0.0348	0.958	0.768	0.192	0.0397
		0.00857	0.0	0.991	0.958	0.0	0.0422
	4.05	0.0	0.441	0.559	0.0	0.974	0.0256
		0.00868	0.289	0.703	0.280	0.692	0.0284
		0.0112 0.0132	0.196 0.103	0.793 0.884	0.472 0.694	0.504 0.283	0.0240 0.0233
		0.0132	0.0382	0.949	0.863	0.115	0.0211
		0.0146	0.0	0.985	0.977	0.0	0.0228
	6.08	0.0	0.751	0.249	0.0	0.977	0.0233
		0.0160	0.450	0.534	0.261	0.716	0.0238
		0.0211	0.314	0.664	0.437	0.543	0.0203
		0.0229 0.0216	0.210 0.112	0.767 0.866	0.607 0.765	0.377 0.220	0.0166 0.0151
		0.0216	0.0	0.978	0.986	0.0	0.0131
	8.11	0.0286	0.507	0.465	0.315	0.662	0.0222
		0.0283	0.448	0.523	0.365	0.615	0.0200
		0.0319	0.343	0.625	0.496	0.486	0.0174
		0.0349	0.164	0.801	0.741	0.245	0.0143
248.2	2.03	0.0275 0.0	0.0 0.149	0.972 0.851	0.988 0.0	0.0 0.858	0.0119 0.142
240.2	2.03	0.00326	0.149	0.896	0.231	0.634	0.134
		0.00545	0.0679	0.927	0.403	0.459	0.137
		0.00687	0.0371	0.956	0.593	0.268	0.139
		0.00802	0.0179	0.974	0.726	0.135	0.139
		0.00977	0.0	0.990	0.863	0.0	0.137
						(con	it.)

^{*} The mole fraction of propylene in the gas phase at 173.15 K was too small for accurate estimation.

1

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. Propene (Propylene); C₃H₆;
  [115-07-1]

### ORIGINAL MEASUREMENTS:

Sagara, H.; Mihara, S.; Arai, Y.;

Saito, S.

J. Chem. Engng. Japan <u>1975</u>, 8,

98-104.

### EXPERIMENTAL VALUES:

		Mole fra	actions in	liquid	Mole :	fractions :	in vapor
T/K	P/MPa	$x_{ m H_{2}}$	^x CH ₄	^ж С ₃ Н ₆	$y_{\rm H_{2}}$	^y CH₄	y C ₃ H ₆
248.2	4.05	0.0	0.334	0.666	0.0	0.913	0.0872
		0.00436	0.273	0.723	0.100	0.812	0.0877
		0.0119	0.174	0.814	0.350	0.567	0.0829
		0.0159	0.0994	0.885	0.586	0.334	0.0800
		0.0175	0.0468	0.936	0.753	0.170	0.0768
		0.0183	0.0	0.982	0.914	0.0	0.0857
	6.08	0.0	0.505	0.495	0.0	0.927	0.0733
		0.0147	0.330	0.655	0.245	0.690	0.0646
		0.0226	0.232	0.745	0.422	0.516	0.0616
		0.0306	0.0969	0.873	0.705	0.236	0.0580
		0.0295	0.0864	0.884	0.728	0.212	0.0598
		0.0292	0.0	0.971	0.949	0.0	0.0512
	8.11	0.0	0.712	0.288	0.0	0.921	0.0790
		0.0216	0.445	0.533	0.207	0.726	0.0661
		0.0331	0.248	0.719	0.496	0.452	0.0516
		0.0365	0.229	0.734	0.542	0.407	0.0507
		0.0416	0.0931	0.865	0.775	0.181	0.0446
		0.0409	0.0	0.959	0.956	0.0	0.0438

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Cosway, H. F.; Katz, D. L. 2. Nitrogen; N₂; [7727-37-9] Am. Inst. Chem. Engnrs. J. 3. Methane; CH₄; [74-82-8] 1959, 5, 46-50. 4. Ethane; C₂H₆; [74-84-0] VARIABLES: PREPARED BY: Temperature, pressure, composition C. L. Young

### EXPERIMENTAL VALUES:

Mole	fractions	in liquid		Мо	le fracti	ons in g	as
$x_{ m H_{2}}$	$x_{ m N_{2}}$	$x_{ ext{CH }_4}$	x C ₂ H ₆	y H 2	$y_{N_2}$	$^{\mathcal{Y}}$ CH 4	y C ₂ H ₆
	T/K =	199.8	P/psia	= 1000	P/MP	a = 6.89	
0.00296 0.0146	0.1880 0.1410	0.0852 0.0791	0.7239 0.7653	0.0410 0.2073	0.6196 0.6282	0.0866 0.0814	0.2528 0.0831
	T/K =	144.3	P/psia	= 500	P/MP	a = 3.45	
0.00462 0.00626 0.00698 0.00743 0.00882	0.1215 0.0973 0.0795 0.0705 0.0633	0.0880 0.0873 0.0841 0.0844 0.0848	0.7859 0.8091 0.8295 0.8377 0.8431	0.2454 0.3448 0.4476 0.5044 0.5676	0.7087 0.6101 0.5096 0.4532 0.3932	0.0398 0.0391 0.0374 0.0371 0.0346	0.00606 0.00608 0.00549 0.00525 0.00456

### AUXILIARY INFORMATION

### METHOD APPARATUS/PROCEDURE:

Recirculating vapor flow system based on that described in ref. (1). Details of present apparatus in source and ref. (2). Temperature measured with thermocouple. Pressure measured with Bourdon gauge. High pressure magnetic circulating pump employed.

Cell charged under pressure.

Samples of each phase expanded to room temperature and pressure; analysed by mass spectrometry.

### SOURCE AND PURITY OF MATERIALS:

- 1 and 2. No details given.
- 3 and 4. Phillips Petroleum Co. samples.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/MPa = \pm 0.03$ ;  $\delta x$ ,  $\delta y = \pm 2\%$  (estimated by compiler)

- Dodge, B. F.; Dunbar, A. K.
   J. Am. Chem. Soc. 1927, 49, 591.
- Aroyan, H. J.; Katz, D. L.
   Ind. Eng. Chem. 1951, 43, 185.

COMPONENTS:		ORIGINAL MEASUREMENTS:								
	1. Hydrogen; H ₂ ; [1333-74-0]					Benham, A.L.; Katz. D.L.;				
2. Methane; CH 3. Ethene; C ₂				Am.Inst. Chem. Engnrs. J. <u>1957</u> ,3,						
4. Ethane; C2	4. Ethane; C ₂ H ₆ ; [74-84-0]					33-36.				
	<ol> <li>Propene; C₃H₆; [115-07-1]</li> <li>Propane; C₃H₈; [74-98-6]</li> </ol>									
VARIABLES:				PREPARED	BY:					
Temperature,	pressure,	compositi	on		С	L. Young				
EXPERIMENTAL VAL	LUES:				···					
T/K		255.37	199.	82 19	99.82	255.37	199.82			
P/bar		34.47	34.	47	34.47	68.95	68.95			
	$x_{ m H_{2}}$	0.0104	0.01	34 0	.0148	0.0236	0.0197			
Liquid Composition	$x_{\mathrm{CH_4}}$	0.0767	0.14	84 0	.1277	0.1645	0.1782			
Mole fractions	$x_{C_2H_4}$	0.0942	0.09	06 0.	.1823	0.1732	0.1797			
riactions	x C ₂ H ₆	0.0507	0.04	66 0	.0421	0.0402	0.0374			
	[∞] C₃H ₆	0.0839	0.07	77 0	.0707	0.0667	0.0600			
	$x_{C_3H_8}$	0.6841	0.62	33 0.	.5624	0.5318	0.5250			
	$y_{\mathrm{H}_2}$	0.3828	0.65	79 0.	.6860	0.4693	0.7726			
	$y_{\mathrm{CH_{4}}}$	0.3137	0.30	45 0.	.2545	0.3518	0.1966			
Vapor compositions	$y_{C_2H_4}$	0.0856	0.02	00 0.	.0406	0.0964	0.0209			
Mole fractions	$y_{C_2H_6}$	0.0344	0.00	65 0	.0060	0.0173	0.0038			
	y C ₃ H ₆	0.0263	0.00	26 0.	.0024	0.0086	0.0010			
	^у С ₃ Н ₈	0.1572	0.00	85 0.	.0105	0.0566	0.0051			
		Afivi	TTADV	INFORMATI	row.					
Milmuo			LIAKI				_			
METHOD:/APPARA'	TUS/PROCEDU	JRE:		SOURCE AND PURITY OF MATERIALS: 1. Purity better than 99.5 mole per						
described in	ref. l. T $\epsilon$	mperature		cent; further purified to remove water						
measured with measured with	thermocoup	ole. Press	sure	2,3,4,5 and 6. Purity better than 99.0 mole per cent; further purified to remove water and higher hydro-						
recirculated h	by high pre	essure magn	netic							
Pump. Cell cl Samples of eac	narged unde ch phase ex	er pressure spanded to	e. room	carbons	•					
pressure and a spectrometer.		[			j					
Postioneter.										
				ESTIMATED ERROR:						
				$\delta T/K = \pm 0.6$ ; $\delta P/bar = \pm 0.5$ %;						
				$\delta x, \ \delta y = \pm 0.5 \%.$						
				REFERENC	CES:					
				l. Aro	yan, H.J	.; Katz, D	).L.			
				Ind. Eng. Chem. <u>1951</u> ,43,185.						

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Benzene; C₆H₆; [71-43-2]
- 3. Cyclohexane;  $C_6H_{12}$ ; [110-82-7]

### ORIGINAL MEASUREMENTS:

Brainard, A.J. Williams, G.B.

Am. Inst. Chem. Engnrs.J. 1967, 13, 60-69.

4. Hexane; C₆H₁₄; [110-54-3]

### VARIABLES:

PREPARED BY:

Temperature, pressure, composition

C.L. Young

EXPERIME	NTAL VALU	ES: I	Liquid co Mole fr		n		K-va	lues	
T/K	P/bar	$x_{ m H_2}$	^x C ₆ H ₆	x _{C6H12}	$x_{C_6H_{14}}$	K _{H₂}	KC6H6	$K_{C_6H_{12}}$	KC6H14
366.48	36.3 71.2 105.9 137.7 35.0 70.5 101.9 136.9 35.9 69.8 102.2 137.0	0.0235 0.0450 0.0655 0.0849 0.0204 0.0401 0.0580 0.0756 0.0245 0.0455 0.0651 0.0854	0.3935 0.3859 0.3766 0.3688 0.4738 0.4608 0.4515 0.4440 0.2341 0.2277 0.2243 0.2193	0.3298 0.3225 0.3156 0.3090 0.3786 0.3754 0.3671 0.3619 0.5558 0.5441 0.5327 0.5234	0.2532 0.2476 0.2423 0.2373 0.1272 0.1237 0.1234 0.1185 0.1856 0.1827 0.1779	40.00 21.46 14.84 11.52 46.13 24.17 16.82 12.94 38.16 21.25 14.98 11.46	0.0582 0.0329 0.0287 0.0226 0.0593 0.0311 0.0240 0.0213 0.0684 0.0356 0.0270 0.0239	0.0546 0.0309 0.0269 0.0212 0.0590 0.0308 0.0247 0.0215 0.0609 0.0308 0.0232 0.0209	0.0794 0.0448 0.0390 0.0307 0.0856 0.0473 0.0379 0.0335 0.0825 0.0442 0.0342
394.26	35.2 70.6 105.8 137.4 38.3 72.2 102.9 137.6 35.8 70.1 102.2 134.7	0.0255 0.0511 0.0741 0.0976 0.0255 0.0464 0.0682 0.0897 0.0258 0.0509 0.0752 0.0957	0.3935 0.3834 0.3742 0.3646 0.4662 0.4562 0.4458 0.4334 0.2266 0.2237 0.2170 0.2178	0.3287 0.3202 0.3124 0.3045 0.3830 0.3748 0.3662 0.3580 0.5660 0.5487 0.5357 0.5189	0.2523 0.2453 0.2393 0.2333 0.1253 0.1226 0.1198 0.1189 0.1816 0.1767 0.1721 0.1676	34.66 18.30 12.85 9.80 35.52 20.34 14.04 10.75 34.98 18.52 12.72 10.07	0.1080 0.0636 0.0470 0.0450 0.0917 0.0544 0.0430 0.0377 0.1069 0.0623 0.0480 0.0399	0.1010 0.0590 0.0433 0.0397 0.0890 0.0530 0.0425 0.0370 0.0895 0.0556 0.0410 0.0350	0.1530 0.0888 0.0688 0.0639 0.1417 0.0862 0.0663 0.0571 0.1344 0.0780 0.0626 0.0521

### AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Stirred equilibrium cell. Pressure measured with Bourdon gauge. Analysis of samples carried out by expanding into an expansion cylinder and freezing out the hydrocarbon; hydrogen measured volumetrically and then total hydrocarbon estimated volumetrically. Composition of hydrocarbon residue measured by mass spectrometer. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Matheson ultrapure sample, purity better than 99.998 mole per cent.
- 2. Phillips Petroleum sample, purity 99.89 mole per cent; major impurity toluene.
- Phillips Petroleum sample, purity 99.99 mole per cent; major impurity 2,4-dimethyl pentane and 2,2diethyl pentane.
- Phillips Petroleum sample, purity 99.97 mole per cent; major impur-ity methyl cyclopentane.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3$ ;  $\delta P/bar = \pm 0.15$ ;  $\delta x, \delta y = \pm 2.0\%.$ 

(estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Benzene;  $C_6H_6$ ; [71-43-2]
- 3. Cyclohexane; C₆H₁₂; [110-82-7]
- 4. Hexane; C₆H₁₄; [110-54-3]

### ORIGINAL MEASUREMENTS:

Brainard, A.J. Williams. G.B.

Am. Inst. Chem. Engnrs. J. 1967, 13, 60-69.

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EXPERI	MENTAL	VALUES:		compositi fraction	on		K-Va	lues	
T/K	P/bar	$x_{ m H_{2}}$	^ж С ₆ Н ₆	x C $_{6}$ H $_{1}$ $_{2}$	^ж С ₆ Н _{1 4}	K _{H2}	K C $_{6}$ H $_{6}$	$K_{C_6H_{12}}$	K C ₆ H ₁₂
422.04	34.8	0.0272	0.4022	0.3127	0.2579	29.32	0.1980	0.1810	0.2590
	71.8 103.1	0.0578 0.0844	0.3896 0.3786	0.3028 0.2943	0.2498 0.2427	15.38 10.82	0.1073 0.0859	0.1050 0.0854	0.1496 0.1205
	139.5 37.9	0.1105 0.0277	0.3678 0.4670	0.2859 0.3818	0.2358 0.1235	8.41 29.58	0.0715 0.1769	0.0719 0.1716	0.1008 0.2510
	70.4	0.0530	0.4511	0.3714	0.1245	16.75 11.63	0.1148	0.1126 0.0791	0.1538 0.1142
	138.8	0.1018	0.4333	0.3492	0.1157	9.20	0.0673	0.0673	0.0978
	35.3 70.3	0.0278 0.0561	0.2261 0.2195	0.5649 0.5485	0.1812 0.1759	29.52 16.01	0.1827 0.1060	0.1685 0.0985	0.2380 0.1351
	103.6 132.4	0.0829 0.1062	0.2133 0.2079	0.5329 0.5193	0.1709 0.1666	11.12 8.81	0.0847 0.0750	0.0775 0.0640	0.1098 0.0923
1									

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. 1,2,3,4-Tetrahydronaphthalene
   (Tetralin); C₁₀H₁₂; [119-64-2]

### ORIGINAL MEASUREMENTS:

Simnick, J. J.; Sebastian, H. M.; Lin, H.-M.; Chao, K.-C. J. Chem. Eng. Data 1980, 25, 147-149.

### VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

					Mole fractio	ons
T/K	P/atm	P/MPa	Phase	$x_{ m H_{2}}$	[∞] CH ₄	^ж С ₁₀ Н ₁
462.3	49.7	5.04	liquid	0.0256	0.00834	0.9661
			vapor	0.8825	0.1033	0.0141
462.2	101.0	10.23	liquid	0.0508	0.01513	0.9341
			vapor	0.8892	0.1031	0.0076
462.2	150.3	15.23	liquid	0.0742	0.0204	0.9054
			vapor	0.8934	0.1014	0.0051
462.4	249.4	25.27	liquid	0.1194	0.0309	0.8497
			vapor	0.8929	0.1031	0.0039
462.2	49.9	5.06	liguid	0.0232	0.01525	0.9616
			vapor	0.7780	0.2068	0.0151
462.2	100.5	10.18	liquid	0.0459	0.0289	0.9252
			vapor	0.7899	0.2009	0.0092
462.2	150.1	15.21	liquid	0.0695	0.0403	0.8902
			vapor	0.7921	0.2007	0.0071
462.3	252.8	25.61	liguid	0.1105	0.0556	0.8338
			vapor	0.8154	0.1785	0.0062
462.3	50.0	5.07	liquid	0.0171	0.0339	0.9490
			vapor	0.5489	0.4344	0.0167
462.2	100.4	10.17	liquid	0.0333	0.0639	0.9029
			vapor	0.5514	0.4377	0.0109
462.2	150.5	15.25	liquid	0.0506	0.0922	0.8573
			vapor	0.5501	0.4403	0.0096
462.3	249.1	25.24	liquid	0.0863	0.1301	0.7836
			vapor	0.5830	0.4076	0.0093 nt.)

### AUXILIARY INFORMATION

### METHOD 'APPARATUS/PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top of cell. Details in ref. (1). Composition of liquid and vapor determined by stripping out hydrogen and methane and analysing by gas Amount of gas chromatography. determined volumetrically and amount of liquid determined gravimetrically. Details in source.

### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.95 mole per cent.
- 2. Purity better than 99 mole per cent.
- Purity better than 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \quad \delta P/MPa = \pm 0.02; \\ \delta x_{\rm H_2}, \quad \delta x_{\rm CH_4}, \quad \delta x_{\rm C_4H_{10}} = \pm 2 .$ 

### REFERENCES:

Simnick, J. J.; Lawson, C. C.;
 Lin, H. M.; Chao, K. C.
 Am. Inst. Chem. Engnrs. J.
 1977, 23, 469.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Methane; CH4; [74-82-8]
- 3. 1,2,3,4-Tetrahydronaphthalene (Tetralin); C₁₀H₁₂; [119-64-2]

## ORIGINAL MEASUREMENTS:

Simnick, J. J.; Sebastian, H. M.; Lin, H.-M.; Chao, K.-C. J. Chem. Eng. Data 1980, 25, 147-149.

### EXPERIMENTAL VALUES:

				Мо	le fractio	ns
T/K	P/atm	P/MPa	Phase	$x_{ m H_{2}}$	x CH4	xC ₁₀ H ₁₂
663.4	50.0	5.07	liquid	0.0435	0.0065	0.9491
663.3	101.5	10.28	vapor liquid	0.4608 0.1080	0.0428 0.0156	0.4965 0.8762
663.3	151.3	15.33	vapor liquid	0.6471 0.1666	0.0609 0.0211	0.2920
663.5	250.2	25.35	vapor liquid	0.7182 0.2762	0.0595 0.0315	0.2223
663.4	50.0	5.07	vapor liquid	0.7631 0.0393 0.4135	0.0601 0.0124 0.0854	0.1768 0.9483 0.5012
663.3	99.9	10.12	vapor liquid vapor	0.4135 0.0981 0.5741	0.0303	0.8717 0.3080
663.4	146.3	14.82	liquid vapor	0.1387 0.6105	0.0450 0.1356	0.8163
663.4	252.1	25.54	liquid vapor	0.2604 0.6754	0.0732 0.1368	0.6664
663.3	50.1	5.08	liquid vapor	0.0284	0.0308 0.2081	0.9408
663.3	100.9	10.22	liquid vapor	0.0722 0.3931	0.0764 0.2819	0.8514 0.3250
663.3	150.5	15.25	liquid vapor	0.1129 0.4227	0.1114 0.3055	0.7745 0.2718

- 1. Hydrogen; H₂; [1333-74-0]
- 1,2,3,4-Tetrahydronaphthalene, (Tetralin);C₁₀H₁₂;[119-64-2]
- 3. 1,3-Dimethylbenzene,(m-xylene);
  C₈H₁₀;[108-58-3]

### ORIGINAL MEASUREMENTS:

Oliphant, J.L.; Lin, H.-M.; Chao, K.-C.

Fluid Phase Equil. 1979, 3, 35-46

### VARIABLES:

Temperature, pressure, liquid composition.

### PREPARED BY:

C.L. Young

L								
EXPERIMENT.	AL VALUES:	Mole	fraction	in liquid	Mole	fraction	in vapor,	
T/K	P/10 ⁵ Pa	$x_{ m H_{2}}$	$x_{\mathrm{C}_{10}\mathrm{H}_{12}}$	x C $_{8}$ H $_{1}$ $_{0}$	$y_{ m H_2}$	y C ₁₀ H ₁₂	$y_{C_8H_{10}}$	
462.15 462.15 462.45	19.8 19.8 50.7	0.0130 0.0130 0.0327	0.497 0.498 0.488	0.486 0.486 0.479	0.892 0.894 0.952	0.0204 0.01923 0.00823	0.0872 0.0868 0.0394	
462.45 462.35 462.35 462.35	50.7 151.7 151.8 253.5 253.5	0.0336 0.0919 0.0927 0.1461 0.1463	0.486 0.461 0.455 0.432 0.434	0.480 0.447 0.453 0.422 0.420	0.955 0.978 0.978 0.983 0.982	0.00785 0.00348 0.00345 0.00257 0.00289	0.0370 0.0184 0.01832 0.01489 0.01522	
462.35 502.65 502.65 502.85 502.65 502.65 502.65	20.3 20.3 51.2 51.2 151.4 151.4 253.0	0.01342 0.01337 0.0368 0.0369 0.1076 0.1079	0.599	0.388 0.389 0.412 0.419 0.397 0.394 0.366	0.796 0.797 0.907 0.909 0.958 0.959	0.0594 0.0598 0.0237 0.0232 0.01021 0.00986 0.00749	0.1445 0.1437 0.0688 0.0674	
502.55 542.75 542.75 542.65 542.65 542.65 542.65 542.65	253.0 19.8 19.8 50.7 50.7 151.1 151.1 253.0 253.0	0.1689 0.01255 0.01247 0.0407 0.0412 0.1265 0.1253 0.1987 0.1993	0.468	0.364 0.384 0.437 0.438 0.420 0.427 0.382 0.378	0.968 0.589 0.598 0.813 0.922 0.920 0.940 0.941	0.00750 0.1394 0.1391 0.0541 0.0538 0.0211 0.0215 0.01642 0.01605	0.0240 0.272 0.263 0.1327 0.1332 0.0570 0.0587	

### AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which the phases separated under gravity. Liquid sample removed from the bottom of cell and vapor sample from top. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Composition of solvent determined by GC. Temperature measured with thermocouple and pressure with Bourdon gauge.

### SOURCE AND PURITY OF MATERIALS:

- Air Products sample, minimum purity 99.95 mole per cent.
- and 3. Aldrich Chemical Company samples, purity better than 99 mole per cent.

### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3$ ;  $\delta P/MPa = \pm 0.02$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = \pm 1\%$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 1,2,3,4-Tetrahydronaphthalene, [Tetralin);  $C_{10}H_{12}$ ; [119-64-2]
- 3. 1,3-Dimethylbenzene, (m-xylene);  $C_0H_{10}$ ; [108-58-3]

### ORIGINAL MEASUREMENTS:

Oliphant, J.L.; Lin, H.-M.; Chao, K.-C.

Fluid Phase Equil. <u>1979</u>, 3, 35-46.

EXPERIMENTAL VALUES: Mole fraction in liquid, Mole fraction in vapo	EXPERIMENTAL	VALUES: Mo	e fraction	in liquid,	Mole	fraction	in	vapor,
---------------------------------------------------------------------	--------------	------------	------------	------------	------	----------	----	--------

T/K	<i>P</i> /10 ⁵ Pa	$x_{ m H_{2}}$	x C ₁₀ H ₁₂	^ж С _в н ₁₀	$y_{\rm H_2}$	$y_{C_{10}H_{12}}$	^у С ₈ Н ₁₀
582.45	20.2	0.00986	0.645	0.345	0.352	0.283	0.363
582.45	20.2	0.00989	0.640	0.350	0.357	0.275	0.368
582.35	50.6	0.0432	0.581	0.376	0.691	0.1201	0.189
582.35	50.6	0.0430	0.582	0.375	0.687	0.1224	0.1907
582.65	151.6	0.1459	0.484	0.370	0.859	0.0500	0.0911
582.65	151.6	0.1459	0.484	0.370	0.860	0.0493	0.0903
582.35	252.9	0.232	0.434	0.325	0.900	0.0356	0.0644
582.35	252.9	0.231	0.434	0.335	0.899	0.0361	0.0649

- Hydrogen; H₂; [1333-74-0]
- 1,2,3,4-Tetrahydronaphthalene, (Tetralin); C₁₀H₁₂; [119-64-2]
- 1,1'-Methylenebisbenzene, (Diphenylmethane); C₁₃H₁₂; [101-81-5]

# ORIGINAL MEASUREMENTS:

Oliphant, J.L.; Lin, H.-M.; Chao, K.C Fluid Phase Equil. 1979, 3, 35-46.

#### VARIABLES:

Temperature, pressure, liquid composition.

PREPARED BY:

C.L. Young

<u></u>							
EXPERIMENTA		Mole fra	ction in	liquid	Mole fr	action in	vapor,
T/K	<i>P/</i> 10 ⁵ Pa	$x_{ m H_{2}}$	x C ₁₀ H ₁₂	x C $_{1}$ $_{3}$ H $_{1}$ $_{2}$	$y_{\rm H_2}$	$^{\mathcal{Y}}$ C ₁₀ H ₁₂	^у С ₁₃ Н ₁₂
462.45 461.15 461.15 461.25 461.25 461.05 541.55 541.55 541.45 541.45	20.6 20.7 20.7 50.7 152.7 252.3 20.0 51.1 51.1 152.3 152.3	0.01188 0.01171 0.01168 0.0294 0.0828 0.1292 0.01457 0.0398 0.0388 0.1195 0.1147	0.4866 0.4684 0.4688 0.4768 0.4546 0.4352 0.3729 0.4396 0.4441 0.4184 0.4203	0.5016 0.5198 0.5195 0.4938 0.4626 0.4356 0.6125 0.5205 0.5172 0.4621 0.4649	0.9815 0.9818 0.9820 0.9919 0.9966 0.9974 0.8981 0.9531 0.9533 0.9816 0.9801	0.01532 0.01462 0.01436 0.00642 0.00265 0.00204 0.0652 0.0334 0.0336 0.01336	0.00320 0.00355 0.00363 0.00162 0.00078 0.00060 0.0366 0.01345 0.01313 0.00505 0.00551
541.45 541.55 541.55	152.3 252.3 252.3	0.1186 0.1790 0.1688	0.4208 0.3885 0.3910	0.4605 0.4325 0.4402	0.9806 0.9865 0.9860	0.01404 0.00964 0.00995	0.00537 0.00383 0.00403
621.65 621.65 621.55 621.55 621.45 621.45 621.45 621.45	20.6 20.6 51.1 51.1 152.0 152.0 253.0 253.0	0.01515 0.01513 0.0486 0.0486 0.1444 0.1432 0.229 0.225 0.228	0.448 0.445 0.445 0.439 0.417 0.372 0.373 0.366	0.537 0.540 0.506 0.512 0.439 0.440 0.399 0.402 0.406	0.598 0.597 0.822 0.819 0.927 0.925 0.949 0.951	0.255 0.255 0.1139 0.1160 0.0476 0.0489 0.0329 0.0316 0.0326	0.1469 0.1480 0.0642 0.0650 0.0253 0.0261 0.01818 0.01740 0.01842

#### AUXILIARY INFORMATION

# METHOD APPARATUS / PROCEDURE:

Flow apparatus with both liquid and gas components continually passing into a mixing tube and then into a cell in which the phases separated under gravity. Liquid sample removed from bottom of cell and vapor sample from top. Composition of samples found by stripping out gas and estimating amount of solute volumetrically and solvent gravimetrically. Composition of solvent determined by GC. Temperature measured with thermocouple and pressure with Bourdon gauge.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Air Products sample, minimum purity 99.95 mole per cent.
- and 3. Aldrich Chemical Company samples, purity better than 99 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.3$ ;  $\delta P/MPa = \pm 0.02$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 1$ %.

(estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. 1,2,3,4-Tetrahydronaphthalene, [Tetralin);  $C_{10}H_{12}$ ; [119-64-2]
- 3. 1,1'-Methylenebisbenzene,
   (Diphenylmethane); C₁₃H₁₂;
   [101-81-5]

# ORIGINAL MEASUREMENTS:

Oliphant, J.L.; Lin, H.-M.; Chao, K.-C.

Fluid Phase Equil. 1979, 3, 35-46.

T/K	<i>P</i> /10 ⁵ Pa	^x H ₂	xC ₁₀ H ₁₂	^x C ₁₃ H ₁₂	$y_{\rm H_2}$	y _{C₁₀H₁₂}	^у С ₁₃ Н ₁₂
01.05	30.2	0.01920	0.446	0.534	0.251	0.421	0.328
01.05	30.2	0.01912	0.446	0.535	0.252	0.429	0.328
701.15	30.9	0.0212	0.409	0.570	0.274	0.376	0.349
700.75	50.4	0.0539	0.428	0.518	0.497	0.282	0.221
700.75	50.4	0.0538	0.428	0.518	0.495	0.283	0.223
701.05	151.0	0.202	0.392	0.406	0.761	0.1397	0.0993
701.05	151.0	0.203	0.398	0.405	0.760	0.1405	0.0993
701.05	253.0	0.328	0.311	0.361	0.828	0.0947	0.0773
701.05	253.0	0.316	0.316	0.368	0.835	0.0908	0.0742
701.05	253.0	0.321	0.313	0.365	0.835	0.0909	0.0745

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hydrogen sulfide;  $H_2S$ ; [7783-06-4]
- 3. Nonane;  $C_9H_{20}$ ; [111-84-2]

ORIGINAL MEASUREMENTS:

Eakin, B.E.; DeVaney, W.E.

Am. Inst. Chem. Eng. Symp. Ser., 1974, 70, 80-90.

VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMENTA	L VALUES:			Mole	fractions		
			in liqu	id		in vapor	
T/K	p/MPa	^ж н ₂	^x H ₂ S	^ж С ₉ Н _{2 0}	^у н ₂	y _{H2} S	^у С ₉ Н ₂₀
310.9	3.45	0.0265	0.0207	0.9528	0.9829	0.0167	0.00041
	6.89	0.0506	0.0212	0.9282	0.9902	0.0095	0.00029
	13.79	0.0927	0.0231	0.8842	0.9943	0.0056	0.00019
366.5	3.45	0.0348	0.0227	0.9425	0.9602	0.0348	0.00502
	6.89	0.0624	0.0237	0.9139	0.9773	0.0197	0.00302
	13.79	0.1188	0.0269	0.8543	0.9853	0.0129	0.00187
477.6	3.45	0.0490	0.0213	0.9297	0.8244	0.0680	0.1075
	6.89	0.0991	0.0227	0.8782	0.8880	0.0387	0.0733
	13.79	0.1859	0.0243	0.7898	0.9270	0.0218	0.0512
310.9	3.45	0.0202	0.1563	0.8235	0.8499	0.1498	0.00036
	6.89	0.0392	0.1541	0.8067	0.9225	0.0772	0.00025
	13.79	0.0846	0.1518	0.7636	0.9530	0.0468	0.00017
366.5	3.45	0.0212	0.1540	0.8248	0.7314	0.2647	0.00396
	6.89	0.0495	0.1462	0.8042	0.8534	0.1430	0.00365
	13.79	0.1042	0.1461	0.7497	0.9166	0.0819	0.00158
477.6	3.45	0.0232	0.1427	0.8341	0.3729	0.4866	0.1405
	6.89	0.0635	0.1627	0.7738	0.6400	0.2822	0.0778
	13.79	0.1570	0.1459	0.6971	0.8083	0.1603	0.0314

#### AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Stainless steel rocking equilibrium cell fitted with liquid and gas sampling ports. Pressure measured with Bourdon gauge. Components charged into cell under pressure, equilibrated and samples withdrawn. Samples analysed by GC using a termal conductivity detector and Porapak P column.

# SOURCE AND PURITY OF MATERIALS:

- 1. Liquid Carbonic sample, purity 99.999 mole per cent.
- Matheson sample, purity better than 99 mole per cent.
- Phillips Petroleum sample, purity better than 99.6 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$   $\delta p/MPa = \pm 0.05;$   $\delta x, \delta y = \pm 0.001$  (estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hydrogen sulfide; H₂S; [7783-06-4]
- 3. 1,3,5-Trimethylbenzene,
   (Mesitylene); C₉H₁₂; [108-67-8]

#### ORIGINAL MEASUREMENTS:

Eakin, B.E.; DeVaney, W.E.,

Am. Inst. Chem. Eng. Symp. Ser., 1974, 70, 80-90.

# VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMENT	AL VALUES:			Mole	fractions		
T/K	p/MPa	x _{H₂}	x _{H2} S in_liquid	^ж с ₉ н ₁₂	<i>y</i> _{H 2}	^y H ₂ S in vapor	^у С ₉ Н ₁₂
310.9	3.45	0.0124	0.0202	0.9674	0.9811	0.0187	0.00013
	6.89	0.0271	0.0203	0.9526	0.9889	0.0110	0.00014
	13.79	0.0525	0.0253	0.9224	0.9926	0.0073	0.00008
366.5	3.45	0.0174	0.0235	0.9590	0.9520	0.0465	0.00156
	6.89	0.0349	0.0273	0.9378	0.9719	0.0264	0.00171
	13.79	0.0702	0.0234	0.9064	0.9865	0.0123	0.00113
477.6	3.45	0.0274	0.0188	0.9538	0.8103	0.1008	0.0889
	6.89	0.0575	0.0192	0.9233	0.9013	0.0455	0.0532
	13.79	0.1135	0.0218	0.8647	0.9384	0.0279	0.0338
310.9	3.45	0.0121	0.1547	0.8332	0.8632	0.1367	0.00015
	6.89	0.0266	0.1523	0.8211	0.9265	0.0733	0.00016
	13.79	0.0521	0.1400	0.8079	0.9596	0.0403	0.00008
366.5	3.45	0.0156	0.1418	0.8426	0.7154	0.2808	0.00379
	6.89	0.0288	0.1624	0.8089	0.8238	0.1739	0.00226
	13.79	0.0615	0.1656	0.7729	0.9091	0.0897	0.00118
477.6	3.45	0.0104	0.1468	0.8428	0.2707	0.6308	0.0985
	6.89	0.0414	0.1465	0.8121	0.6147	0.3378	0.0475
	13.79	0.0965	0.1518	0.7518	0.8071	0.1905	0.0241

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Stainless steel rocking equilibrium cell fitted with liquid and gas sampling ports. Pressure measured with Bourdon gauge. Components Charged into cell under pressure, equilibriated and samples withdrawn. Samples analysed by GC using thermal conductivity detector and Porapak P column.

# SOURCE AND PURITY OF MATERIALS:

- 1. Liquid Carbonic sample, purity 99.999 mole per cent.
- Matheson sample, purity better than 99 mole per cent.
- 3. Eastman Kodak sample, normal boiling point 160-163°C.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.05$ ;  $\delta x, \delta y = \pm 0.001$  (estimated by compiler)

- 1. Hydrogen; H,; [1333-74-0]
- 2. Hydrogen sulfide; H₂S; [7783-06-4]
- 3 1-Methylethylcyclohexane, (isopropylcyclohexane);  $C_9H_{18}$ ;

ORIGINAL MEASUREMENTS:

Eakin, B.E.; DeVaney, W.E.

Am. Inst. Chem. Eng. Symp. Ser., 1974, 70, 80-90.

VARIABLES:

[696-29-7]

PREPARED BY:

Temperature, pressure

C. L. Young

EXPERIMENT	TAL VALUES:			Mole :	fractions		
			in liqu	iđ	in vapor		
T/K	p/MPa	ж _{Н 2}	x _{H2} S	^ж С ₉ Н ₁₈	^у н ₂	y _{H2} S	^у С ₉ Н ₁₈
310.9	3.45	0.0171	0.0210	0.9619	0.9809	0.0188	0.00027
	6.89	0.0350	0.0194	0.9456	0.9901	0.0097	0.00016
	13.79	0.0662	0.0216	0.9122	0.9933	0.0066	0.00019
366.5	3.45	0.0211	0.0210	0.9579	0.9533	0.0431	0.00364
	6.89	0.0455	0.0189	0.9356	0.9802	0.0181	0.00164
	13.79	0.0872	0.0251	0.8877	0.9839	0.0140	0.00213
477.6	3.45	0.0322	0.0166	0.9512	0.8419	0.0643	0.0937
	6.89	0.0683	0.0223	0.9094	0.9031	0.0477	0.0492
	13.79	0.1344	0.0225	0.8431	0.9240	0.0265	0.0495
310.9	3.45	0.0154	0.1403	0.8443	0.8575	0.1421	0.00031
	6.89	0.0323	0.1446	0.8231	0.9226	0.0772	0.00019
	13.79	0.0617	0.1448	0.7935	0.9552	0.0447	0.00017
366.5	3.45	0.0171	0.1478	0.8351	0.7057	0.2887	0.00563
	6.89	0.0396	0.1485	0.8119	0.8375	0.1589	0.00364
	13.79	0.0801	0.1493	0.7705	0.9047	0.0931	0.00220
477.6	3.45	0.0138	0.1424	0.8438	0.3303	0.5525	0.1172
	6.89	0.0483	0.1549	0.7968	0.6114	0.3202	0.0684
	13.79	0.1160	0.1560	0.7280	0.7696	0.1912	0.0392

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Stainless steel rocking equilibrium cell fitted with liquid and gas sampling ports. Pressure measured with Bourdon gauge. Components charged into cell under pressure, equilibriated and samples withdrawn. Samples analysed by GC using a thermal conductivity detector and Porapak P column.

- SOURCE AND PURITY OF MATERIALS:
- 1. Liquid Carbonic sample, purity 99.999 mole per cent.

- 2. Matheson sample, purity better than 99 mole per cent.
- 3. Phillips Petroleum sample, purity better than 99.9 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.05$ ;  $\delta x, \delta y = \pm 0.001$  (estimated by compiler)

- 1. Hydrogen; H,; [1333-74-0]
- 2. Hydrogen sulfide; H₂S; [7783-06-4]
- 3. Methane; CH₄; [74-82-8]
- 1-Methylethylcyclohexane, (isopropylcyclohexane); C₉H₁₈; [696-29-7]

#### ORIGINAL MEASUREMENTS:

Eakin, B.E.; DeVaney, W.E.

Am. Inst. Chem. Eng. Symp. Ser., 1974, 70, 80-90.

# VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

#### Temperature, pressure

# EXPERIMENTAL VALUES:

T/K	=	31	Λ	Q

			-,	
p/MPa		3.45	6.89	13.79
	$x_{ m H_2}$	0.0110	0.0284	0.0613
Mole fraction	$x_{\text{H}_2}$ S	0.1408	0.1451	0.1362
in liquid	n₂5 ^x CH₄	0.0301	0.0314	0.0339
	^x C ₉ H ₁₈	0.8181	0.7951	0.7686
	$y_{ m H_2}$	0.5870	0.7740	0.8664
Mole fraction in vapor	y _{H2} s	0.1451	0.0809	0.0444
	y _{CH} ,	0.2676	0.1449	0.0890
	^у С ₉ Н ₁₈	0.00035	0.00028	0.000230

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Stainless steel rocking equilibrium cell fitted with liquid and gas sampling ports. Pressure measured with Bourdon gauge. Components charged into cell under pressure, equilibriated and samples withdrawn. Samples analysed by GC using thermal conductivity detector and Porapak P column.

# SOURCE AND PURITY OF MATERIALS:

- 1. Liquid Carbonic sample, purity 99.999 mole per cent.
- 2. Matheson sample, purity better than 99 mole per cent.
- 3. No details given.
- 4. Phillips Petroleum sample, purity better than 99.9 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta p/MPa = \pm 0.05$ ;  $\delta x, \delta y = \pm 0.001$  (estimated by compiler)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hydrogen sulfide; H₂S; [7783-06-4]
- 3. Methane; CH4; [74-82-8]

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4. 1-Methylethylcyclohexane, (isopropylcyclohexane); C₉H₁₈; [696-29-7]

# ORIGINAL MEASUREMENTS:

Eakin, B. E.; DeVaney, W. E. Am. Inst. Chem. Eng. Symp. Ser., 1974, 70, 80-90.

			T/K = 366.5	
p/MPa		3.45	6.89	13.79
	$x_{ m H_{2}}$	0.0100	0.0235	0.0754
Mole fraction	x _H ,S	0.1408	0.1405	0.1412
in liquid	^x CH₄	0.0313	0.0317	0.0332
	^x C ₉ H ₁₈	0.8180	0.7953	0.7503
	^у н,	0.3996	0.6824	0.8104
Mole fraction	y _{H₂S}	0.2592	0.1445	0.0878
in vapor	y _{CH} ,	0.3347	0.1696	0.0993
	yC9H18	0.0065	0.0035	0.0025

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<u>p/MPa</u>		3.45	6.89	13.79
	$x_{ m H_{2}}$	0.0014	0.0381	0.1027
Mole fraction	x _H ,s	0.1437	0.1476	0.1514
in liquid	xCH,	0.0281	0.0308	0.0309
	^х С ₉ Н _{1 в}	0.8268	0.7835	0.7150
	^у н,	0.0325	0.4444	0.6700
Mole fraction	y _{H,S}	0.5395	0.3164	0.1876
in vapor	y _{CH} "	0.3103	0.1685	0.0976
	^у С ₉ Н ₁₈	0.1178	0.0707	0.0448

	1111000110110000	Organic Flaids		J	
COMPONENTS:		ORIGINAL·MEASU	REMENTS:		
1. Hydrogen; H2;	[1333-74-0]	Yorizane, M.; Sadamoto, S.;			
2. Hydrogen sulfide;	H ₂ S;	Masuoka, H.; Eto, Y.			
[7783-06-4]	Kogyo Kaga	ku Zasshi <u>1969</u>	, 72,		
<ol><li>Methanol; CH₄O;</li></ol>	[67-56-1]	2174-7.			
VARIABLES:		DDEDARED DV.			
	e, pressure,	PREPARED BY:			
gas compos			C. L. Young		
EXPERIMENTAL VALUES:					
AFERIMENIAL VALUES:					
T/K P/MPa	Mole fractions			_	
	$x_{ m H_2}$	$x_{ m H_{2}S}$	^у н ₂	$y_{\rm H_2S}$	
273.15 1.01	0.003	0.043	0.925	0.075	
2,3,13 1.01	0.006	0.107	0.813	0.187	
	0.002 0.003	0.205 0.379	0.702 0.400	0.298 0.600	
	0.002	0.617	0.237	0.763	
	0.002	0.688	0.163	0.837	
3.04	0.007 0.007	0.043 0.161	0.974 0.928	0.026 0.072	
	0.007	0.195	0.924	0.076	
	0.009	0.197	0.904	0.096	
	0.007 0.009	0.327 0.409	0.781 0.760	0.219 0.240	
	0.010	0.685	0.672	0.327	
5.07	0.012	0.050	0.988	0.012	
	0.014 0.014	0.149 0.194	0.962 0.945	0.038 0.055	
	0.014	0.221	0.945	0.055	
	0.013	0.353	0.868	0.132	
	0.015 0.018	0.401 0.675	0.854 0.796	0.146 0.204	
243.15 1.01	0.003	0.397	0.813	0.187	
	0.010	0.668	0.692	0.308	
		(cc	ont.)		
	AUXILIARY	INFORMATION			
ETHOD/APPARATUS/PROCEDURI	G:	SOURCE AND PUR	ITY OF MATERIALS:		
Vapor-liquid equilib	rium cell.	l. Purity	99.9 mole per	cent.	
Diagram given in sou		1	•		
(Original in Japanes		2. Purity	99.0 mole per	cent.	
v-raginar in oupunes	·· <i>,</i>		,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		
		}			
		ESTIMATED ERRO	R:		
		1	.1; $\delta x_{\rm H_2}$ , $\delta x_{\rm H}$	= ±0.001	
		1	_	_	
			d by compiler)	•	
		REFERENCES:			
		l			

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Hydrogen sulfide;  $H_2S$ ; [7783-06-4]
- 3. Methanol; CH₄O; [67-56-1]

# ORIGINAL MEASUREMENTS:

Yorizane, M.; Sadamoto, S.; Masuoka, H.; Eto, Y.

Kogyo Kagaku Zasshi 1969, 72, 2174-7.

# EXPERIMENTAL VALUES:

T/K	P/MPa	Mole fraction $^x{ m H}_2$	s in liquid ^x H ₂ S	Mole fract $y_{ m H_2}$	ions in gas ^y H ₂ S
	· · · · · · · · · · · · · · · · · · ·			<del></del>	
243.15	1.01	0.004	0.721	0.702	0.298
	3.04	0.006 0.006	0.776 0.397 0.652	0.655 0.813 0.896	0.345 0.187 0.104
	3.07	0.005 0.006 0.010	0.652 0.704 0.333	0.896 0.971 0.977	0.104 0.030 0.023
<u> </u> 	3.07	0.013 0.012	0.621 0.813	0.941 0.929	0.059 0.071

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COMPONENTS:  1. Hydrogen, H ₂ ; [1333-74-0]  2. Methylbenzene, (toluene);  C ₇ H ₆ ; [108-88-3]  3. Hexacarbonylbis (tributyl- phosphine) dicobalt;  C ₃₀ H ₅₄ Co ₂ O ₆ P ₂ ; [12101-96-1]	ORIGINAL MEASUREMENTS: Kharchenko, A.A.; Legtyareva, L.V.; Zhesko, T.E. Barinov, N.S.  Zhur. Fiz. Khim. 1975, 49, 2405-6				
VARIABLES: Pressure, composition	PREPARED BY: C.L. Young.				
EXPERIMENTAL VALUES:	328,15				
$P_{\rm H_2}$ /atm Conc. of (3)					
40 0.0 60 80 100 120 140 160	0.12 - 0.18 - 0.23 - 0.29 - 0.34 - 0.40 - 0.46 - 0.52 -				
40 1.5 mass% 60 (0.0192 M) 80 100 120 140 160	0.16 2.1 0.24 3.6 0.32 4.3 0.38 5.1 0.46 6.1 0.53 6.6 0.59 7.0 0.66 7.5				
40 4 mass% 60 (0.0512 M) 80 100 120	0.19 1.3 0.29 2.3 0.39 4.1 0.50 4.2 0.60 5.0				
AUXILIA	RY INFORMATION				
METHOD/APPARATUS/PROCEDURE:  Method stated as an analytical high pressure method and ref. (1) given as reference.	SOURCE AND PURITY OF MATERIALS:  1. Purity 99.82 mole per cent.  2. Analytical reagent quality  3. No details given.				
	ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta M = \pm 8\%.$ (estimated by compiler)  REFERENCES:  1. Tsiklis, D.S.  Technique of Physicochemical  Investigations at High and Ultra- High Pressures.				

- 1. Hydrogen; H₂; [1333-74-0]
- Methylbenzene, (toluene); C₇H₈; [108-88-3]
- 3. Hexacarbonylbis (tributyl-phosphine) dicobalt; C₃₀H₅₄Co₂O₆P₂; [12101-96-1]

#### ORIGINAL MEASUREMENTS:

Kharchenko, A.A. Legtyareva, L.V.; Zhesko, T.E.; Barinov, N.S.

Zhur. Fiz. Khim. 1975, 49, 2405-6.

#### **EXPERIMENTAL VALUES:**

$P_{ m H_2}/{ m atm}$	Conc. of (3)	T/K = 328.15  H solubility,  M	Mol (1)/mol (3)
140	4 mass %	0.74	6.6
160	(0.0512 M)	0.84	7.4
180		0.98	9.0
40	8 mass %	0.19	0.7
60	(0,1025 M)	0.29	1.2
80		0.41	1.8
100		0.54	2.5
120		0.68	3.3
140		0.83	4.2
160		1.00	5.7

M appears to be moles per litre and column headed mol (1)/mol (3) appears to be deduced by subtracting the amount of hydrogen dissolved in the toluene from the total amount of hydrogen dissolved.

NOTE: Table taken from Russ J. Phys. Chem. 1975, 49, 1409-10.

May, 1980

	COMPONENTS:	EVALUATOR:
-	1. Hydrogen; H ₂ ; [1333-74-0]	Colin L. Young,
	2. Argon; Ar; [7440-37-1]	Department of Chemistry,
		University of Melbourne,
i		Parkville, Victoria 3052,

AUSTRALIA.

#### CRITICAL EVALUATION:

Although this system has been studied by five different groups (1-5) there is a surprising lack of agreement between the various workers. The most extensive study is that of Calado and Streett (1), who studied coexisting vapor and liquid compositions at temperatures from 83 K to 141 K and pressures up to 52 MPa. Volk and Halsey (2) determined liquid phase compositions only, in the temperature range 87 to 140 K and pressures to 10 MPa. Mullins and Zeigler (3) studied coexisting vapor and liquid compositions in the temperature range 68 to 108 K and pressures to 12 MPa. Augood (4) made measurements at 87.4 K at two pressures of 18.4 and 11.6 MPa. Ostronov et al. (5) made measurements from 86 to 113 K at pressures between 1 and 4 MPa.

The very limited data of Augood (4) are consistent with those of Calado and Streett (1). The vapor composition given by Calado and Streett (1) are about 0.03 to 0.05 mole fraction higher than those of Mullins and Zeigler (3) but are sometimes higher and sometimes lower than those given by Ostronov et al. (5). There is reasonable agreement between the data of Volk and Halsey (2), and Calado and Streett (1) for the liquid compositions at 2 MPa but considerable differences at the higher pressures above 100 K. The liquid composition values of Calado and Streett (1) are smaller by about 0.005 than those of Mullins and Zeigler (3). There is fair agreement between the liquid phase compositions of Mullins and Zeigler (3) and Ostronov et al. (5).

The measurements of Calado and Streett (1) were made on ultra high purity samples using a well tried apparatus design and are probably the most accurate. However, in view of the differences between the various workers, the data of Volk and Halsey (2), Mullins and Zeigler (3), Ostronov et al. (5) and Calado and Streett (1) are all classified as tentative. Further measurements with carefully purified samples are needed.

# References

- Calado, J. C. G.; Streett, W. B. Fluid Phase Equilibria 1979, 2, 275.
- 2. Volk, H.; Halsey, G. D. J. Chem. Phys. 1960, 33, 1132.
- 3. Mullins, J. C.; Zeigler, W. T. Intern. Adv. Cryog. Engng. 1960, 10, 171.
- 4. Augood, D. R. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 5. Ostronov, M. G.; Shatskaya, L. V.; Finyagina, R. A.; Brodskaya, L. F.; Zhironova, N. A. Zhur. Fiz. Khim. 1977, 51, 2396.

# COMPONENTS: ORIGINAL MEASUREMENTS: Augood, D. R. 1. Hydrogen; H₂; [1333-74-0] 2. Argon; Ar; [7440-37-1] Trans. Instn. Chem. Engnrs. 1957, 35, 394-408. VARIABLES: PREPARED BY: Pressure C. L. Young

#### EXPERIMENTAL VALUES:

т/к	P/psig ⁺	P/MPa	Mole fraction in liquid, $x_{\rm H_2}$	of hydrogen in gas, y _{H2}	
87.4	2650 2650 1670 1670	18.37 18.37 11.62 11.62	0.187 0.181 0.103 0.091	0.941 - 0.948 0.912	

# AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid 2. British Oxygen Company sample. phases taken. The argon was condensed out and both components estimated volumetrically. Ratio of H2/HD in liquid estimated by mass spectrometry.

- SOURCE AND PURITY OF MATERIALS:
  - 1. Electrolytic sample containing 0.09 mole per cent HD.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; P/MPa = \pm 0.1;$  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = 4$ % (estimated by compiler)

⁺ psig - pounds per square inch gauge pressure

COMPONE	NTS:			ORIGINA	L MEASUREMEN	TS:	
	ydrogen;	TT . [7.7	222-74-01-		H.; Hals		,
	yarogen; rgon; Ar;			]		_	33, 1132-1139.
2. A.	rgon; AL	; [7440-	.37-1]	0. cn	em. rnys.	1900,	78, 1132-1139.
				ľ			
VARIABL	•	-		PREPARE		· · · · · · · · · · · · · · · · · · ·	
Tempe:	rature, pi	ressure		C. L.	Young		
EXPERIM	ÆNTAL VALUE			<u> </u>			
T/K	P/bar	P [†] /bar	Mole fraction	T/K	P/bar	P [†] /bar	Mole fraction
1/K	P/Dar	P /bar	of hydrogen in liquid, ^x H ₂	17 K	P/Dar	P /bar	of hydrogen in liquid, $x_{ m H_2}$
			H 2				H 2
87.0	22.51	24.54	0.0253	87.0	91.26	97.74	0.0860
	24.91 28.01	26.96 30.24	0.0278 0.0308	94.2	14.39 16.04	16.74 18.43	0.0189 0.0210
	31.97	34.44	0.0349		18.25	20.69	0.0233
	37.39	40.23	0.0402		21.01 24.83	23.87 27.93	0.0268 0.0314
	37.75 41.91	40.58 45.02	0.0408 0.0451		24.83	32.20	0.0314
	45.22	48.61	0.0481		30.39	33.89	0.0384
	47.22 54.22	50.69 58.22	0.0499 0.0565		31.99 35.90	35.42 39.58	0.0405 0.0450
	57.87	62.19	0.0595		40.80	44.94	0.0504
	64.27	69.19	0.0652		42.29	46.46	0.0525
	66.53 68.87	71.48 73.98	0.0671 0.0691		46.62 52.31	51.00 57.00	0.0578 0.0642
	71.38	76.67	0.0091		55.07	59.98	0.0672
	74.16	79.63	0.0733		59.29	64.46	0.0711
	77.04 80.22	82.70 86.09	0.0758 0.0780		61.05 69.19	66.40 74.88	0.0735 0.0810
	83.67	89.74	0.0804		69.37	75.05	0.0820
	87.23	93.49	0.0829				(cont.)
P =	fugacity	of hydro	gen.	$_{P}^{\dagger}$	= total	pressure	·.
			AUXILIARY	INFORMA	TION		
METHOD	/APPARATUS	5/PROCEDU	IRE:	SOURCE	AND PURITY (	OF MATERIA	ALS:
	ng equilib	-					•
ture :	measured v	vith ther	mocouple and	1			
			Bourdon gauge ad weight	1	No det	ails giv	en.
teste			f liquid	Ì		-	
calcu.	lated from	n number	of moles in				
gas pl	hase and t	total num	ber of moles.	}			
				}			
}				ESTIMAT	TED ERROR:		
					$= \pm 0.1; \delta$	P/bar =	±0.05;
				δx _{H2}	< ±2%.		
				REFERE	NCES:		

#### 574 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: [1333-74-0]; 1. Hydrogen; H₂; Volk, H.; Halsey, G. D. Argon; Ar; [7440-37-1] 2. J. Chem. Phys. 1960, 33, 1132-1139. EXPERIMENTAL VALUES: Mole fraction Mole fraction P[†]/bar P[†]/bar T/K P/bar of hydrogen T/K P/bar of hydrogen in liquid, in liquid, x H 2 $x_{\rm H_2}$ 86.32 0.0915 94.2 80.00 120.0 22.42 36.82 0.0418 82.95 89.36 0.0945 24.60 39.21 0.0455 95.51 102.39 0.1056 27.34 42.13 0.0499 100.0 13.68 0.0197 17.69 30.65 45.71 0.0552 19.16 0.0214 15.10 34.88 50.27 0.0639 16.79 20.92 0.0236 36.07 51.57 0.0660 18.89 23.15 0.0264 37.33 53.54 0.0680 21.68 0.0306 26.11 40.82 56.61 0.0740 25.53 30.72 30.10 0.0360 44.91 61.07 0.0814 35.42 0.0428 49.98 66.30 0.0902 31.17 35.76 0.0435 0.1000 56.19 73.05 34.08 38.82 0.0475 64.12 81.64 0.1129 42.88 0.0530 95.83 38.06 76.41 0.1299 43.49 48.47 0.0600 130.0 25.99 50.20 0.0558 45.63 50.65 0.0632 28.59 53.16 0.0613 50.02 55.33 0.0676 31.71 56.67 0.0670 50.14 55.43 0.0684 36.64 62.24 0.0771 56.02 61.57 0.0760 40.32 66.36 0.0845 59.43 65.09 0.0801 44.83 71.43 0.0932 0.0952 63.47 69.26 0.0848 72.33 45.64 66.11 71.98 0.0878 45.68 72.40 0.0952 0.0975 73.68 79.77 73.63 0.0975 46.83 74.53 80.53 0.0978 52.06 79.08 0.1078

85.64

87.28

23.25

25.66

28.73

32.65

38.06

38.24

42.48

47.74

54.51

63.67

63.74

65.71

67.87

70.25

81.42

85.51

110.0

91.97

93.63

31.76

34.34

37.52

41.64

47.22

47.40

51.97

57.52

64.81

74.61

74.68

76.74

78.91

81.47

93.22

97.58

0.1095

0.1115

0.0372

0.0410

0.0458

0.0515

0.0596

0.0602

0.0662

0.0742

0.0834

0.0961

0.0960

0.0986

0.1010

0.1042

0.1178

0.1229

52.23

57.09

62.85

24.96

27.54

29.30

32.21

32.77

34.20

34.57

35.90

39.22

39.92

41.46

43.76

44.36

50.78

52.92

55.18

140.0

79.44

85.01

91.35

61.29

63.95

66.67

69.77

70.39

71.70

72.40

73.85

77.71

78.53

80.26

82.94

83.63

91.01

93.35

95.90

0.1080

0.1169

0.1275

0.0615

0.0670

0.0723

0.0779

0.0796

0.0824

0.0833

0.0863

0.0943

0.0953

0.0990

0.1044

0.1060

0.1199

0.1245

0.1295

P = fugacity of hydrogen.

 $P^{\dagger}$  = total pressure.

			inorganic (	ompounas	3		57
COMPONENT	rs:		<u></u>	ORIGINAL	MEASUREMEN	NTS:	
1. Det	terium;	D ₂ ; [7	7782-39-0];	Volk,	H.; Hals	sey, G. I	) <b>.</b>
2. Arc	jon; Ar	; [7440-	-37-1]	J. Cher	m. Phys.	<u>1960</u> , 3	33, 1132-1139.
VARIABLE	S:			PREPARED	RY:		
Tempera	ature, p	ressure		C. L.			
EXPERIME	NTAL VALUE	cs:					
T/K	P/bar	P [†] /bar	Mole fraction of deuterium in liquid, $x_{D_2}$	T/K	P/bar	P [†] /bar	Mole fraction of deuterium in liquid, "D ₂
87.0	22.42 24.52 27.12 30.42 34.73 40.31 48.75 51.26 53.65 17.54 19.10 20.90 23.10	24.34 25.57 29.34 32.85 37.15 43.44 52.54 55.16 57.85 21.75 23.38 25.30 27.63	0.0317 0.0348 0.0381 0.0424 0.0480 0.0557 0.0669 0.0693 0.0721 0.0298 0.0353 0.0388	100.0	44.71 48.87 53.95 60.39 68.94 80.90 83.31 18.66 26.26 32.90 35.64 39.01 43.15	50.44 54.82 60.16 66.92 75.84 88.25 90.74 32.86 41.25 48.19 51.16 55.02 59.50	0.0734 0.0782 0.0860 0.0970 0.1088 0.1236 0.1270 0.0409 0.0574 0.0720 0.0771 0.0840 0.0920
	25.89 29.46 34.15		0.0432 0.0489 0.0564 fugacity of description		48.32 53.54	65.08	0.1021
			AUXILIARY				
Rocking ture me pressur calibra tester. lated f	g equilible asured we measured againg Composition number	with ther sed with inst a de desition oper of mo	JRE:  1. Tempera- mocouple and Bourdon gauge ad weight f liquid calcu- les in gas of moles.		ND PURITY (	OF MATERIA	
				ESTIMATE $\delta T/K = \delta x_{D_2} < \epsilon$	±0.1; δ	P/bar =	±0.05;

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Mullins, J. C.; Ziegler, W. T. Internat. Adv. Cryogen. Eng. 2. Argon; Ar; [7440-73-1] 1964, 10, 171-181. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young

_							
	TAL VALUES	of hydi	ogen			Mole fra of hydi	cogen
T/K	<i>P/</i> bar	in liquid,	in vapor,	T/K	P/bar	in liquid,	in vapor,
		$x_{ m H_{2}}$	$^{\mathcal{Y}}_{ ext{H}_{2}}$			$x_{ m H_{2}}$	$^{\mathcal{Y}}_{ ext{H}_{2}}$
		2	2			2. 2	2
86.95	60.87	_	0.9395	105.01	80.99	_	0.8347
86.97	121.89	-	0.9316	86.95	60.87	0.0636	-
86.94	101.53	_	0.9397		101.60	0.1024	_
	81.06	-	0.9459		81.06	0.0847	_
	40.87	-	0.9479	86.94	40.87	0.0432	_
	20.25	_	0.9290		20.25	0.02143	-
94.21	121.93	-	0.8955	94.21	121.93	0.1458	-
94.20	101.67	-	0.9054	94.20	101.67	0.1207	-
94.21	81.06	-	0.9119	94.21	81.06	0.0962	-
	60.80	-	0.9143		60.80	0.0720	_
	40.33	-	0.9056		40.33	0.0471	-
	20.40	-	0.8648	94.20	20.40	0.02301	-
99.95	61.21	-	0.8746	99.95	40.53	0.0506	-
	40.53	-	0.8585	99.97	20.29	0.02311	-
99.96	20.29	-	0.7888	99.94	121.32	0.1644	-
99.94	121.32	_	0.8582		101.67	0.1351	-
	101.67	-	0.8688	99.96	81.06	0.1058	-
99.95	81.06	-	0.8754	99.94	61.48	0.0789	-
	61.48	-	0.8749	105.01	61.00	0.0827	-
105.01	61.00	-	0.8306	105.00	40.95	0.0529	-
105.00	40.95	-	0.8046	105.01	20.53	0.02292	-
105.01	20.53	-	0.7065		121.17	0.1801	-
105.00	121.17	-	0.8168	105.02	101.60	0.1473	-
105.02	101.60	-	0.8291	105.01	80.99	0.1138	-

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Single pass flow apparatus with two compartment equilibrium cell. Temperature measured with platinum resistance thermometer; pressure measured with Bourdon gauge. Pure hydrogen bubbled through liquid argon. Samples analysed by gas chromatography Details in source.

## SOURCE AND PURITY OF MATERIALS:

1. and 2. Commercial samples with stated purities better than 99.995 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.03$ ;  $\delta P/bar = \pm 0.5\%$ ;  $\delta x_{\rm H_2}$  <  $\pm 2\%$ ;  $\delta (1-y_{\rm H_2})$  <  $\pm 3\%$ .

#### Inorganic Compounds COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Ostronov, M.G. Shatskaya, L.V.; 1. Finyagina, R.A.; Brodskaya, L.F.; Zhironova, N.A. Argon; Ar; [7440-37-1] Zhur. Fiz. Khim. 1977, 51, 2396-2398 VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/atm P/MPa in liquid, in gas, $x_{\rm H_2}$ $y_{\rm H_2}$ 112.8 10 1.01 0.0041 0.224 0.0084 0.350 1.22 12 0.0128 0.434 14 1.42 0.493 0.0171 16 1.62 0.538 1.82 0.0225 18 0.574 20 2.03 0.0258 2.53 0.0367 0.639 25 30 3.04 0.0475 0.683 3.55 0.0584 0.720 35 4.05 0.0692 0.746 40 0.51 0.0022 0.300 102 5 0.61 0.0030 0.412 6 0.477 7 0.71 0.0047 0.0064 0.524 8 0.81 0.561 9 0.91 0.0080 10 1.01 0.0098 0.591 0.0132 0.638 1.22 12 1.42 14 0.0165 0.675 0.706 16 1.62 0.0198 1.82 0.730 18 0.0232 0.754 20 2.03 0.0266 0.800 25 2.53 0.0350 30 3.04 0.0434 0.826 0.0518 0.830 35 3.55

#### AUXILIARY INFORMATION

0.0600

# METHOD/APPARATUS/PROCEDURE:

Recirculating flow method with magnetic recirculating pump. The liquid and gaseous samples were analysed by GC using a 5A Molecular sieve. Details in source.

40

4.05

# SOURCE AND PURITY OF MATERIALS:

1. Electrolytic grade oil vapor and oxygen removed, dried

0.834

2. Grade A purity 99.987 mole per cent.

#### ESTIMATED ERROR:

$$\delta T/K = \pm 0.01; \ \delta P = \pm 0.38; \ \delta (1-x_{H_2}), \ \delta (1-y_{H_2}) = \pm 18.$$

#### 578 Hydrogen and Deuterium Solubilities above 200kPa COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Ostronov, M.G.; Shatskaya, L.V.; 1. Finyagina, R.A.; Brodskaya, L.F.; 2. Argon; Ar; [7440-37-1] Zhironova, N.A. Zhur. Fiz. Khim. 1977, 51, 2396-2398 EXPERIMENTAL VALUES: Mole fraction of hydrogen in liquid, T/K P/atm P/MPa in gas, $x_{\rm H_2}$ $y_{\rm H_2}$ 93 0.51 0.0042 0.636 0.0055 0.667 0.61 6 7 0.71 0.0068 0.694 8 0.0088 0.81 0.718 9 0.91 0.0096 0.739 10 1.01 0.0107 0.758 0.0135 12 1.22 0.789 14 1.42 0.0162 0.815 16 1.62 0.0188 0.835 18 1.82 0.0215 0.851 0.0242 20 2.03 0.865 25 2.53 0.0310 0.887 0.0376 30 3.04 0.899 35 3.55 0.0443 0.906 40 4.05 0.0510 0.916 0.51 85.93 5 0.0051 0.828 6 0.61 0.0062 0.845 7 0.71 0.0074 0 858 8 0.81 0.0086 0.871 0.0096 9 0.881 0.91 10 1.01 0.0107 0.892 12 1.22 0.0130 0.908 14 1.42 0.0152 0.920 1.62 16 0.0174 0.930 18 1.82 0.0196 0.936 20 2.03 0.0218 0.940 25 2.53 0.0274 0.948 30 3.04 0.0327 0.952 3.55 0.0384 0.953 35 40 4.05 0.0440 0.953

#### Inorganic Compounds COMPONENTS: ORIGINAL MEASUREMENTS: Calado, J. C. G.; Streett, W. B. 1. Hydrogen; H₂; [1333-74-0] Fluid Phase Equilibria 2. Argon; Ar; [7440-37-1] 1979, 2, 275-282. VARIABLES: PREPARED BY: C. L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of Mole fraction of hydrogen hydrogen T/K P/MPa in liquid, in gas, T/K P/MPa in liquid, in gas, $x_{\rm H_2}$ $y_{\rm H_2}$ $x_{\rm H_2}$ $y_{\rm H_2}$ 83.09 10.34 0.0865 0.9820 84.50 35.30 0.3022 0.9764 0.8170 13.93 39.64 0.3476 0.1131 17.24 0.1378 0.9698 43.09 0.3934 0.7770 0.4508 0.1630 46.54 0.7260 0.9527 21.03 28.48 0.9366 48.40 0.4902 0.6968 0.2212 0.2404 0.6835 49.23 0.5142 31.03 0.9180 0.5495 33.09 0.2549 0.9065 49.92 0.6584 0.9427 0.0026 83.40 4.83 0.0403 0.9836 85.65 1.38 8.27 0.0706 0.9820 2.21 0.0130 0.9688 0.9828 0.0354 10.34 0.0876 0.9798 3.65 13.79 0.1152 0.9740 4.20 0.0404 0.9800 0.9764 17.44 0.1426 0.9670 4.83 0.0466 0.9585 20.68 0.1676 5.79 0.0563 0.9802 0.9800 24.34 0.1922 0.9467 6.89 0.0674 27.78 0.2144 0.9333 8.38 0.0806 0.9808 31.03 0.2393 0.9200 9.44 0.0908 0.9745 0.9722 34.47 0.8970 10.89 0.1036 0.2722 39.30 0.3166 0.8590 13.10 0.1226 0.9760 0.1577 83.74 17.37 0.9652 45.30 0.4005 0.7623

#### AUXILIARY INFORMATION

0.7680

0.6890

0.6762

0.6532

#### METHOD/APPARATUS/PROCEDURE:

46.54

49.71

50.68

51.43

84.05

Recirculating vapor flow apparatus fitted with magnetically operated Pressure measured with manganin pressure gauge.

0.4158

0.4992

0.5190

0.6246

Temperature measured with platinum resistance thermometer. Samples of liquid and gas analysed using thermal conductivity gas analyser. Details in ref. (1).

# SOURCE AND PURITY OF MATERIALS:

20.75

23.86

28.37

1. and 2. Linde Division of Union Carbide Co. samples, ultra high purity grade with minimum purity of 99.999 mole per cent.

0.1852

0.2128

0.2540

0.9502 0.9393

0.9057

(cont.)

#### ESTIMATED ERROR:

 $\delta P/\text{MPa} = \pm 0.05;$  $\delta T/K = \pm 0.2;$  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 0.005$  (may be larger near critical point).

#### REFERENCES:

1. Streett, W. B.; Calado, J. C. G. J. Chem. Thermodynamics 1978, 10, 1089.

1. Hydrogen; H₂; [1333-74-0]

2. Argon; Ar; [7440-37-1]

Calado, J. C. G.; Streett, W. B.

Fluid Phase Equilibria

1979, 2, 275-282.

# EXPERIMENTAL VALUES: .

		Mole frac hydro	gen			Mole frac hydro	gen
T/K	P/MPa	in liquid,	in gas,	T/K	<i>P/</i> MPa	in liquīd,	in gas,
		x H $_2$	$y_{\rm H_2}$			$x_{ m H_{2}}$	$y_{_{ m H_{2}}}$
85.65	.31.03	0.2796	0.8765	104.11	22.82	0.4340	0.6930
	35.58	0.3284	0.8375		23.59	-	0.6582
	40.95	0.4004	0.7765	111.46	1.72	0.0157	0.0544
	41.78	0.4066	0.7620		2.83	0.0311	0.6648
	43.16	0.4278	0.7507		4.41	0.0565	0.7490
	44.82	0.4590	0.7260		6.41	0.0884	0.7870
i	46.47	0.4917	0.6740		9.03	0.1352	0.7990
00.16	47.57	-	0.6333		11.03	0.1744	0.7890
90.16	24.27	0.2492	0.9056		14.13	0.2440	0.7533
	27.85	0.2973	0.8605		16.06 17.58	0.3071 0.3664	0.7138 0.6762
	33.30 36.54	0.3884 0.4311	0.7863 0.7270		18.75	0.4427	0.6020
	37.58	0.4714	0.7068	122.73	3.45	0.0375	0.4406
	38.26	0.4714	0.6795	122.73	4.20	0.0480	0.4986
95.77	1.38	0.0132	0.7877		5.93	0.0802	0.5768
,,,,	2.07	0.0213	0.8735		6.45	0.0933	0.5875
	3.45	0.0397	0.9383		7.72	0.1235	0.6089
	5.38	0.0621	0.9513		8.93	0.1501	0.6118
ı	7.58	0.0891	0.9613		10.34	0.1891	0.6050
	9.17	0.1025	0.9497		11.03	0.2158	0.5900
	10.27	0.1142	0.9503		12.06	0.2449	0.5811
	13.10	0.1495	0.9407		12.55	0.2655	0.5654
	14.96	0.1734	0.9243		13.41	0.2854	0.5383
	18.48	0.2223	0.8965		14.27	0.3487	_
	20.41	0.2514	0.8645	134.91	4.83	0.0520	0.3110
	21.99	0.2774	0.8550		5.27	0.0682	0.3309
	24.48	0.3245	0.8060		5.65	0.0744	0.3425
	25.79 27.44	0.3459 0.3914	0.7703 0.7553		6.27 6.55	0.0804	0.3579 0.3751
	28.96	0.4458	0.7553		6.89	0.0930 0.1099	0.3768
	29.54	0.4486	0.6910		7.31	0.1147	0.3889
	30.40	0.5375	0.6442		7.86	0.1332	0.3963
104.11	1.10	-	0.6002		8.34	0.1510	0.3961
	1.52	0.0172	0.6892		8.93	0.1692	0.3947
	1.72	0.0177	0.7028		9.24	0.1929	0.3895
	2.07	0.0226	0.7367		9.65	0.2177	0.3667
	2.90	0.0336	0.7990		10.14	0.2577	0.2606
	4.07	0.0482	0.8495	141.42	5.10	0.0442	0.1769
	6.20	0.0787	0.8925		5.51	0.0532	0.2003
	8.69	0.1142	0.9053		6.03	0.0680	0.2202
	11.44	0.1572	0.8900		6.48	0.0838	0.2357
	14.00	0.1965	0.8590		7.03	0.1129	0.2441
	17.44	0.2664	0.8170		7.41	0.1247	0.2481
	20.96	0.3600	0.7397		7.86	0.1445	-

- 2. Neon; Ne; [7440-01-9]

#### **EVALUATOR:**

Colin L. Young,
Department of Chemistry,
University of Melbourne,
Parksville, 3052: Vic.
AUSTRALIA: June, 1980

The deuterium and neon system has been studied by Simon (1,2) at the triple point of neon. The limited nature of the measurements make evaluation difficult but the same worker's data on the neon and hydrogen system (3) are not consistent with data thought to be reliable (see below). Therefore the data are classified as doubtful. Brouwer  $et\ al.\ (4)$  have studied the liquid-liquid and solid-liquid phase boundaries of the neon-deuterium system.

The hydrogen and neon system has been studied by Simon (3), Streett and Jones (5), Heck and Barrick (6) and by Van't Zelfde and Dokoupil (7).

The data of Heck and Barrick (6) cover vapor-liquid equilibrium from 26 to 42.5 K whereas those of Streett and Jones (5) cover the temperature range 24.6 to 33.7 K. These two sets of data are in good agreement and are classified as tentative.

The data of Simon (3) were presented in graphical form and are not consistent with the data Streett and Jones (5) and are not considered further here. There are considerable inconsistencies between the data of Van't Zelfde and Dokoupil (7) and those of Streett and Jones (5). The former worker's data are claimed to be more accurate but are restricted to a much smaller pressure range. The experimental method of Van't Zelfde and Dokoupil (7) is generally less reliable than that of Streett and Jones (5) or of Heck and Barrick (6) and the evaluator suggests that the more recent data of Van't Zelfde and Dokoupil are in error. The error may be partly due to impurities in the gases (to which the method is very sensitive) or may be due to a systematic error in the volume of the apparatus.

- 1. Simon, M. Physica, 1963, 29, 1079
- 2. Simon, M. Phys. Lett 1962 2, 234
- 3. Simon, M. Phys. Lett 1963, 5, 319
- 4. Brouwer, J.P.; Hermans, L.J.F.; Knapp, H.F.P.; Beennakker, J.J.M. *Physica*, <u>1964</u>, *30*, 1409.
- 5. Streett, W.B.; Jones, C.H. J. Chem. Phys. 1965, 42, 3989
- 6. Heck, C.H.; Barrick, P.L. Advan. Crogenic. Eng. 1965, 11, 349
- 7. Van't Zelfde, P.; Dokoupil, Z. Physica, 1974, 74, 423.

# COMPONENTS: 1. Deuterium; nD₂; [7782-39-0] Simon, M. 2. Neon; Ne; [7440-01-9] Physica 1963, 29, 1079-1086. VARIABLES: Pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction of neon in liquid, in vapor,

EXPERIMENTAL	VALUES:			
ļ			Mole fraction	on of neon
T/K	P/cmHg	P/kPa	in liquid,	in vapor,
	_		$x_{ m Ne}$	y Ne
24.56	98.2	130.92	0.0000	_
	108.33	144.43	0.0645	_
ļ	111.62	148.81	0.1015	-
İ	114.16	152.20	0.1480	-
	115.78	154.36	0.2118	_
	116.13	154.83	0.2641	_
ĺ	116.15	154.85	0.3110	_
1	116.10	154.79	0.4897	_
1	116.15	154.85	0.6104	_
]	116.15	154.85	0.8208	_
Į.	110.87	147.81	0.8724	-
	84.15	112.19	0.9337	-
1	32.51	43.34	1.0000	-
1	98.1	130.79	-	0.0000
	105.7	140.92	-	0.1019
1	112.5	149.99	-	0.1947
}	115.75	154.32	-	0.2501
ĺ	115.7	154.3	-	0.2781
}	99.8	133.1	-	0.3264
	67.5	90.0	-	0.4802
[	50.5	67.3	-	0.6339
}	32.51	43.34	-	1.0000

# AUXILIARY INFORMATION

#### METHOD APPARATUS / PROCEDURE:

Static equilibrium cell.

Temperature measured with Platinum resistance thermometer. Composition at dew and bubble points estimated from a knowledge of total volume and amount of substance in systems.

Details in source and ref. (1).

#### SOURCE AND PURITY OF MATERIALS:

- 1. Prepared by electrolysis of heavy water. Mass spectrometry indicated about 1% of HD.
- 2. At least 99.99 mole per cent pure.

# ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.003; \quad \delta^P/\text{cmHg} = \pm 0.05;$   $\delta x_{\text{Ne}}, \quad \delta y_{\text{Ne}} = \pm 1 \text{%}.$ 

#### REFERENCES:

Mathot, V.; Staveley, L. A.;
 Young, J. A.; Parsonage, N. G.
 Trans. Faraday Soc. 1956, 52,
 1488.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Neon; Ne; [7440-01-9]

#### ORIGINAL MEASUREMENTS:

Heck, C. K.; Barrick, P. L.

Adv. Cryogen. Engng.

1965, 11, 349-355.

#### VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

EXPERIMEN	TAL VALUE	S: Mole fra	action			Mole fra	action
		of hydr				of hydi	ogen
T/K	<i>P/</i> bar	in liquid,	in vapor,	T/K	<i>P/</i> bar	in liquid,	in vapor,
		$x_{ m H_{2}}$	$y_{\rm H_2}$			$x_{ m H_{2}}$	$y_{ m H_{2}}$
26.00	0.72	0.0000	0.0000	28.00	5.43	0.0691	
	2.15	_	0.6370		5.84	-	0.7180
	2.28	_	0.6580		5.89	0.6010	0.7350
	2.87	_	0.7190		5.93	0.6510	0.7400
	3.07	0.0224	_		5.96	0.6740	0.7490
	3.41	-	0.7580		6.01	0.7980	0.8050
	3.68	0.0409	-		6.03	0.8400	0.8340
	3.84	0.0413	-		5.88	-	0.9274
	3.88	0.0412	-		5.81	0.9578	0.9428
	3.92	0.0469	-		5.76	1.0000	1.0000
	4.03	-	0.7950	30.00	2.24	0.0000	0.0000
	4.05	0.7680	0.8010		2.26	_	0.0307
	4.11	0.8120	0.8270		3.26	-	0.3160
	4.13	0.8220	0.8210		4.12	_	0.4150
	4.11	0.8420	0.8400		5.12	0.0283	0.5070
	4.11	0.8630	0.8550		6.09	0.0550	0.5880
	4.09	0.9115	0.9035		6.79	-	0.6140
•	3.92	1.0000	1.0000		6.93	0.0893	-
28.00	1.32	0.0000	0.0000		6.99	-	0.6310
	2.89	-	0.5030		7.02	0.0937	_
	3.57	-	0.5910		7.68	-	0.6630
	3.78	0.0137	-		7.80	0.2360	-
	4.44	-	0.6650		7.84	-	0.6740
l	4.57	0.0311	-			(c	ont.)

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Vapor recirculated through cell.
Liquid and vapor samples analysed by
gas chromatography. Pressure
measured by Bourdon gauge and
temperature measured with platinum
resistance thermometer. Details in
source and ref. 1.

# SOURCE AND PURITY OF MATERIALS:

- 1. Maximum impurity 10 parts per million.
- Matheson research grade. maximum impurity 80 parts per million.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.05; \quad \delta P/\text{bar} = \pm 0.01 \text{ below} \\ 10 \text{ bar}; \quad \pm 0.1 \text{ above 10 bar}; \\ \delta x_{\text{H}_2} = \pm 2 \text{\$}.$ 

#### REFERENCES:

Herring, R. N.; Barrick, R. L.
 Adv. Cryogen. Engng. 1965,
 10, 151.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Neon; Ne; [7440-01-9]

# ORIGINAL MEASUREMENTS:

Heck, C. K.; Barrick, P. L.

Adv. Cryogen. Engng.

<u>1965</u>, *11*, 349-355.

# EXPERIMENTAL VALUES:

T/K	P/bar	Mole fra of hydr in liquid, ^x H ₂	ogen	т/к	P/bar	Mole fra of hydr in liquid, ^x H ₂	ogen
30.00	7.98 8.24 8.49 8.55 8.56 8.56 8.38 8.36 8.31 8.29 8.11 6.45 8.00 9.84 9.84 10.23 11.8 13.1 14.5 14.5	0.4400 0.6270 0.7160 0.7890 0.8310 0.8540 0.8720 0.9137 	0.6960 0.7430 0.7880 0.8200 0.8400 0.8550 - 0.8980 - 0.9218 1.0000 0.0000 0.1780 0.2120 0.3410 0.3480 0.3630 0.4180 0.4600 0.5070 0.5160 0.5410	34.66 37.64 39.57	16.0 10.1 11.6 13.3 14.0 15.4 16.2 18.0 19.0 21.1 13.7 16.5 17.0 19.0 21.3 21.7 20.8 21.9 23.9 24.1 24.6 25.1	0.5220 0.0000 0.0182 0.0439 - 0.1110 0.1780 0.2040 0.3500 0.0000 0.0428 0.0503 0.0896 0.1590 0.1690 0.0176 - 0.0511 0.0627 0.0693	0.5600 0.0000 0.1060 0.1900 0.2230 0.2740 0.3060 0.3500 0.3640 0.3980 0.0000 0.1390 0.1510 0.2100 0.2550 0.2620 0.0000 0.0369 0.0817
		9.4550	0.5410				

# Inorganic Compounds 585 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Streett, W. B.; Jones, C. H. J. Chem. Phys. 1965, 42, 3989-3994. 2. Neon; Ne; [7440-01-9] VARIABLES: PREPARED BY: C. L. Young Temperature, pressure

EXPERIME	NTAL VALUE						
т/к	P/bar	Mole fr of hyd in liquid ^x H ₂	lrogen	т/к	P/bar	Mole fr of hyd in liquid ^x H ₂	lrogen
24.59	1.74 2.15 2.15 2.46 2.77 3.03 3.04 3.05a 3.05a	0.0133 0.0171 	0.7364 0.7840 0.7843 0.8085 0.8265 0.8410 0.8424 0.8416	27.15	4.57 4.88 5.13 5.17a 5.17a 5.17 2.23 3.35 4.97	0.0488 0.0630 0.0762 0.0804 0.0803 0.0803 0.0083 0.0083	0.7439 0.7600 0.7698 0.7714 0.7715 0.7724 0.3598 0.5693 0.6982
26.33	2.14 2.14 3.55 4.03 4.38 4.49a 4.49a 4.48a 4.48a	0.0134 0.0151 0.0329 0.0442 0.0536 0.0589 0.0600 0.0584 0.0579	0.6232 - 0.7485 0.7748 0.7899 0.7950 0.7972	29.0	6.00a 6.000 2.60 3.39 4.61 5.87 6.61 6.67 6.72	0.1232 0.1236 0.0099 0.0203 0.0403 0.0772 0.1322 0.1457 0.1640	0.7440 0.7447 0.3225 0.4668 0.5946 0.6726 0.7049 0.7078
27.15	4.48 ^a 2.31 3.14 3.83	0.0580 0.0156 0.0243 0.0346	0.5422 0.6444 0.7020		6.76 6.77 6.77	0.1729 0.2246 0.2260 (co	0.7133 0.7100 0.7102 nt.)

a Indicates pressure at which 3 phases are present.

#### AUXILIARY INFORMATION

METHOU /	'APPARATUS,	PROCEDURE:
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Recirculating vapor flow apparatus With magnetic pump at ambient temperature. Samples analysed by thermal conductivity. Temperature measured with platinum resistance thermometer. Pressure measured using Bourdon gauge. Details in source.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

 $\begin{array}{lll} \delta {\rm T/K} = \pm 0.1; & \delta P/{\rm bar} = \pm 0.01 \text{ (up to } 10 \text{ bar);} & \pm 0.1 \text{ (above 10 bar);} \\ \delta x_{\rm H_2}, & \delta y_{\rm H_2} = \pm 0.001. \end{array}$ 

1. Hydrogen; H₂; [1333-74-0]

ORIGINAL MEASUREMENTS:

Streett, W. B.; Jones, C. H.

2. Neon; Ne; [7440-01-9]

J. Chem. Phys. 1965, 42, 3989-3994.

T/K	P/bar	Mole fra of hydr in liquid,	ogen	T/K	P/bar	Mole fra of hydr in liquid,	ogen
	, 	<i>x</i> _{H₂}	у _{Н 2}	·		ж _{Н 2}	у _{Н2}
29.00	6.77	0.2243	_	31.51	10.87	0.6971	0.7307
	6.78	0.3248	0.7135		10.98	0.7681	0.7740
	6.78	0.4093	0.7154		10.98	0.8505	0.8396
	6.78	0.5018	0.7211		10.64	0.9441	0.9334
	6.83	0.5552	0.7255		10.65	0.9436	0.9325
	6.88	0.6000	0.7319		10.43	0.9719	0.9645
	6.94	0.6375	0.7402	33.73	7.27	0.0308	0.2793
	6.98	0.6940	0.7586		9.34	0.0723	0.4109
	7.10	0.7318	0.7733		11.03	0.1254	0.4830
	7.14	0.7640	0.7873		12.58	0.2486	0.5370
	7.15	0.7933	0.8027		13.65	0.4203	0.5782
	7.16	0.8168	0.8184		13.82	0.4735	0.5899
	7.12	0.8509	0.8423		13.84	0.4766	0.5914
	7.06	0.9183	0.9008		13.89	0.4847	0.5938
	6.92	0.9620	0.9495		13.88	0.4860	0.5941
31.51	4.14	0.0099	0.1908	28.65	6.51 ^a	0.1708	0.7265
	5.48	0.0291	0.3784		6.51	0.1695	-
	7.75	0.0803	0.5428		6.51	0.4682	-
	9.20	0.1814	0.6054	28.80	6.67 ^a	0.1955	0.7175
	9.83	0.3254	0.6295		6.67	0.1968	-
	10,20	0.4693	0.6504		6.67	0.4282	-
	10.24	0.4827	0.6560		6.67	0.4282	-
	10.48	0.5605	0.6721	28.91	6.76 ^a	0.2323	-
	10.58	0.5970	0.6976		6.76	0.3771	-
	10.70	0.6304	0.6847				

 $^{^{\}mathrm{a}}$  Indicates pressure at which 3 phases are present.

#### Inorganic Compounds 587 COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Van't Zelfde, P.; Dokoupil, Z. Physica 1974, 74, 423-434. 2. Neon; Ne; [7440-01-9] VARIABLES: PREPARED BY: C. L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction Mole fraction of hydrogen of hydrogen T/K P/mmHgP/kPa T/K P/mmHq P/kPa in liquid, in liquid, $x_{\rm H_2}$ $x_{\rm H_2}$ 20.38 40 5.3 0 24.54 392 52.3 0.0010 5.3 20.44 40 0 24.88 421 56.1 0.0010 20.68 47 6.3 0 25.00 434 57.9 0.0010 21.46 72 9.6 0 25.00 438 58.4 0.0010 22.06 101 13.5 0 25.18 464 61.9 0.0010 22.71 143 19.1 0 25.19 465 62.0 0.0010 23.19 178 23.7 0 25.36 474 63.2 0.0010 24.00 255 0 34.0 25.67 541 72.1 0.0010 24.24 278 37.1 0 25.94 576 76.8 0.0010 24.66 45.6 342 0 20.41 106 14.1 0.0020 24.93 377 50.3 0 21.49 149 19.9 0.0020 25.76 499 0 25.5 66.5 22.23 191 0.0020 0.0020 25.82 0 511 68.1 23.06 254 33.9 25.88 44.7 520 69.3 0 23.84 335 0.0020 25.90 529 70.5 0 24.56 410 54.7 0.0020 25.95 537 71.6 0 24.81 420 56.0 0.0020 89.6 59.3 26.64 0 672 24.94 445 0.0020 27.05 758 101.1 0 24.96 446 59.5 0.0020 23.83 305 40.7 0.0010 25.07 462 61.6 0.0020 24.10 336 44.8 0.0010 25.42 513 68.4 0.0020 24.37 49.1 368 0.0010 25.86 581 77.5 0.0020 24.60 51.2 384 0.0010 26.55 712 94.9 0.0020 24.59 388 51.7 0.0010 (cont.) AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Static vapor equilibrium cell fitted 1. Purity 99.9 mole per cent. 2. Purity 99.99 mole per cent.

with a bellows pressure transducer. Cell filled with known amount of components. Bubble points determined from change in slope of pressure-temperature curves. Details of apparatus in ref. (1).

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$ ;  $\delta P/kPa = \pm 0.4$ .

# REFERENCES:

 Van't Zelfde, P.; Omar, M. H.; Le Pair-Schroten, H. G. M.; Dokoupil, Z.

Physica 1968, 38, 241.

25.53

25.66

25.66

648

652

654

86.4

86.9

87.2

1. Hydrogen; H₂; [1333-74-0]

2. Neon; Ne; [7440-01-9]

Van't Zelfde, P.; Dokoupil, Z.

0.0087

0.0087

0.0087

Physica 1974, 74, 423-434.

EXPERI	MENTAL V	ALUES:					
т/к	P/mmHg	P/kPa	Mole fraction of hydrogen in liquid, $^x{ m H}_2$	T/K	P/mmHg	P/kPa	Mole fraction of hydrogen in liquid, $^{x}{ m H}_{2}$
20.38	225	30.0	0.0043	25,85	694	92.5	0.0043
20.42	228	30.4	0.0043	25.85	696	92.8	0.0043
20.42	249	33.2	0.0043	25.88	688	91.7	0.0043
20.86	249	33.2	0.0043	25.96	710	94.7	0.0043
20.98	261	34.8	0.0043	20.46	289	38.5	0.0074
21.62	283	37.7	0.0043	21.61	350	46.7	0.0074
22.30	338	45.1	0.0043	22.30	392	52.3	0.0074
22.33	331	44.1	0.0043	23,23	459	61.2	0.0074
23.0	401	53.5	0.0043	23.71	467	62.3	0.0074
23.06	391	52.1	0.0043	23.71	474	63.2	0.0074
23.77	472	62.9	0.0043	24.32	624	83.2	0.0074
24.39	551	73.5	0.0043	24.55	561	74.8	0.0074
24.46	524	69.9	0.0043	24.55	567	75.6	0.0074
24.51	55 <i>7</i>	74.3	0.0043	25.15	640	85.3	0.0074
24.53	556 555	74.1	0.0043	25.36	686	91.5	0.0074
24.53	552	74.0 73.6	0.0043 0.0043	25.56 25.83	702 730	93.6 97.3	0.0074
24.53	547	72.9	0.0043	20.58	352	46.9	0.0074 0.0087
24.54	536	71.5	0.0043	21.67	471	62.8	0.0087
24.54	530	70.7	0.0043	22.32	547	72.9	0.0087
24.54	527	70.3	0.0043	23.03	616	82.1	0.0087
24.54	525	70.0	0.0043	23.92	725	96.7	0.0087
24.54(		69.6	0.0043	24.29	756	100.8	0.0087
24.54(	5) 518	69.1	0.0043	24.42	774	103.2	0.0087
24.54(		68.7	0.0043	24.46	624	83.2	0.0087
24.54(	5) 508	67.7	0.0043	24.48	779	103.8	0.0087
24.54(	5) 506	67.5	0.0043	24.48	775	103.3	0.0087
24.67	514	68.5	0.0043	24.48	761	101.5	0.0087
24.69	526	70.1	0.0043	24.48	754	100.5	0.0087
24.86	540	72.0	0.0043	24.74	691	92.1	0.0087
24.88	551	73.5	0.0043	24.77	702	93.6	0.0087
25.02	567	75.6	0.0043	25.00	742	98.9	0.0087
25.07	570 648	76.0	0.0043	25.01	751 750	100.1	0.0087
/n n 1	6/14	H h //	11 1111/14	/ S 13/1	/ h U	1017	O DOR (

0.0043

0.0043

0.0043

25.04

25.31 25.84

759

795

835

101.2

106.0

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]

#### **EVALUATOR:**

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

#### CRITICAL EVALUATION:

This system has been studied by several groups but apart from the work of Streett and Calado (1) there has been no work over a wide range of temperature and pressure. Streett and Calado (1) studied the system from 63 to 110 K and at pressures up to 57 MPa. The first reported measurements on this system were those of Verschoyle (2) who studied four isotherms between 63 and 88 K in the pressure range 0.012 to Although the results are less precise than those of Streett and Calado (1) they are in fair agreement. The measurements of Tsin and coworkers (3), (4) between 78 and 117 K were presented in graphical form and are not considered further. Gonikberg et al. (5) studied this system between 79 and 109 K up to pressures of 18 MPa. are in fair agreement with the measurements of Streett and Calado (1). The liquid phase data of Akers and Eubanks (6) for the three isotherms they studied (83, 100, 122 K) are in good agreement with the data of Streett and Calado (1) but their vapor phase data are in fairly poor agreement. Streett and Calado (1) suggested this was partly due to the relatively low purity of Akers and Eubanks (6) samples. The evaluator is inclined to agree as impurities in the samples would be expected to have widely different physical properties from those of the major components (except for argon as an impurity in the nitrogen). There are considerable discrepancies between the data of Augood (7) and Streett and Calado (1) at 67 and 78 K. This is not entirely unexpected in view of the scatter and low precision of Augood's data which are classified as doubtful. and coworker (8), (9) studied the solid-gas equilibrium in the temperature range 35 to 60 K and some vapor compositions up to 75 K. This work is not considered further here as it falls outside the scope of solubility. Yorizane et  $\alpha l$ . (11) studied this system at 77.35 K and the data are in reasonable agreement with those of Streett and Calado (1). their results show considerable scatter. Maimoni (12) studied this system at 90 and 95 K. The data are limited and show considerable scatter and are therefore classified as doubtful.

The data of Streett and Calado (1) are classified as tentative. Their measurements were carried out in a well-tried apparatus design with ultra pure samples. However their technique does not allow very accurate measurements to be made in the lower pressure region (below 1 MPa).

(cont.)

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]

#### **EVALUATOR:**

August 1980

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

#### CRITICAL EVALUATION:

#### References:

- Streett, W. B.; Calado, J. C. G. J. Chem. Thermodynamics <u>1978</u>, 10, 1089.
- Verschoyle, T. T. H. Phil. Trans. Roy. Soc. London A <u>1931</u>, 230, 189.
- 3. Ruhemann, M.; Tsin, N. M. Phys. Z. USSR 1937, 12, 389.
- 4. Steckel, F. A.; Tsin, N. M. Zhur. Khim. Prom. 1939, 16, 24.
- 5. Gonikberg, M. G.; Fastowsky, W. G.; Gurwitsch, J. G. Acta Physiochim. URSS 1939, 11, 865.
- 6. Akers, W. W.; Eubanks, L. S. Adv. Cryogenic Engng. 1960, 3, 275.
- 7. Augood, D. R. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 8. Dokoupil, Z.; Van Soest, G.; Swenker, M. D. P. Appl. Sci. Res. 1955, A5, 182.
- 9. Omar, M. H.; Dokoupil, Z. Physica 1962, 28, 33.
- 10. Dokoupil, Z. Adv. Cryogenic Engng. 1961, 6, 446.
- 12. Maimoni, A. Am. Inst. Chem. Eng. J. 1961, 7, 371.

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Nitrogen; N₂; [7727-37-9] Variables: Temperature, pressure ORIGINAL MEASUREMENTS: Verschoyle, T. T. H. Phil. Trans. A 1931,230, 189-220. PREPARED BY: C. L. Young

				<u> </u>			
EXPERIMENTAL VALUES: Mole fraction of hydrogen							ction of ogen
T/K	P/bar	in liquid,	in vapor,	T/K	P/bar	in liquid,	in vapor,
		$x_{ m H}$	${\cal Y}_{ m H}$			$x_{ m H}$	$y_{\mathrm{H}}$
88.16	17,24	0.024	0.770	68.14	225.79	0.307	0.881
88.14	27.11	0.053	0.833	68.12	227.79	0.311	0.854
88.13	41.58	0.092	0.853	63.15	12.31	0.020	0.987
88.14	56.83	-	0.862	63.17	12.35	0.019	_
88.14	81.06	0.207	0.866	63.16	12.37	0.025	0.984
88.15	105.38	0.283	0.821	63.15	17.32	0.027	0.980
78.13	17.42	0.023	0.905	63.16	27.05	0.041	0.981
78.14	37.07	0.073	0.930	63.17	36.78	0.057	0.984
78.13	56.30	0.119	0.937	63.17	46.72	0.075	0.982
78.13	80.96	0.175	0.922	63.15	56.24	0.083	0.984
76.13	115.11	0.248	0.895	63.15	56.33	0.085	0.974
78.14	149.32	0.334	0.840	63.15	56.77	0.078	-
68.12	17.42	0.033	0.973	63.16	90.74	0.121	-
68.14	26.93	0.046	0.976	63.14	90.77	0.120	0.963
68.12	36.46	0.066	0.976	63.16	199.98	0.143	0.948
68.15	46.50	0.076	0.979	63.15	120.01	0.147	0.957
68.10	56.62	0.094	0.973	63.16	120.02	0.152	-
68.10	90.74	0.154	0.955	63.15	120.05	0.146	0.968
68.12	90.86	0.147	0.953	63.16	149.30	0.163	-
68.10	120.04	0.181	0.944	63.17	149.35	0.172	0.957
68.12	149.36	0.219	0.922	63.16	149.36	0.173	_
68.14	149.39	0.220	0.908	63.15	149.39	0.168	-
68.14	178.74	0.252	0.903				
68.11	206.54	0.296	0.870				
68.12	213.07	0.296	0.883				

#### AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

Static equilibrium cell fitted with liquid and vapor sampling ports and magnetically operated stirrer.

Pressure measured on pressure balance (dead weight gauge). Temperature measured with platinum resistance thermometer. Gas analysed by combustion and absorption. Some details in source.

# SOURCE AND PURITY OF MATERIALS:

- Commercial sample passed over hot copper and through silica gel at liquid air temperature.
- Prepared by action of sodium nitrite on ammonium sulfate, chemically purified by passing through chromic acid and hot copper.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$ ;  $\delta P/bar = \pm 0.05$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 0.005$ .

COMPONENTS: ORIGINAL MEASUREMENTS:					
COMPONENTS:			ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]			Gonikberg, M.; Fastowsky, W.; Gurwitsch, J.		
2. Nitrogen; N ₂ ; [7727-37-9]			Acta Physicochimica URSS <u>1939</u> , 11, 865-881.		
VARIABLES:	<del></del>		PREPARED BY:		
	Temperature,	pressure	C. L.	Young	
EXPERIMENTAL VALUES:			<u> </u>		
	P/kg cm ⁻²	P /MD a	Mole fraction in liquid,	of hydrogen in gas,	
т/к	F/kg Cm	1/MPa	TH 11quia,	y _{H2}	
79.0	1.2	0.12	0.0	0.0 0.910	
79.0 79.0	18.9 34.4	1.85 3.37	0.042 0.069	0.910	
79.0	53	5.2	0.107	0.936 0.922	
79.0 79.0	69 81	6.7 7.9	0.158 0.173	0.922	
79.0	98	9.6	0.199	0.915	
79.0 79.0	103 111	10.1 10.9	0.213 0.224	0.902 0.889	
78.95	124	12.2	0.266	-	
78.9	126	12.4 14.5	0.271 0.337	0.820	
79.0 79.0	148 158	15.5	0.364	0.805	
79.0	181	17.8	0.457	0.697	
86.1 86.1	2.5 24.1	0.25 2.36	0.000 0.052	0.000 0.830	
86.1	45.0	4.41	0.098	0.865	
86.0 86.1	69 80	6.8 7.8	0.160	0.870	
86.05	106	10.4	0.255	0.841	
86.05 86.1	113 126	11.1 12.4	0.269 0.337	0.801	
86.1	134	13.1	0.375	0.770	
86.1	141	13.8	0.430 (cont.	0.566	
		AUXILIARY	INFORMATION	·	
METHOD/APPAR	ATUS/PROCEDURE:		SOURCE AND PURITY OF MATE	RIALS:	
Recircula	ting vapor flow	apparatus.			
ſ	sed by method o				
_	.) using a gas d		No details given.		
balance.					
source re		-			
			ESTIMATED ERROR:		
			$ \begin{cases} \delta T/K = \pm 0.07; & \delta^P/MP \\ 5 & MPa, \pm 0.1 \text{ above 5} \\ \delta x_{H_2}, & \delta y_{H_2} = \pm 2.0\$. \end{cases} $		
			REFERENCES:		
			1. Stock, A.; Ritte	r, G.	
			Z. Phys. Chem. 19		
				· ·	

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]

# ORIGINAL MEASUREMENTS:

Gonikberg, M.; Fastowsky, W.;

Gurwitsch, J.

Acta Physicochimica URSS 1939, 11,

865-881.

# EXPERIMENTAL VALUES:

			Mole fraction of hydrogen		
T/K	P/kg cm ⁻²	P/MPa	in liquid,	in gas,	
			$x_{ m H_{2}}$	$y_{\rm H_2}$	
95.4	5.5	0.54	0.000	0.000	
95.35	13.5	1.32	0.027	0.516	
95.35	25.7	2.52	0.042	0.692	
95.4	43.8	4.30	0.102	0.730	
95.4	63	6.2	0.162	0.733	
95.45	79	7.7	0.221	0.727	
95.35	94	9.2	0.277	0.722	
95.4	113	11.1	0.394	0.691	
95.35	119	11.7	0.417	0.635	
95.35	120	11.8	0.432	0.473	
109.0	13.3	1.30	0.000	0.000	
109.0	19.6	1.92	0.018	0.207	
109.0	35.0	3.43		0.423	
109.0	46.4	4.55	0.103	0.489	
108.95	59	5.8	0.156	0.500	
109.05	80	7.8	0.284	0.457	

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]	Augood, D. R.		
2. Nitrogen; N ₂ ; [7727-37-9]	Trans. Instn. Chem. Engnrs.,		
	<u>1957</u> , <i>35</i> , 394-408		
VARIABLES:	BDD 1919 NV		
VARIABLES:	PREPARED BY:		
Pressure	C. L. Young		
EXPERIMENTAL VALUES:			

т/к	P/psig ⁺	P/MPa	Mole fraction in liquid, $x_{ m H_2}$	
77.7	2580 2430 2250 2225 1660 1260 400 380	17.89 16.86 15.62 15.44 11.55 8.79 2.86 2.72	0.451 0.407 0.473 0.411 0.307 0.217 0.071	0.882 0.835  0.870 0.920  0.923 0.942
67.0	1270 1250	8.86 8.72	0.035 0.039	0.971

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The nitrogen was condensed out and both components estimated volumetrically. Ratio of H₂/HD in liquid estimated by mass spectrometry.

- SOURCE AND PURITY OF MATERIALS;
- 1. Electrolytic sample containing 0.09 mole per cent HD.
- 2. British Oxygen Company sample.

#### ESTIMATED ERROR:

$$\delta T/K = \pm 0.1;$$
  $P/MPa = \pm 0.1;$   $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = 4\%$  (estimated by compiler)

⁺ psig - pounds per square inch gauge pressure

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Nitrogen; N₂; [7727-37-9] VARIABLES: Temperature, pressure ORIGINAL MEASUREMENTS: Akers, W. W.; Eubanks, L. S. 2. Adv. Cryogenic Engng. 1960, 3, 275-293. C. L. Young

EXPERIMENTAL VALUES:

T/K	P/psia	P/MPa	Mole fraction in liquid, $^{w}{ m H}_{2}$	of hydrogen in gas, ${}^{y}_{\mathrm{H}_{2}}$
83.15	315	2.17	0.0487	0.8655
	500	3.45	0.0763	0.8948
	1400	9.65	0.2300	0.8700
	2000	13.79	0.3446	0.7977
99.82	315	2.17	0.0377	0.5509
	500	3.45	0.0741	0.6686
	800	5.52	0.1384	0.72795
	1100	7.58	0.2116	0.7175
	1400	9.65	0.3030	0.6530
122.04	500	3.45	0.0261	0.0821

# AUXILIARY INFORMATION

# METHOD /APPARATUS / PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetic pump at ambient temperature. Cell made of type 303 stainless steel. Pressure measured with Bourdon gauge and temperature measured with copper-constantan thermocouples. Samples of both phases analysed by gas chromatography using a thermal conductivity detector. Details in source.

# SOURCE AND PURITY OF MATERIALS:

1 and 2. Purity 99.7 mole per cent. Dried.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.06; \quad \delta P/MPa = \pm 0.02;$  $\delta x_{H_2}, \quad \delta y_{H_2} = \pm 2 \%.$ 

90.03

90.02

90.03

90.04

89.99

90.01

90.01

90.06

90.04

95.00

95.02

95.00

94.99

COMPONENTS:			ORIGINAL MEASUREMENTS:	· · · · · · · · · · · · · · · · · · ·
ł			1	
1. Hydro	gen; $H_2$ ; [1333	-74-0]	Maimoni, A.	
2. Nitro	gen; N ₂ ; [7727	-37-9]	Am. Inst. Chem. Engnr	s. J.
			<u>1961</u> , 3, 371-375.	
VARIABLES:			PREPARED BY:	
	Temperature, pr	essure	C. L. Yo	ung
EXPERIMENTA	L VALUES:			
T/K	P/lbs in ⁻²	P/MPa	Mole fraction in liquid, $^x{ m H}_2$	of hydrogen in gas, ${}^{y}_{\mathrm{H}_{2}}$
90.00	52.14	0.3595	0	0
90.02	259.0	1.7857	-	0.7324
90.02	196.76	1.3566	0.0248	0.6732
90.01	188.20	1.2976	0.0232	0.6619

1.1853

1.1336

0.9842

1.0209

0.8436

0.6134

1.0066

2.4421

4.5954

5.4076

1.1092

2.6217

4.5329

#### AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Recirculating vapor flow apparatus. The vapor was recirculated by a double acting mercury piston pump situated outside the low temperature cryostat. Liquid and gas samples analysed by optical interferometry. Temperature measured with thermocouples and pressure with dead weight piston gauge.

171.91

164.42

142.74

148.07

88.96

146.00

354.19

666,51

78.43

160.87

380,24

657.44

122.35

#### SOURCE AND PURITY OF MATERIALS:

0.0207

0.0164

0.0119

0.0159

0.0534

0.1115

0.0149

0.0566

0.1121

0

1. Purified by passing over activated charcoal at liquid nitrogen temperature. Purity 99.970 mole per cent by mass spectrometry.

0.6367

0.6247

0.5791

0.5903

0.5217

0.3753

0.5855

0.7800

0.8304

0

0.4492

0.7005

0.7643

Purified by passing over activated charcoal at dry ice temperature. Purity 99.974 mole per cent by mass spectrometry.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.02; \quad \delta^P/MPa = \pm 0.002;$  $\delta x_{H_2}, \quad \delta y_{H_2} = \pm 0.001.$ 

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Deuterium; D ₂ ; [7752-39-0]	Maimoni, A.
2. Nitrogen; N ₂ ; [7727-37-9]	Am. Inst. Chem. Engnrs. J.
	<u>1961</u> , 3, 371-375.
VARIABLES:	PREPARED BY:
Temperature, pressure	C. L. Young

#### EXPERIMENTAL VALUES:

T/K	P/lbs in ⁻²	P/MPa	Mole fraction in liquid, $x_{D_2}$	of deuterium in gas, ^y D ₂
90.00	52.14	0.3595	0	0
89.99	172.86	1.1918	0.0250	0.6403
90.05	112.29	0.7742	0.0122	0.4910
89.99	351.57	2.4240	0.0639	0.7819
90.05	613.40	4.2292	0.1214	0.8268
90.00	1011.59	0.6975	0.2169	0.8264
95.00	78.43	0.5408	0	0
95.01	987.71	6.8100	0.2160	0.7678
95.00	517.83	3.5703	0.9077	0.7446

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Recirculating vapor flow apparatus. The vapor was recirculated by a double acting mercury piston pump situated outside the low temperature cryostat. Liquid and gas samples analysed by optical interferometry. Temperature measured with thermocouples and pressure with dead weight piston gauge.

# SOURCE AND PURITY OF MATERIALS:

- Purified by passing over activated charcoal at liquid nitrogen temperature. Purity 99.61 mole per cent by mass spectrometry.
- Purified by passing over activated charcoal at dry ice temperature. Purity 99.974 mole per cent by mass spectrometry.

ESTIMATED ERROR:  $\delta T/K = \pm 0.02; \quad \delta P/\text{MPa} = \pm 0.002;$   $\delta x_{\text{D}_2}, \quad \delta y_{\text{D}_2} = \pm 0.001.$ 

#### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Yorizane, M.; Yoshimura, S.; Masuoko, H.; Toyama, A. 2. Nitrogen; N₂; [7727-37-9] Proc. ICECI, 1968, p.59. Heywood Temple, London. VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen T/K P/atm P/MPa in liquid in vapor $x_{\rm H_2}$ $x_{\rm H_2}$ 77.35 0.51 0.749 10 1.01 0.018 0.858 20 2.03 0.036 0.913 0.926 30 3.04 0.042 50 5.07 0.107 0.933 0.925 70 7.09 0.156 90 9.12 0.190 0.911 100 10.13 0.903 0.196 110 11.15 0.214 0.889

13.17

15.20

15.20

# AUXILIARY INFORMATION

#### METHOD APPARATUS/PROCEDURE:

Vapor recycle equilibrium cell with magnetic pump. Temperature measured with platinum resistance thermometer and pressure measured with Bourdon gauge. Vapor and liquid sampled simultaneously and expanded to 200 cm³ at room temperature, analysed using GC. Details in source.

130

150

150

#### SOURCE AND PURITY OF MATERIALS:

0.337

0.347

0.362

1. and 2. Purities 99.99 mole per cent or better.

0.876

0.843

0.831

# ESTIMATED ERROR:

 $\delta$ T/K = ±0.2;  $\delta$ P/MPa = ±0.03 up to 7.5 MPa; ±0.1 above 7.5 MPa;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2}$  = ±2%. (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]

# ORIGINAL MEASUREMENTS:

Streett, W.B.; Calado, J.C.G.

J. Chem. Thermodynamics,  $\underline{1978}$ , 10,  $\underline{1089-1100}$ .

VARIABLES:

PREPARED BY:

Temperature, pressure

C.L. Young

EXPERIMENTAL VALUES:			
T/K	Pressure	Mole fraction	of hydrogen
	/MPa	in liquid	in gas
		$x_{ m H_{2}}$	y H $_{2}$
}		11 2	11 2
63.19	19.17	0.201	
	20.82	0.214	0.916
	25.30	0.211	0.898
<b>\</b>	27.85	0.255	0.890
Į	30.61	0.276	0.884
	33.57	0.294	0.877
	35.99	0.298	0.869
	39.02	0.325	0.853
1	42.33	0.352	0.833
)	46.40	0.372	0.815
	49.64	0.407	0.785
	52.05	0.434	0.771
]	53.36	0.471	0.735
	57.22	0.536	0.696
70.35	1.45	0.032	0.961
	3.52	0.068	0.967
[	5.93	0.105	0.962
	8.27	0.138	0.954
	12.13	0.197	0.936
	15.51	0.242	0.897
(	19.37	0.290	0.874
	24.68	0.383	0.808
1	26.41	0.414	0.783
	27.44	0.447	0.771
L			

#### AUXILIARY INFORMATION

# METHOD /APPARATUS/PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetically operated pump. Pressure measured with manganin pressure gauge. Temperature measured with platinum resistance thermometer. Samples of liquid gas analysed using a thermal conductivity gas analyser.

# SOURCE AND PURITY OF MATERIALS:

Both gases were obtained from the Linde Div. of Union Carbide Corp. and had a stated purity of 99.999 moles per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.01$ ;  $\delta P/MPa = \pm 0.05$ ;  $\delta x, \delta y = \pm 0.001$ .

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]

# ORIGINAL MEASUREMENTS

Streett, W.B.; Calado, J.C.G.

J. Chem. Thermodynamics, 1978, 10, 1089-1100.

משקעש	ንፐ ለም አም አ ፐ.	WALLIES:

T/K	Pressure /MPa	Mole fraction in liquid,	of hydrogen in gas,
		ж _{Н 2}	у _{Н2}
70.35	28.68 29.30	0.487 0.536	0.725 0.690
77.55	1.03 2.07 3.44 4.48 7.03 8.62 10.48 13.79 14.55 15.58 17.10 18.62 19.30 19.44	0.026 0.046 0.064 0.086 0.140 0.173 0.214 0.286 0.306 0.335 0.373 0.433	0.886 0.914 0.931 0.928 0.921 0.919 0.918 0.873 0.862 0.840 0.820 0.762
83.67	11.27 12.72 13.86 14.34 14.96 15.31 15.68	0.273 0.325 0.360 0.384 9.410 0.429 0.465	0.826 0.798 0.765 0.747 0.711 0.683
90.79	1.86 2.48 3.45 4.55 6.07 7.31 9.17 10.55 11.86 12.76	0.034 0.047 0.072 0.099 0.144 0.178 0.237 0.289 0.349 0.407	0.685 0.748 0.794 0.816 0.823 0.822 0.803 0.779 0.746 0.698
100.00	1.45 2.07 2.96 4.14 5.34 6.34 7.48 8.55 9.45 10.34	0.018 0.031 0.056 0.090 0.128 0.158 0.207 0.248 0.301 0.361	0.338 0.490 0.587 0.656 0.682 0.688 0.689 0.674 0.645
110.30	2.38 3.17 3.90 4.69 5.07 5.72 6.17 6.62 7.55 7.79	0.029 0.055 0.080 0.107 0.125 0.153 0.172 0.202 0.206 0.286	0.253 0.361 0.426 0.463 0.477 0.489 0.491 0.486 0.456 0.421

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon monoxide; CO; [630-08-0]

#### **EVALUATOR:**

Colin L. Young
Department of Chemistry,
University of Melbourne,
Parkville, 3052, Victoria,
AUSTRALIA:

September, 1980.

The most extensive study of this system has been undertaken by Tsang and Streett (1) who reported seven isotherms in the temperature range 70 to 125K up to pressures of 53 MPa. They located the mixture critical line over the same temperature range. Verschoyle (2) reported the first work on this system and reported four isotherms, 68.2K, 73.2K, 83.2K and 88.2K in the pressure range 1.7 to 22.8 MPa. He also made some measurements in the vapor-solid region at 58.2 and 63.2K at pressures up to 18 MPa.

Ruhemann and Tsin (3) investigated this system at three temperatures, 78, 83 and 90K at pressures up to 5 MPa. However, their data were presented in graphical form and are not considered further here. Dokoupil  $et\ al$  (4) studied the vapor-solid region in the temperature range 32 to 70K and pressures up to 5MPa but did not study liquid-vapor equilibrium in detail and their results are not considered further. Augood (5) studied this system at the isolated temperature of 81.4K at two pressures and his results deviate somewhat from the data of Tsang and Streett (1) and are classified as doubtful.

Akers and Eubanks (6) studied three isotherms at 83, 100 and 122 K up to pressures of 24 MPa and Yorizane et al (7) studied three isotherms at 77.2, 103 and 123 K up to pressures of 15 MPa. The latter work was not extensive. The data of Verschoyle (2) Akers and Eubanks (6), Tsang and Streett (1) and Yorizane et al (7) are all in fair agreement in the overlapping ranges of temperature and pressure. The data of Tsang and Streett (1) are probably the most reliable and are classified as tentative. Compared with Tsang and Streett's data (1) those of Akers and Eubanks (6) were obtained on gases of lower purity, the data of Yorizane et al (7) are limited and of lower precision and the data of Verschoyle were determined fifty years ago with consequent lower precision in analysis.

- 1. Tsang, C.Y.; Streett, W.B. in press
- 2. Verschoyle, T.T.H. Phil. Trans. 1931, A230, 189.
- Ruhemann, M.; Tsin, N. Phys. Z. Sovietunion, 1937, 12, 389. C A.1938, 32, 2416.
- Dokoupil, Z.; Van Soest, G.; Swenker, M.D.P. Appl. Sci. Res. 1955, A5, 182.
- 5. Augood, D.R. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 6. Akers, W.W.; Eubanks, L.S.; Adv. Cryogenic. Engng. 1960, 3, 275.
- Yorizane, M.; Yoshimura, S.; Masouka, H.; Toyama, A. Proc. ICECI, p.57. Heywood Temple Industrial Publ. London, 1968

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Verscholye, T. T. H. 2. Carbon monoxide; CO; [630-08-0] Phil. Trans. 1931, A230, 189-220. VARIABLES: Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen in liquid in vapor

XPERIMENTA	L VALUES.			
T/K	P/atm	P/MPa	Mole fraction in liquid, x H ₂	of hydrogen in vapor,
	2.10	0.223	0.00	0.00
88.15	2.18	0.221	0.00	0.00 0.840
88.13 88.15	17.2 22.1	1.74 2.24	0.036 0.052	0.846
88.15	31.4	3.18	0.032	0.888
88.15	55.4	5.61	0.071	0.000
88.15	55.8	5.65	0.120	0.893
88.14	55.9	5.66	0.134	0.902
88.16	89.3	9.05	0.203	0.888
88.13	89.6	9.08	0.217	0.887
88.15	128.0	12.97	-	0.867
88.16	128.1	12.98	0.304	-
88.12	128.2	12.99	0.303	0.848
83.14	166.7	16.89	0.410	0.771
83.15	181.3	18.37	0.454	0.704
83.15	1,18	0.120	0.00	0.00
83.13	17.2	1,74	0.027	0.899
83.13	51,2	5,19	0.102	0.931
83.14	51.2	5.19	0.125	0.932
83.14	89.5	9.07	0.195	0.918
83.16	89.3	9.05	0.170	0.920
83.13	109.6	11.11	0,206	0.906
83.13	109.8	11.13	0.210	0.907
83.13	109.8	11.13	0.228	0.904
			(cont.	.)

# AUXILIARY INFORMATION

# METHOD APPARATUS/PROCEDURE:

Static equilibrium cell fitted with liquid and vapor sampling ports and magnetically operated stirrer.

Pressure measured with pressure balance (dead weight gauge).

Temperature measured with platinum resistance thermometer. Gas analysed by combustion and absorption. Some details in source.

# SOURCE AND PURITY OF MATERIALS:

- Commercial sample passed over hot copper and through silica gel at liquid air temperature.
- Prepared by the action of sulfuric acid on sodium formate. Distilled.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.02; \quad \delta P/MPa = \pm 0.005; \\ \delta x_{H_2}, \quad \delta y_{H_2} = \pm 0.005.$ 

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon monoxide; CO; [630-08-0] | Phil. Trans. 1931, A230, 189-220.

Verscholye, T. T. H.

EXPER	TMENTAT.	VALUES:	
-METIN	THUMTAN	ANDOUS .	

r/ĸ	P/atm P/MPa		Mole fraction of hydrogen in liquid, in vapor,		
			$x_{ m H_{2}}$	$y_{\rm H_2}$	
3.15	128.1	12.98	0.254	0.888	
33.13	128.1	12.98	0.249	0.889	
3.18	166.7	16.89	(0.292)	0.840	
3.13 3.15	166.8 176.4	16.90 17.87	0.329 0.344	0.843 0.831	
3.13	186.1	18.86	0.368	0.808	
3.14	190.9	19.34	0.381	0.805	
3.15	195.8	19.84	0.401	0.795	
3.13	200.6	20.33	0.415	0.777	
3.14	200.6	20.33	0.411	0.767	
3.15	205.4	20.81	0.435	0.766	
3.11	205.4	20.81	0.430	(0.800)	
3.13 3.17	205.4	20.81 21.32	0.422	(0.735) 0.759	
3.11	210.4 215.1	21.32	0.448 0.470	0.737	
3.15	215.2	21.81	(0.389)	0.725	
3.12	220.9	22.38	0.486	0.694	
3.13	224.8	22.78	0.541	0.663	
3.15	0.33	0.033	0.00	0.00	
3.17 3.14	17.3	1.75	0.033	0.967	
3.14	22.2 31.5	2.25 3.19	<u>-</u>	0.954 0.964	
3.14	31.8	3.22	0.056	0.975	
3.15	50.9	5.16	-	0.970	
3.14	51.0	5.17	0.084	0.967	
3.17	79.7	8.08	-	0.963	
3.14	80.1	8.12	0.120	0.964	
3.15	80.2	8.13	0.127	0.959	
'3.17 '3.15	113.7 113.8	11.52 11.53	0.165 0.154	0.948 0.955	
3.14	113.9	11.54	0.166	0.951	
3.14	128.0	12.97	_	0.942	
3.16	142.5	14.44	-	0.935	
3.12	152.4	15.44	0.206	0.930	
3.15	152.4	15.44	-	0.931	
3.19 3.14	176.4	17.87	0.218 0.230	0.917 0.920	
3.14	176.4 186.2	17.87 18.87	0.236	0.914	
3.15	186.2	18.87	0.229	0.916	
3.12	205.4	20.81	0.257	0.902	
3.12	205.6	20.82	0.250	0.912	
3.15	224.8	22.78	0.265	0.893	
3.16	224.9	22.79	0.275	0.890	
8.19 8.17	17.02 21.69	1.725 2.198	0.030 0.033	0.979 0.982	
8.15	26.61	2.198	0.033	0.982	
8.15	31.67	3.209	0.042	0.986	
8.11	41.26	4.181	-	0.987	
8.15	41.41	4.196	0.062	0.985	
8.15	41.45	4.200	0.063	0.975	
8.14 8.14	79.86	8.092	- 103	0.977	
8.14 8.16	79.89	8.095 11.986	0.102	0.977 0.962	
8.15	118.29 118.38	11.986	0.138	0.962	
8.15	152.17	15.419	0.158	(0.968)	
8.15	152.33	15.435	0.163	0.946	
8.15	190.97	19.350	0.188	0.939	
8.14	215.16	21.801	0.202	0.934	

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] Augood, D. R. 2. Carbon monoxide; CO; Trans. Instn. Chem. Engnrs. [630-08-0] 1957, 35, 394-408. VARIABLES: PREPARED BY: C. L. Young

#### EXPERIMENTAL VALUES:

T/K	P/psig ⁺	P/MPa	Mole fraction of in liquid, $x_{ m H_2}$	of hydrogen in gas, $y_{\rm H_2}$	
81.4	2620 2600 1430 1380	18.17 18.03 9.96 9.62	0.312 0.334 0.184 0.174	0.913 0.941 0.940 0.912	

#### AUXILIARY INFORMATION

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The carbon monoxide was condensed out and both components estimated volumetrically. Ratio of  $\rm H_2/HD$  in liquid estimated

METHOD/APPARATUS/PROCEDURE:

by mass spectrometry.

- SOURCE AND PURITY OF MATERIALS:
- Electrolytic sample containing 0.09 mole per cent HD.
- 2. British Oxygen Company sample.

ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/MPa = \pm 0.1$ ;  $\delta x_{H_2}$ ,  $\delta y_{H_2} = 4$ % (estimated by compiler)

⁺ psig - pounds per square inch gauge pressure

# COMPONENTS: ORIGINAL MEASUREMENTS: Akers, W. W.; Eubanks, L. S. 1. Hydrogen; H₂; [1333-74-0] Adv. Cryogenic Engng. 1960, 3, 2. Carbon monoxide; CO; [630-08-0] 275-293. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES:

T/K	<i>P/</i> psia	<i>P/</i> MPa	Mole fraction in liquid, $^{x}{ m H}_{2}$	of hydrogen in gas, ^y H ₂
83.15	315	2.17	0.0398	0.9084
	500	3.45	0.0609	0.9320
	1400	9.65	0.1745	0.9143
	2000	13.79	0.2490	0.8790
99.82	315 500	2.17	0.0389 0.0674	0.6803 0.7619
	800	5.52	0.1163	0.7844
	1100	7.58	0.1727	0.7848
	1400	9.65	0.2399	0.7739
122.04	500	3.45	0.0449	0.2260
	800	5.52	0.1382	0.3349

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetic pump at ambient Cell made of type 303 temperature. stainless steel. Pressure measured with Bourdon gauge and temperature measured with copper-constantan thermocouples. Samples of both phases analysed by gas chromatography using a thermal conductivity detector. Details in source.

#### SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.7 mole per cent. Dried.
- 2. Prepared from reaction of formic acid and sulfuric acid. Dried. Purity about 97 mole per cent.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.06; \delta P/MPa = \pm 0.02;$  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 2$ %.

- Hydrogen; H₂; [1333-74-0]
- 2. Carbon monoxide; CO; [630-08-0]

#### ORIGINAL MEASUREMENTS:

Yorizane, M.; Yoshimura, S.; Masuoko, H.; Toyama, A.

Proc. ICECI 1968, p.59. Heywood, Temple, London.

#### VARIABLES:

Temperature, pressure

#### PREPARED BY:

C.L. Young

PERIMENTAL VA	TOE2:		Mole fraction	of hydrogen
T/K	P/atm	P/MPa	in liquid	in vapor,
			$x_{ m H_{2}}$	$^{\mathcal{Y}}$ H 2
123.15	30	3.04	-	0.140
	40	4.05	0.047	0.235
	50	5.07	0.084	0.288
	60	6.08	0.167	-
	62	6.28	0.200	0.291
	62.7	6.35	0.247	0.293
103.15	10	1.01	-	0.270
	20	2.03	-	0.528
	30	3.04	~	0.637
	40	4.05	-	0.692
	50	5.07	0.136	0.710
	75	7.60	0.192	0.726
	100	10.13	0.267	0.673
	123.5	12.48	0.395	0.563
77.35	6	0.61	~	0.887
	11	1.11	~	0.928
	21	2.13	~	0.954
	31	3.14	~	0.958
	46	4.66	0.075	0.947
	51	5.17	0.083	0.960
	75	7.60	0.113	0.944
	100	10.13	0.160	0.941
	125	12.67	0.200	0.929
	150	15.20	0.250	0.909

# AUXILIARY INFORMATION

# METHOD APPARATUS/PROCEDURE:

Vapor recycle equilibrium cell with magnetic pump. Temperature measured with platinum resistance thermometer and pressure measured with Bourdon gauge. Vapor and liquid sampled simultaneously and expanded to 200 cm³ at room temperature, analysed using GC. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. Purity 99.99 mole per cent or better.
- Purity 99.67 mole per cent oxygen and nitrogen being principle impurities.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2$ ;  $\delta P/MPa = \pm 0.03$  up to 7.5 MPa;  $\pm 0.01$  above 7.5MPa;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = 2\%$ . (estimated by compiler).

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon monoxide; CO; [630-08-0]

# ORIGINAL MEASUREMENTS:

Tsang, C. Y.; Streett, W. B.

in press

VARIABLES:

PREPARED BY:

Temperature, pressure

C. L. Young

	NTAL VALUE	Mole from of hyd	rogen		<b></b>	Mole fra of hydr	ogen
T/K	P/MPa	in liquid, $^{x}_{ m H_{2}}$	in vapor,  yH2	T/K	P/MPa	in liquid, [#] H ₂	in vapor
70.0	0.49	0.0110	0.9500	70.0	40.44	0.3726	0.8275
	0.79	0.0152	0.9696		42.01	0.3890	0.8173
	1.46	0.0260	0.9804		44.23	0.4130	0.8070
	2.15	0.0349	0.9864		46.91	0.4430	0.7926
	3.49	0.0546	0.9901		49.75 50.93	0.4750 0.4975	0.7600 0.7387
	4.90 6.28	0.0704 0.0871	0.9878 0.9864		51.64	0.4973	0.7307
	7.59	0.1012	0.9818		52.61	0.5374	0.6951
	9.80	0.1243	0.9654		52.94	0.5561	0.6753
	10.78	0.1327	0.9612	77.3	0.65	0.0136	0.974
	11.86	0.1433	0.9577	, , , ,	1.51	0.0292	0.9437
	13.98	0.1624	0.9491		2.10	0.0369	0.9554
	15.78	0.1764	0.9406		2.86	0.0498	0.9602
	19.18	0.2030	0.9301		3.60	0.0619	0.9615
	22.38	0.2270	0.9155		4.27	0.0732	0.9628
	25.02	0.2468	0.9018		4.95	0.0847	0.9622
	28.09	0.2716	0.8881		5.64	0.0948	0.9647
	30.58	0.2900	0.8798		6.36	0.1058	0.9634
	32.63	0.3053	0.8666		7.03	0.1165	0.9641
	33.44	0.3112	0.8602		7.66	0.1241	0.9570
	34.89	0.3222	0.8547		8.36	0.1355	0.9538
	35.74	0.3314	0.8482		10.47	0.1648	0.9418
	37.94	0.3502	0.8335			(6)	ont.)

#### AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetically operated pump. Pressure measured with manganin pressure gauge.

Temperature measured with platinum resistance thermometer. Samples of liquid gas analysed using a thermal conductivity gas analyser.

# SOURCE AND PURITY OF MATERIALS:

- Matheson ultra high purity sample, purity 99.999 mole per cent or better.
- Matheson sample, purity 99.99
   mole per cent. Passed through
   cold trap at boiling point of
   nitrogen.

# ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.02; \quad \delta P/\text{MPa} = \pm 0.5\$; \\ \delta x_{\text{H}_2}, \delta y_{\text{H}_2} = \pm 0.005 \text{ (but may be as large as } \pm 0.02 \text{ near critical point).}$ 

# REFERENCES:

Streett, W. B.; Calado, J. C. G. J. Chem. Thermodyn. <u>1978</u>, 10, 1089.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon monoxide; CO; [630-08-0]

# ORIGINAL MEASUREMENTS:

Tsang, C. Y.; Streett, W. B.

in press

# EXPERIMENTAL VALUES:

		Mole fra of hydr				Mole fra of hydr	
T/K	<i>P/</i> MPa	in liquid,	in vapor,	T/K	P/MPa	in liquid,	
		$x_{ m H_{2}}$	$y_{ m H_2}$			$x_{ m H_{2}}$	$y_{ m H_{2}}$
77.3	11.13	0.1743	0.9362	105.0	2.21	0.0364	0.5504
	12.31	0.1914	0.9313		2.87	0.0541	0.6177
1	13.94 15.99	0.2155 0.2410	0.9200 0.9053		3.57	0.0731	0.6628
	18.90	0.2851	0.8804		4.62 5.62	0.1034 0.1322	0.6953 0.7101
	22.15	0.3334	0.8520		6.64	0.1644	0.7138
Į.	24.90	0.3814	0.8178		7.73	0.2015	0.7155
)	26.99	0.4270	0.7877		8.58	0.2329	0.7048
	29.13	0.4916	0.7378		9.15	0.2556	0.6964
	29.67 30.14	0.5176 0.5458	0.7218 0.6983		9.75 10.56	0.2813 0.3248	0.6840 0.6612
85.0	0.52	0.0090	0.6970		11.22	0.3698	0.6262
""	0.78	0.0142	0.8181		11.56	0.4026	0.5966
}	1.45	0.0266	0.8730		11.73	0.4314	0.5726
	2.86	0.0543	0.9110	115.0	1.71	0.0084	0.1095
}	4.20	0.0814	0.9218		1.95	0.0159	0.1838
}	4.94 5.63	0.0957 0.1084	0.9230 0.9233		2.26 2.92	0.0249 0.0444	0.2596 0.3684
	7.01	0.1364	0.9194		3.62	0.0663	0.4393
ĺ	8.38	0.1640	0.9167		4.20	0.0859	0.4765
	10.10	0.1977	0.9053		4.98	0.1142	0.5087
ļ	11.84	0.2321	0.8919		5.80	0.1447	0.5319
	13.86 15.42	0.2760 0.3122	0.8702 0.8506		6.36	0.1680	0.5400
	17.02	0.3122	0.8366		7.02 7.50	0.1964 0.2227	0.5349 0.5273
	18.41	0.3936	0.7941		8.04	0.2553	0.5048
Í	19.44	0.4312	0.7694		8.50	0.2945	0.4784
1	20.09	0.4610	0.7452		8.59	0.3068	0.4659
	20.79	0.5103	0.7067	105.0	8.68	0.3195	0.4559
95.0	21.07 0.91	0.5358 0.0120	0.6930 0.5894	125.0	2.98 3.30	0.0217 0.0330	0.1065 0.1487
73.0	1.47	0.0240	0.7231		3.63	0.0461	0.1860
	2.83	0.0543	0.8086		3.95	0.0594	0.2130
ļ	4.22	0.0881	0.8311		4.47	0.0820	0.2446
	5.62	0.1221	0.8380		4.71	0.0953	0.2572
	7.01 8.40	0.1560 0.1933	0.8369 0.8309		4.92 5.07	0.1050 0.1131	0.2617 0.2650
Į.	9.53	0.2255	0.8207		5.19	0.1131	0.2661
	10.51	0.2522	0.8099		5.32	0.1303	0.2674
	11.83	0.2972	0.7877		5.45	0.1402	0.2645
	13.17	0.3464	0.7565		5.51	0.1457	0.2611
1	14.61	0.4264	0.7088		5.61	0.1550	0.2579
105.0	14.93 1.21	0.4635 0.0121	0.6719 0.3010		5.74	0.1680	0.2530
103.0	1.51	0.0121	0.4056				
1	1.90	0.0291	0.4972				-
}							_

- 1. Hydrogen;  $H_2$ ; [1333-74-0]
- Nitrogen oxide, (Nitric oxide);
   NO; [10102-43-9]

#### ORIGINAL MEASUREMENTS:

Augood, D. R.

Trans. Instn. Chem. Engnrs.,

1957, 35, 394-408.

#### VARIABLES:

PREPARED BY:

Pressure

C. L. Young

# EXPERIMENTAL VALUES:

т/к	P/psig ⁺	P/MPa	Mole fraction of hydrogen in liquid, $x_{ m H_2}$ in gas, $y_{ m H_2}$
119.5	2540	17.61	0.017 0.991
	2240	15.55	0.009 0.992
	1620	11.27	0.005 ~

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The nitric oxide was condensed out and both components estimated volumetrically. Ratio of H /HD in liquid estimated by mass spectrometry.

# SOURCE AND PURITY OF MATERIALS:

- 1. Electrolytic sample containing 0.09 mole per cent HD.
- Prepared by the method of Johnstone and Giauque (1).

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/MPa = \pm 0.1$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 4$ % (estimated by compiler)

# REFERENCES:

Johnstone, H.L.; Giauque, W.F. J. Amer. Chem. Soc. 1929, 5, 3194.

⁺ psig - pounds per square inch gauge pressure

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon dioxide; CO₂; [124-38-9]

#### **EVALUATOR:**

Colin Young
Department of Chemistry
University of Melbourne
Parkville,
Victoria. 3052
AUSTRALIA

September, 1980

This system has been extensively investigated by Tsang and Streett (1) who measured vapor-liquid equilibrium isotherms at ten temperatures between 220K and 290K at pressures up to 172 MPa. Their measurements were carried out with high purity samples in an apparatus of proven reliability. The results of Kaminishi and Toriumi (2), who studied six isotherms between 233.15K and 298.15K at pressures up to 20 MPa, are in good agreement with the more extensive data of Tsang and Streett (1) although the mole fractions of hydrogen in the liquid phase from reference (2) are slightly smaller than those obtained by interpolation of the data of Tsang and Streett (1).

Spano et al (3) studied this system at six temperatures ranging from 219.9K to 289.9K at pressures up to 20 MPa. At the three lowest temperatures there is good agreement with the data of Kaminishi and Toriumi (2) and Tsang and Streett (1) but there are significant deviations at the higher temperatures. The hydrogen mole fractions in the liquid phase are smaller in the work of Spano et al (3) than in that of the two other groups (1) and (2).

The data of Yorizane et al (4), which are restricted to 273.15K and pressure up to 37 MPa give interpolated liquid phase hydrogen compositions which are slightly smaller than those of Tsang and Streett (1) and agree better with the slightly smaller values of Kaminishi and Toriumi (2).

Augood (5) reported data at the single temperature of 239.7K which are in fair agreement with interpolated values from the measurements of Spano  $et\ al$  (3) but his data are not considered further in view of their very limited nature.

The earliest reported measurements of vapor-liquid equilibrium for this system are those of Abdullayev (6) who studied the system at 298.2K and pressures between 8 and 20 MPa. The results, which were presented in graphical form, differ widely from any other data on this system and are rejected. Similarly the data of Mills and Miller (7), who reported two isotherms at 288.2K and 281.2K at pressures up to 11 MPa, are rejected. Their data were presented only in graphical form and deviate somewhat from the data given in reference (1), (2), (3) and (4). The results of Greco et al (8) were presented in graphical form and appear to agree with the data of Tsang and Streett (1) within a few percent. However in view of the uncertainty in the graphical presentation the data are not considered further here.

The data of Spano  $et\ al$  (3), Tsang and Streett (1) Kaminishi and Toriumi (2) and Yorizane  $et\ al$  (4) are all classified as tentative. The solubility of hydrogen in carbon dioxide at the highest temperatures varies by several per cent between these workers but there is insufficient evidence to make a definite choice between the four sets of data.

- 1. Tsang, C.Y.; Streett, W.B. in press
- Kaminishi, G.; Toriumi, T.; J. Chem. Soc. Japan. Ind. Chem. Sec. 1966, 69, 175.
- 3. Spano, J.O.; Heck, C.K.; Barrick, P.L. J. Chem. Engng. Data, 1968, 13, 168.

# References (continued).

- 4. Yorizane, M.; Yoshimura, S.; Masouku, H. Kagaku Kogaku, 1970, 34, 953.
- 5. Augood, D.R.; Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 6. Abdullayev, Y.A. Zh. Fiz. Khim. 1939, 13, 986.
- 7. Mills, J.R.; Miller, F.J.L. Can. Chem. Process. Ind. 1945, 29, 651.
- 8. Greco, G.; Casale, C.; Negri, G. Comp. rend. Congr. intern. chim. ind. 27 Congr. Brussels, 1954, 251.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon dioxide; CO,; [124-38-9]

#### ORIGINAL MEASUREMENTS:

Augood, D. R.

Trans. Instn. Chem. Engnrs.

1957, 35, 394-408.

VARIABLES:

PREPARED BY:

Pressure

C. L. Young

# EXPERIMENTAL VALUES:

T/K	P/psig ⁺	Р/мРа	Mole fraction in liquid, $x_{\rm H_2}$		
239.7	2780 2720 2680	19.27 18.86 18.58	0.064 0.071 0.062	0.910 0.871 0.873	

# AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrers. After equilibrium had been established samples of gas and liquid phases taken.

The carbon dioxide was condensed out and both components estimated volumetrically. Ratio of  $\rm H_2/HD$  in liquid estimated by mass spectrometry.

#### SOURCE AND PURITY OF MATERIALS:

- Electrolytic sample containing 0.09 mole per cent HD.
- 2. British Oxygen Company sample.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$   $\delta P/MPa = \pm 0.1;$   $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = 4%$  (estimated by compiler)

⁺ psig - pounds per square inch gauge pressure

#### COMPONENTS: ORIGINAL MEASUREMENTS: Hydrogen; H₂; [1333-74-0] Kaminishi, G.; Toriumi, T. 2. Carbon dioxide; CO₂; [124-38-9] Kogyo Kagaku Zasshi, 1966, 69, 175-172. VARIABLES: PREPARED BY: C.L. Young Temperature, pressure EXPERIMENTAL VALUES: Mole fraction of hydrogen P/MPa in liquid, T/K in vapor $x_{\rm H2}$ $y_{\rm H_2}$ 9.64 298.15 0.044 0.041. 12.41 0.099 0.191 293.15 9.64 0.044 0.213 14.57 0.109 0.321 19.50 0.179 0.260 283.15 7.45 0.246 9.64 0.044 0.086 0.439 14.57 0.134 19.51 0.469 0.011 273.15 5.08 0.212 9.64 0.043 0.478 10.18 0.045 0.483 14.53 0.081 0.568 19.51 0.118 0.606 19.99 0.603 0.016 253.15 5.27 0.522 10.18 0.038 0.696 15.09 0.061 0.753 0.084 20.00 0.775 233.15 5.27 0.014 0.746 10.18 0.029 0.835 15.09 0.046 0.864 20.00 0.061 0.875 AUXILIARY INFORMATION METHOD /APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Better than 99.5 mole per cent. Static equilibrium cell with agitator. Pressure measured with Bourdon gauge. After equilibrium established sample removed and analysed by volumetric and gravimetric techniques. Carbon dioxide absorbed in potassium hydroxide solution. ESTIMATED ERROR: $\delta T/K = \pm 0.05$ ; $\delta P/MPa = \pm 0.01$ ; $\delta x_{\rm H_2}$ , $\delta y_{\rm H_2} = \pm 0.003$ . (estimated by compiler). REFERENCES:

COMPONENTS:		ORIGINAL MEASUR	EMENTS:		
l. Hydrogen; $H_2$	; [1333-74-0]	Spano, J.O.;	Heck, C.K.; Barrick, P.L		
2. Carbon Dioxi	de; CO ₂ ; [124-38-9]	J. Chem. Engng. Data, <u>1968</u> , 13, 168-171			
VARIABLES:		PREPARED BY:			
	ture, pressure		L. Young		
EXPERIMENTAL VALUES	:		<del> </del>		
T/K p/10 5 Pa		Mole fraction in liquid, $x_{\rm H_2}$	of hydrogen in gas, ${}^x{ m H}_2$		
		H ₂	H ₂		
219.9	10.8 21.6 35.9 52.8 70.6 73.2 102.8 154.4 198.3  16.6 25.8 31.8 36.5 45.7 46.5 66.6 73.3 87.1 106.9 121.6 161.6 203.0	0.0013 0.0044 0.0081 0.0128 0.0175 - 0.0258 0.0385 0.0487 - 0.0056 0.0077 0.0092 0.0121 - 0.0216 - 0.0365 0.0477 0.0586	0.428 0.693 0.800 0.852 - 0.885 0.9090 0.9267 0.9335 0.420 0.6140 - - 0.765 0.822 0.832 0.850 0.864 0.878 0.896 0.9046		
	AUXILIARY	INFORMATION			
METHOD/APPARATUS/PF		<del></del>	ITY OF MATERIALS:		
ref. (1). Temp platinum resist pressure measur Details of appa ref. (1). Cel components. Va vapor and liqui	ibed in detail in erature measured with ance thermometer and ed with Bourdon gauge ratus in source and 1 charged with por recirculated and d samples withdrawn gas chromatography.	cent.	purity 99.999 mole per purity 99.99 mole per		

ESTIMATED ERROR:  $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$  (up to 10.0 MPa),  $\pm 0.3$  (up to 30.0 MPa);  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 1\%$  or 0.0002 whichever is greater.

# REFERENCES:

 Herring, R.N.; Barrick, P.L.
 Int. Adv. Cryogenic Engng. 1965, 10, 151.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon Dioxide; CO₂; [124-38-9]

# ORIGINAL MEASUREMENTS:

Spano, J.O.; Heck, C.K.; Barrick, P.L.

J. Chem. Engng. Data. <u>1968</u>, 13, 168-171.

XPERIMENTAL VALUES:		Mala function	of huduages	
m /12	p/10 ⁵ Pa	Mole fraction of hydrogen in liquid, in gas,		
T/K	p/10 Fa		- ·	
		$x_{ m H_{2}}$	${m y}_{{f H}_{f 2}}$	
244.9	20.8	0.0027	-	
	21.8	-	0.265	
	38.0	0.0100	0.523	
	52.6	0.0159	0.634	
	80.5	0.0276	0.733	
	113.0	0.0407	0.789	
	161.0	0.0589	0.826	
	165.2	0.0605	0.828	
	201.1	0.0727	0.839	
	203.2	0.0732	0.841	
259.9	31.0	-	0.174	
	32.7	0.0047	0.206	
	50.7	0.0146	0.420	
	73.9	0.0269	0.550	
	92.6	0.0363	0.618	
	123.2	-	0.675	
	135.0	0.0598	0.695	
	153.5	0.0688	0.711 .	
	156.7	0.0700	0.712	
	203.2	0.0927	0.745	
274.9	49.9	0.0097	0.180	
	66.1	0.0213	0.300	
	95.0	0.0405	0.442	
	123.1	0.0588	0.518	
	160.5	0.0860	-	
	166.0	-	0.588	
	177.3	0.1000		
	192.0	-	0.610	
	200.6	0.115	-	
289.9	65.8	0.0130	0.102	
	90.0	0.0258	0.176	
	102.3	0.0490	0.280	
	153.7	0.110	0.391	
	162.1	0.121	0.400	
	175.3	0.139	0.422	
	182.9	-	0.425	

#### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Yorizane, M.; Yoshimura, S.; Masuoka, H. 2. Carbon dioxide; CO₂; [124-38-9] Kagaku Kogaku 1970, 34, 953-7. VARIABLES: PREPARED BY: Pressure C.L. Young EXPERIMENTAL VALUES: Mole fraction of hydrogen P_{total}/MPa T/K in liquid, in vapor $x_{\rm H_2}$ y H 2 6.08 273.15 0.283 10.44 0.047 0.474 0.563 13.88 0.0789 18.34 0.104 0.596 23.30 0.156 0.625 27.76 0.180 0.649 30.30 0.214 0.651 31.31 0.223 33.94 0.286 0.604 35.46 0.317 0.580 36.27 0.321 0.534 37.49 0.472 0.478 AUXILIARY INFORMATION METHOD APPARATUS / PROCEDURE: SOURCE AND PURITY OF MATERIALS: Vapor recycle equilibrium cell with magnetic pump. Temperature measured with platinum resistance thermometer No details given. and pressure measured with Bourdon gauge. Vapor and liquid sampled simultaneously and expanded to 200 cm3 at room temperature, analysed using GC. Details in source. ESTIMATED ERROR: $\delta T/K = \pm 0.1; \ \delta P/MPa = \pm 0.03;$ $\delta x_{\rm H_2}, \ \delta y_{\rm H_2} = \pm 1-2\%.$ (estimated by compiler). REFERENCES:

1

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon dioxide; CO₂; [124-38-9]

#### ORIGINAL MEASUREMENTS:

Tsang, C. Y.; Streett, W. B.

in press

#### VARIABLES:

PREPARED BY:

Temperature, pressure

C. L. Young

EXPERIMENTAL	TEAT TIEC .
EXPERIMENTAL	VALUES:

EXPERIME	NTAL VALUE						
Mole fraction of hydrogen				m /**	D /un -	Mole fraction of hydrogen	
T/K	P/MPa	in liquid, ^x H ₂	in vapor,  y H2	т/к	P/MPa	in liquid, $^{x}_{ m H_{2}}$	in vapor
220.0	0.93 1.00	0.0015	0.2898 0.3445	225.0	1.47 2.16	0.0039 0.0068	0.4372 0.5997
	1.07	0.0028	0.3871		2.78	0.0089	0.6757
	1.18		0.4309		3.56	0.0117	0.7409
	1.27	0.0032	0.4642		4.85	0.0159	0.7965
	1.35	0.0035	0.5025		7.00	0.0218	0.8507
	2.23	0.0067	0.6755		10.65	0.0312	0.8890
	3.51	0.0112	0.7810		14.22	0.0393	0.9036
	5.13 7.13	0.0159 0.0218	0.8369 0.8737		21.15 27.88	0.0567 0.0740	0.9178 0.9225
	11.01	0.0218	0.9055		34.69	0.0740	0.9232
	14.00	0.0297	0.9162		41.44	0.1073	0.9240
	15.46	0.0394	0.9189		48.37	0.1235	0.9228
	16.93	0.0427	0.9213		55.35	0.1390	0.9209
	18.79	0.0463	0.9209		69.99	0.1690	0.9131
	20.99	0.0514	0.9260		79.48	0.1877	0.9070
	24.34	0.0593	0.9299		91.26	0.2112	0.9036
	26.44	0.0647	0.9307	235.0	1.49	0.0039	0.2127
	27.59	0.0663	0.9303		2.14	0.0069	0.4228
	31.50	0.0721	0.9307		3.38	0.0121	0.6088
	35.40	0.0838	0.9315		5.22	0.0185	0.7286
225.0	1.18	0.0023	0.3102			(00)	nt.)

# AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetically operated pump. Pressure measured with manganin pressure gauge. Temperature measured with platinum resistance thermometer. Samples of liquid gas analysed using a thermal conductivity gas analyser.

#### SOURCE AND PURITY OF MATERIALS:

- Matheson ultra high purity sample, purity 99.999 mole per cent or better.
- 2. Matheson sample, purity 99.99 mole per cent or better.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.02$ ;  $\delta P/MPa = \pm 0.5\%$ ;  $\delta x_{\rm H_2}$ ,  $\delta y_{\rm H_2} = \pm 0.005$  (but may be as large as  $\pm 0.02$  near critical).

# REFERENCES:

Streett, W. B.; Calado, J. C. G.
 J. Chem. Thermodyn. 1978, 10,
 1089.

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Carbon dioxide; CO₂; [124-38-9]

# ORIGINAL MEASUREMENTS:

Tsang, C. Y.; Streett, W. B.

in press

# EXPERIMENTAL VALUES:

т/к	P/MPa	Mole from of hydronic liquid $^x{ m H}_2$		T/K	P/MPa	Mole fra of hydr in liquid, $x_{ m H_2}$	
235.0	7.06 10.46 14.03 20.73	0.0243 0.0342 0.0450 0.0659	0.7806 0.8322 0.8562 0.8755	250.0	88.39 91.61 3.37 5.58	0.4317 0.4680 0.0081 0.0208	0.7030  0.2083 0.4511
	27.71 35.22 41.38 55.17	0.0881 0.1123 0.1307 0.1707	0.8828 0.8868 0.8864 0.8813		7.23 10.53 13.49 21.62	0.0208 0.0284 0.0450 0.0596 0.1044	0.5382 0.6348 0.6787 0.7342
	73.10 93.03 117.61 137.35 152.00	0.2184 0.2728 0.3371 0.3928 0.4365	0.8704 0.8562 0.8343 0.8102 0.7877		28.15 34.70 41.71 48.44 55.59	0.1414 0.1777 0.2197 0.2640 0.3199	0.7483 0.7483 0.7370 0.7217 0.6965
237.0	165.58 168.96 171.79 132.08	0.4884 0.5062 0.5264 0.4067	0.7556 0.7455 0.7328 0.7949	270.0	62.04 65.64 4.38 5.31	0.3908 0.4768 0.0118 0.0191	0.6471 0.5773 0.1768 0.2749
	138.00 144.90 148.35 150.28 152.07	0.4281 0.4530 0.4731 0.4789 0.4908	0.7837 0.7698 0.7524 0.7486 0.7390		7.08 10.62 13.86 17.44 21.93	0.0301 0.0564 0.0817 0.1095 0.1388	0.3971 0.5282 0.5852 0.6201 0.6440
245.0	154.90 156.97 158.83 160.41 83.68	0.5049 0.5238 0.5401 0.5566 0.3251	0.7300 0.7190 0.7046 0.6921 0.7918		25.26 27.97 34.76 39.99 44.14	0.1706 0.1956 0.2457 0.2950 0.3560	0.6496 0.6475 0.6399 0.6157 0.5751
243.0	89.58 96.65 101.54 105.06	0.3521 0.3521 0.3882 0.4155 0.4379	0.7776 0.7600 0.7441 0.7303	280.0	45.69 7.44 9.15 11.27	0.3967  	0.5332 0.2891 0.3612 0.4251
250.0	108.51 111.83 113.23 2.31 3.04	0.4657 0.5010 0.5262 0.0044 0.0086	0.7094 0.6789 0.6603 0.1589 0.3196		13.80 18.35 20.30 22.62 24.56	0.1100 0.1580 0.1791 0.2000 0.2195	0.4731 0.5166 0.5255 0.5264
	3.63 5.20 6.98 10.29	0.0124 0.0186 0.0262 0.0396	0.4090 0.5501 0.6371 0.7179		26.01 27.45 29.25 31.19	0.2358 0.2536 0.2745 0.3043	0.5194 0.5133 0.5039 0.4740
	13.85 17.28 25.44 31.54 35.34	0.0545 0.0695 0.1058 0.1332 0.1488	0.7585 0.7822 0.8044 0.8105 0.8116	290.0	31.96 8.53 9.49 11.29 11.72	0.3270 0.0405 0.0528 0.0804	0.4472 0.1988 0.2342 0.2867 0.2969
	49.66 62.81 75.88 83.22 86.54	0.2121 0.2724 0.3412 0.3887 0.4147	0.8060 0.7834 0.7541 0.7300 0.7126		13.88 15.65 17.27 18.95 19.71	0.1226 0.1449 0.1670 0.1920 0.2065	0.3296 0.3460 0.3525 0.3327 0.3241
			,		• •		

# COMPONENTS: 1. Hydrogen; H₂; [1333-74-0] 2. Hydrogen sulfide; H₂S; [7783-06-4] VARIABLES: Pressure Pressure C. L. Young EXPERIMENTAL VALUES:

T/K	P/psig ⁺	P/MPa	Mole fraction of hydrogen in liquid, $x_{\rm H_2}$ in gas, $y_{\rm H_2}$
213.6	1500	10.44	0.015 0.990
	1500	10.44	0.011 0.990

#### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The hydrogen sulfide was condensed out and both components estimated volumetrically. Ratio of  $\rm H_2/HD$  in liquid estimated by mass spectrometry.

# SOURCE AND PURITY OF MATERIALS:

- Electrolytic sample containing 0.09 mole per cent HD.
- Prepared in Kipp's apparatus liquefied in carbon dioxide/ acetone bath. Non-condensible impurities removed.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1; \ \delta P/MPa = \pm 0.1;$   $\delta x_{\rm H_2}, \ \delta y_{\rm H_2} = \pm 4 \ \mbox{(estimated by compiler)}$ 

⁺ psig - pounds per square inch gauge pressure.

COMPONENTS -		ODICINAL AGACUPPAGNES			
COMPONENTS:	en; H ₂ ; [1333-74-0]	ORIGINAL MEASUREMENTS:			
i, nyaroge	en; n ₂ ; [1333-74-0]	Yorizane, M.; Sadamoto, S.; Masuoka, H.; Eto, Y.			
2 Uridana	on gulfido. H.C.	Kogyo Kagaku Zasshi 1969, 72,			
	en sulfide; H ₂ S;	2174-7.			
[7783-0	16-4]	21/4-/.			
VARIABLES:		PREPARED BY:			
VIKTINDEED.					
	Temperature, pressure	C. L. Young			
EXPERIMENTAL	VALUES:	<u> </u>			
m /	T /ND-	Wala furnish of huduanan			
T/K	P/MPa	Mole fraction of hydrogen in liquid,			
		$x_{ m H_{2}}$			
		-			
273.15	3.04	0.012			
258.15	5.07 1.01	0.020 0.003			
~JU•#J	2.03	0.006			
	3.04 5.07	0.008 0.016			
243.15	1.01	0.002			
	2.03 3.04	0.003 0.005			
	4.05	0.008			
	5.07	0.010			
****	AUXILIARY	INFORMATION			
METHOD/APPAR	ATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
-	aid equilibrium cell.	1. Purity 99.9 mole per cent.			
	ven in source.				
(Original	in Japanese.)	2. Purity 99.0 mole per cent.			
		ESTIMATED ERROR:			
		1			
		$\delta T/K = \pm 0.1;  \delta x_{H_2} = \pm 0.001$ (estimated by compiler).			
		(eactmated by compitel).			
		REFERENCES:			
		I .			

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Sulfur dioxide; SO₂; [7446-09-5]

# ORIGINAL MEASUREMENTS:

Augood, D.R.

Trans. Instn. Chem. Engnrs.,

1957, 35, 394-408.

#### VARIABLES:

Temperature, pressure

PREPARED BY:

C. L. Young

#### EXPERIMENTAL VALUES:

т/к	P/psig ⁺	P/MPa	Mole fraction in liquid, $x_{ m H_2}$	of hydrogen in gas, $y_{\rm H_2}$
293.2	2775	19.24	0.028	0.985
	2760	19.13	0.030	0.988
	1500	10.44	0.017	0.982
263.2	2770	19.20	0.019	0.981
	1860	12.93	0.015	0.979
	1500	10.44	0.016	0.969

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The sulfur dioxide was condensed out and both components estimated volumetrically. Ratio of  $\rm H_2/HD$  in liquid estimated by mass spectrometry.

# SOURCE AND PURITY OF MATERIALS:

- 1. Electrolytic sample containing 0.09 mole per cent HD.
- 2. Brotherton sample.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.1;$   $\delta P/MPa = \pm 0.1;$   $\delta x_{H_2}$ ,  $\delta y_{H_2} = 4\%$  (estimated by compiler)

⁺ psig - pounds per square inch gauge pressure

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Ammonia; NH₃; [7664-41-7]

### **EVALUATOR:**

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

October 1980

# CRITICAL EVALUATION:

The most extensive data on this system are those of Wiebe and coworkers (1), (2) who studied the system over the temperature range 273 K to 373 K and at pressures up to 101 MPa. Their data are thought to be reliable and are classified as tentative. Ipat'ev and Theodorovich (3) studied this system at 298.15 K up to pressures of 25 MPa and from 258 K to 298 K at a pressure of 10.1 MPa. Their mole fraction data at 298 K are significantly lower than those of Wiebe and coworkers (1), (2) and are rejected from further consideration. The data of Zeininger (4) were presented in small graphical form and are rejected for the present purpose.

Reamer and Sage (5) studied the phase behaviour of this system but only made measurements on the composition of the gas phase. They presented a table of coexisting liquid and gas phase compositions but the liquid phase compositions were based on the data of Wiebe and Tremearne (1). Krichevskii and Khazanova (6) and Krichevskii and Efremova (7) also studied the gas phase compositions in this system. Their results are not considered further.

The limited data of Augood (8) at 293.2 K and 239.7 K are consistent with the data of Wiebe and coworkers (1), (2) but of lower precision. The data of Hiese (9) at 298.15 K at pressures up to 20.2 MPa are consistent with those of Wiebe and Tremearne (1).

Lawson and Black (10) have determined the solubility of a mixture of three volumes of hydrogen and one of nitrogen in liquid ammonia at pressures up to 15 MPa over the temperature range of 243 K to 295 K. Their results indicate that the two gases behave independently and that the mole fraction in the liquid phase of either gas is proportional to its partial pressure. Their results are consistent with those of Wiebe and coworkers (1) and (2). The low pressure measurements of Gelperin et al. (11) over the temperature range 203 K to 273 K, and of Moore and Otto (12), over the temperature range 203 K to 303 K are also consistent with the results of Wiebe and coworkers (1), (2) if it is assumed that the mole fraction of hydrogen in the liquid phase is a linear function of pressure.

#### References:

- 1. Wiebe, R.; Tremearne, T. H. J. Am. Chem. Soc. 1934, 56, 2357.
- 2. Wiebe, R.; Gaddy, V. L. J. Am. Chem. Soc. 1937, 59, 1984.
- 3. Ipat'ev, V. V.; Theodorovich, V. P. Zh. Obshch. Khim. 1932, 2, 305.
- 4. Zeininger, H. Chem.-Ing.-Tech. 1973, 45, 1067.
- 5. Reamer, H. H.; Sage, B. H. J. Chem. Engng. Data 1959, 4, 152.
- 6. Krichevskii, I. R.; Khazanova, N. E. Zh. Fiz. Khim. 1939, 13, 1690.
- 7. Krichevskii, I. R.; Efremova, G. D. Zh. Fiz. Khim. 1952, 26, 1117.
- 8. Augood, D. R. Trans. Instn. Chem. Engnrs. 1957, 35, 394.
- 9. Hiese, F. Ber. Bunsenges. Phys. Chem. 1972, 76, 938.
- Larson, A. T.; Black, C. A. J. Am. Chem. Soc. 1925, 47, 1015 and Ind. Eng. Chem. 1925, 17, 715.
- Gel'perin, I. I.; Trubitsyn, B. A.; Kalinina, S. Ye.; Bezyulev, V. V. Khim. Prom. 1974, 8, 619.
- 12. Moore, R. G.; Otto, F. D. Can. J. Chem. Engng. 1972, 50, 355.

#### COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen; H₂; [1333-74-0] Wiebe, R.; Tremearne, T. H. J. Am. Chem. Soc. 1934, 56, 2357-60. 2. Ammonia; NH₃; [7664-41-7] VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: 102 Mole fraction 102 Mole fraction of hydrogen of hydrogen in liquid, T/K P/bar P/bar in liquid, T/K 102xH2 10²x_{H₂} 348.15 101.3 298.15 50.7 0.338 1.227 202.7 3.050 101.3 0.745 202.7 1.503 405.3 6.290 608.0 405.3 2.816 9.052 608.0 3.921 810.6 11.391 1013.3 13.380 810.6 4.887 373.15 5.679 101.3 1.177 1013.3 202.7 323.15 50.7 0.386 4.158 101.3 1.015 405.3 9.652 182.4 1.963 608.0 14.544 202.7 2.184 810.6 18.824 405.3 4.244 1013.3 22.777 608.0 5.965 810.6 7.415 1013.3 8.667 AUXILIARY INFORMATION

# METHOD / APPARATUS / PROCEDURE:

Mixtures equilibrated in rocking autoclave. Pressures measured with piston gauges. Liquid phase analysed by condensing sample in liquid air and removing nitrogen by Toepler pump and then estimating amount volumetrically.

# SOURCE AND PURITY OF MATERIALS:

- Purity 99.9 mole per cent, major impurity nitrogen.
- Contained 0.02 mole per cent of water.

# ESTIMATED ERROR:

 $\delta T/K = \pm 0.1$ ;  $\delta P/bar = \pm 0.1$  or less;  $\delta x_{\rm H_2} = \pm 0.2 - 0.3$ %.

#### REFERENCES:

 Wiebe, R.; Tremearne, T. H.
 J. Am. Chem. Soc. 1933, 55, 975.

COMPONENTS:		ORIGINAL MEASUREMENTS:			
1. Hydrogen; H ₂ ; [133]	3-74-01	ORIGINAL MEASUREMENTS: Weibe, R.; Gaddy, V.L.			
2. Ammonia; NH ₃ ; [7664	±-41-/J	J. Am. Chem. Soc. <u>1937</u> ,59,1984-7			
VARIABLES:		PREPARED BY:			
Pressure		C.L. Young			
EXPERIMENTAL VALUES:					
T/K	P/bar	10 ² x mole fraction of			
		hydrogen in liquid, $10^2 x_{\rm H_2}$			
		н ₂			
273.15	101.32	0.506			
	202.65 405.30	0.986 1.815			
	607.95 810.60	2.518 3.116			
	1013.25	3.644			
	AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:		SOURCE AND PURITY OF MATERIALS:			
Rocking equilibrium cel measured with dead weig Liquid samples analysed out nitrogen at low pre temperatures. Details	ht tester. by stripping ssure and low	No details given but thought to be of high purity as in ref. 1.			
		ESTIMATED EDDOD.			
		ESTIMATED ERROR:			
		ESTIMATED ERROR: $\delta T/K = \pm 0.1;  \delta P/bar = \pm 0.1;  \delta x_{\rm H_2} = \pm 0.5\% \text{ (estimated by compiler)}.$			
		$\delta T/K = \pm 0.1;  \delta P/bar = \pm 0.1;  \delta x_{H_2} =$			
		$\delta$ T/K = ±0.1; $\delta$ P/bar = ±0.1; $\delta x_{\rm H_2}$ = ±0.5% (estimated by compiler).			
		$\delta$ T/K = ±0.1; $\delta$ P/bar = ±0.1; $\delta x_{\rm H_2}$ = ±0.5% (estimated by compiler).			

COMPONENTS:	ORIGINAL MEASUREMENTS:		
1. Hydrogen; H ₂ ; [1333-74-0]	Augood, D. R.		
2. Ammonia; NH ₃ ; [7664-41-7]	Trans. Instn. Chem. Engnrs.,		
	<u>1957</u> , <i>35</i> , 394-408.		
VARIABLES:	PREPARED BY:		
Temperature, pressure	C. L. Young		

T/K P/psig [†]		P/MPa	Mole fractic in liquid, $x_{ m H}$	on of hydrogen in gas, y _{H2}
293.2	2750	19.06	0.014	0.900
	2750	19.06	0.015	0.921
	2250	15.61	0.013	0.954
239.7	2760	19.13	0.005	0.973
	2250	15.61	0.004	0.987
	2090	14.51	0.003	0.972

# AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetically operated stirrer. After equilibrium had been established samples of gas and liquid phases taken. The ammonia was condensed out and both components estimated volumetrically. Ratio of H₂/HD in liquid estimated by mass spectrometry.

# SOURCE AND PURITY OF MATERIALS:

- 1. Electrolytic sample containing 0.09 mole per cent HD.
- 2. Imperial Chemical Industries sample.

# ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.1; \quad \delta P/\text{MPa} = \pm 0.1;$   $\delta x_{\text{H}_2}, \quad \delta y_{\text{H}_2} = \pm 4 \text{% (estimated by compiler)}$ 

⁺ psig - pounds per square inch gauge pressure

298.15

# COMPONENTS: ORIGINAL MEASUREMENTS: 1. Hydrogen, H₂; [1333-74-0] Heise, F., 2. Ammonia, NH₃; [7664-41-7] Ber. Bunsenges, Phys. Chem. 1972, 76, 938-943. VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: T/K P/bar Mole fraction of hydrogen in liquid, in vapor, $x_{\rm H_2}$ $y_{\rm H_2}$

0.00166

0.00370

0.00769

0.01555

# AUXILIARY INFORMATION

#### METHOD /APPARATUS/PROCEDURE:

Static rocking equilibrium cell. Liquid and gas samples removed after equilibrium established. Samples analysed by freezing out ammonia in liquid nitrogen trap. Details in source and ref. 1.

28.90

53.45

100.2

100.7 202.15

# SOURCE AND PURITY OF MATERIALS:

0.6145

0.8751

0.9304

- Messer-Griessheim sample, better than 99.95 mole per cent.
- Gerling and Holtz sample, purity better than 99.8 mole per cent as determined by gas chromatography and mass spectrometry.

### ESTIMATED ERROR:

 $\delta \text{T/K} = \pm 0.1; \quad \delta P/\text{bar} = \pm 0.3 \text{ below 100}$  bar;  $\pm 0.6 \text{ above 100 bar; } \delta x_{\text{H}_2}$ ,  $\delta y_{\text{H}_2} = \pm 2\%$  (estimated by compiler).

#### REFERENCES:

1. Heise, F. Dissertation, Gottengen, 1971.

Inorganic Compounds				
COMPONENTS:  1. Hydrogen; H ₂ ; [1333-74-0]	ORIGINAL MEASUREMENTS: Moore, R.G.; Otto, F.D.			
2. Ammonia; NH ₃ ; [7664-41-7]	Can. J. Chem. Engng. <u>1972</u> , 50, 355-60.			
VARIABLES:	PREPARED BY:			
Temperature	C.L. Young			
EXPERIMENTAL VALUES:	L			
T/K	10"x Mole fraction of hydrogen in liquid, $10^4x_{ m H_2}$			
203.2 213.2 223.2 233.2 243.2 253.2 263.2 273.2 283.2 293.2 303.2 *at a partial pressure	0.1185 0.1573 0.2018 0.2528 0.3119 0.3808 0.4616 0.5565 0.6685 0.8007 0.9567 of 101.3 kPa cont.			
AUXILIARY	INFORMATION			
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:			
Recirculating flow apparatus fitted with magnetic pump. Amine saturated with hydrogen for a minimum of 8 hr. Samples of liquid withdrawn and amine frozen out, hydrogen released collected in calibrated gas buret. Amount of amine determined gravimetrically.	<ol> <li>Matheson sample, purity 99.999     mole per cent. Dried.</li> <li>Matheson sample, purity 99.95     mole per cent. Dried.</li> </ol>			
	ESTIMATED ERROR:			

 $\delta T/K = \pm 0.1$ ;  $\delta x_{\rm H_2} = \pm 4$ %. (estimated by compiler).

- 1. Hydrogen;  $H_2$ ; [1333-74-0]
- 2. Ammonia; NH₃; [7664-41-7]

# ORIGINAL MEASUREMENTS:

Moore, R.G., Otto, F.D.

Can. J. Chem. Engng. <u>1972</u>, 50, 355-60.

# DATA taken from deposited document

		Total	Partial	pressure	Solubil-	Mole fract-
}		pressure	of hydro	ogen	ity +	ion of
T/°C	T/K	P/atm	P/atm	P /MPa		hydrogen [#] H2
-25.01	248.14	7.55	6.06	0.614	0.2837	0.002155
-24.50	248.65	7.54	6.01	0.609	0.2843	0.002159
-24.53	248.62	7.59	6.06	0.614	0.2756	0.002094
-24.31	248.84	16.36	14.81	1.501	0.6669	0.005064
-24.95	248.20	16.35	14.86	1.506	0.6935	0.005266
-24.67	248.48	14.42	12.90	1.307	0.5907	0.004486
-24.39	248.76	14.64	13.10	1.327	0.5996	0.004553
-24.11	249.04	14.57	13.01	1.318	0.5977	0.004539
-23.83	249.32	14.51	12.93	1.310	0.5857	0.004448
-24.39	248.76	16.60	15.06	1.526	0.7101	0.005393
-24.39	248.76	16.58	15.04	1.524	0.6885	0.005228
-35.61	237.54	13.99	13.10	1.327	0.4820	0.003660
-35.61	237.54	13.99	13.10	1.327	0.4777	0.003628
-38.07	235.08	18.07	17.29	1.752	0.5904	0.004484
-38.07	235.08	18.07	17.29	1.752	0.6053	0.004597
19.89	293.04	15.66	7.23	0.733	0.7634	0.005797
19.89	293.04	15.66	7.23	0.733	0.7621	0.005787
-59.83	213.32	17.02	16.80	1.702	0.3472	0.002637
-60.46	212.69	19.17	18.96	1.921	0.3828	0.002908
-62.16	210.99	17.19	17.01	1.724	0.3338	0.002535
-62.16	210.99	17.19	17.01	1.724	0.3303	0.002509
-62.29	210.86	17.37	17.18	1.741	0.3332	0.002531
-62.04	211.11	18.62	18.44	1.362	0.3696	0.002808
-61.09	212.06	15.70	15.50	1.571	0.3098	0.002353
0.19	273.34	15.76	11.50	1.165	0.8378	0.006361
0.19	273.34	21.52	17.25	1.748	1.2692	0.009634
0.19	273.34	21.52	17.25	1.748	1.2625	0.009583
0.13	273.28	18.93	14.67	1.486	1.0732	0.008147
0.11	273.26	18.93	14.68	1.487	1.0725	0.008142
21.96	295.11	17.74	8.74	0.886	0.9450	0.007175
21.96	295.11	17.74	8.74	0.886	0.9595	0.007285

⁺ Volume of hydrogen (cm³) reduced to 101.3 kPa and 273.15K dissolved by 1 gram of ammonia

		ORIGINAL MEASUREMENTS:			
en; H ₂ ;	[1333-74-0]	Gel'perin, I. I.; Trubitsyn, B. A.;			
a; NH ₃ ;	[7664-41-7]	Kalinina. S. Ye.; Bezyulev, V. V.			
		Khim. Prom. <u>1974</u> , 8, 619-20.			
		PREPARED BY:			
Tempe	rature	C. L. Young			
L VALUES:		*			
K³/atm	g cm ³ 10 ⁴ × M	ole fraction of hydrogen at 1 atmosphere partial pressure $10^{+x}{ m H_2}$			
14.	8	0.514			
		0.338			
25. 30.		0.295 0.246			
	3	0.179 0.112			
	Tempe.  L VALUES:  K ^{\$} /atm	K ^{\$} /atm g cm ⁻³ 10 ⁴ × M  14.8 22.5 25.8			

^{*} calculated by compiler assuming molar volume of hydrogen at 101.325 kPa and 273.15 K is 22.4 dm³.

$$p = K \times C$$

where p is the partial pressure of hydrogen and C is concentration in  $\mbox{cm}^{\,3}$  (reduced to NTP) per gram.

#### AUXILIARY INFORMATION

# METHOD/APPARATUS/PROCEDURE:

Measurements made in high pressure cell up to 17.0 MPa. Results only given in terms of K but it was stated Henry's law was obeyed up to a mole fraction of 0.005 of hydrogen. Samples analysed by freezing ammonia in liquid nitrogen and estimating hydrogen volumetrically. Hydrogen removed and ammonia estimated volumetrically. Details in source.

# SOURCE AND PURITY OF MATERIALS:

No details given.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.2; \quad \delta x_{H_2} = \pm 2\%.$ 

solubility coefficient in equation

#### ORIGINAL MEASUREMENTS: COMPONENTS: Hydrogen; $H_2$ ; [1333-74-0] Hu, J.-H.; MacWood, G. R. J. Phys. Chem. 1956, 60, 1483-6. 2. Diborane; $B_2H_6$ ; [19287-45-7] VARIABLES: PREPARED BY: Temperature, pressure C. L. Young EXPERIMENTAL VALUES: Mole fraction Mole fraction of hydrogen of hydrogen P/bar in liquid, in gas, in liquid, T/K T/K P/bar in gas, x_{H2} $x_{\rm H_2}$ $y_{\rm H_2}$ $y_{\rm H_2}$ 115.49 8.89 0.02590 0.9994 146.19 20.93 0.09307 0.9948 112.34 10.27 0.02969 0.9996 146.55 25.78 0.11338 0.9953 0.9998 0.9954 112.43 11.60 0.03365 146.75 0.14406 32.87 113.82 0.9998 0.9960 15.34 0.04435 146.01 42.47 0.18326 0.9998 114.51 21.28 0.06182 158.43 4.09 0.01954 0.9295 158.32 113.46 21.69 0.06285 0.9998 10.07 0.05106 0.9755 0.9998 26.96 0.07501 112.66 158.30 15.15 0.07634 0.9823 112.85 34.58 0.08694 0.9998 158.15 21.51 0.10854 0.9862 0.9999 112.08 42.54 0.09667 158.33 28.58 0.14541 0.9895 0.9986 0.17622 123.83 6.83 0.02330 158.35 34.58 0.9900 123.95 14.61 0.04842 0.9992 159.26 42.04 0.21377 0.9915 20.24 169.55 0.06841 0.9994 123.92 7.89 0.04337 0.9279 124.24 25.92 0.08469 0.9994 169.86 14.79 0.08427 0.9650 124.46 169.88 34.51 0.11180 0.9994 21.69 0.12433 0.9719 124.23 42.68 0.13554 0.9994 169.97 29.12 0.17083 0.9780 134.94 0.9976 169.69 7.12 0.02834 0.9805 36.29 0.21139 169.71 134.93 13.74 0.05381 0.9980 42.54 0.24527 0.9816 135.13 20.86 0.08230 181.56 0.9985 8.42 0.04900 0.8527 134.80 27.52 0.9984 0.10757 181.68 14.28 0.08921 0.9137 134.95 34.19 0.13073 0.9987 181.42 20.39 0.13143 0.9435 134.95 43.02 0.16129 0.9988 181.55 27.24 0.17661 0.9540 145.91 5.55 0.02458 0.9834 181.55 36.29 0.23562 0.9610 145.66 9.25 0.04152 0.9886 181.73 0.9630 42.24 0.27194 AUXILIARY INFORMATION METHOD /APPARATUS/PROCEDURE: SOURCE AND PURITY OF MATERIALS: High pressure cell connected to vapor 1. Electrolytic sample. recirculating pump. Pressure measured with Bourdon gauge calibrated 2. Purity 99.9 mole per cent. against dead weight balance. Temperature measured with thermocouple. Hydrogen analysed volumetrically by stripping the liquid phase mixture. Details in source. ESTIMATED ERROR: $\delta x_{\rm H_2}$ $\delta T/K = \pm 0.3$ ; $\delta P/\text{bar} = \pm 0.03;$ $\delta y_{\rm H_2} = \pm 0.0001$ $= \pm 0.0001;$ (estimated by compiler). REFERENCES:

- 1. Hydrogen; H₂; [1333-74-0]
- 2. Nitrogen; N₂; [7727-37-9]
- 3. Carbon monoxide; CO; [630-08-0]

#### ORIGINAL MEASUREMENTS:

Akers, W.W.; Eubanks, L.S. Adv. Cryogenic Engng. 1960, 3, 275-293.

#### VARIABLES:

PREPARED BY:

Temperature, pressure, composition

C.L. Young

EXPERIMENTAL	VALUES:		Mole fractions in liquid,		Mole fractions in vapor,			
T/K	P/psia	P/MPa	$x_{ m H_{2}}$	^x N ₂	^x co	$y_{\rm H_2}$	$y_{N_2}$	^y co
80.37	315	2.17	0.0398 0.0404 0.0447 0.0460 0.0469 0.0487	0 0.2186 0.7483 0.8270 0.8776 0.9513	0.9602 0.7410 0.2070 0.1270 0.0805	0.9084 0.8865 0.8671 0.8662 0.8658 8655	0 0.0416 0.0181 0.1169 0.1234 0.1345	0.0916 0.0719 0.0242 0.0169 0.0108
	500	3.45	0.0609 0.0658 0.0672 0.0694 0.0706 0.0726 0.0745 0.0755 0.0761	0 0.1165 0.2170 0.3120 0.4030 0.4784 0.6195 0.7185 0.8176 0.9237	0.0301 0.8177 0.7158 0.6186 0.5264 0.4490 0.3060 0.2060 0.1063	0.9320 0.9250 0.9198 0.9050 0.9020 0.9073 0.9018 0.8987 0.8964 0.8948	0 0.0158 0.0285 0.0401 0.0495 0.0583 0.0710 0.0819 0.0932 0.1052	0.0680 0.0592 0.0517 0.0449 0.0385 0.0344 0.0272 0.0194 0.0104
	1400	9.65	0.1745 0.1815 0.1828 0.1943 0.1950 0.2094 0.2190	0 0.0940 0.1122 0.2265 0.2860 0.4796 0.6212	0.8255 0.7245 0.7050 0.5292 0.5190 0.3110 0.1598	0.9143 0.9080 0.9067 0.8956 0.8950 0.8831 0.8765	0 0.0168 0.0201 0.0470 0.0483 0.0810 0.1049	0.0857 0.0752 0.0732 0.0574 0.0567 0.0359 0.0186

#### AUXILIARY INFORMATION

#### METHOD /APPARATUS / PROCEDURE:

Recirculating vapor flow apparatus fitted with magnetic pump at ambient temperature. Cell made of type 303 stainless steel. Pressure measured with Bourdon gauge and temperature measured with copper-constantan thermocouples. Samples of both phases analysed by gas chromatography using a thermal conductivity detector. Details in source.

# SOURCE AND PURITY OF MATERIALS:

- 1. and 2. Purity 99.7 mole per cent.
- Prepared from reaction of formic acid and sulfuric acid. Dried. Purity about 97 mole per cent.

#### ESTIMATED ERROR:

 $\delta T/K = \pm 0.06$ ;  $\delta P/MPa = \pm 0.02$ ;  $\delta x$ ,  $\delta y = \pm 2$ %.

# COMPONENTS:

- Hydrogen; H₂; [1333-74-0]
   Nitrogen; N₂; [7727-37-9]
   Carbon monoxide; CO; [630-08-0]

# ORIGINAL MEASUREMENTS:

Akers, W.W.; Eubanks, L.S.

Adv. Cryogenic Engng. 1960, 3, 275-293.

EXPERIMENTAL VALUES:			Mole fraction in liquid			Mole fractio in vapor,		ns
T/K	P/psia	P/MPa	ж _{Н 2}	x _{N₂}	^x co	^у н ₂	y _{N2}	^y co
80.37	1400	9.65	0.2231 0.2300	0.6864 0.7700	0.0905	0.8731 0.8700	0.1159 0.1300	0.0110
	2000	13.79	0.2490 0.2815 0.3000 0.3317 0.3446	0 0.2270 0.3500 0.5644 0.0654	0.7510 0.4915 0.3500 0.1039	0.8790 0.8508 0.8356 0.8090 0.7977	0 0.0440 0.0743 0.1550 0.2023	0.1210 0.1052 0.0901 0.0360 0
99.82	315	2.17	0.0389 0.0393 0.0398 0.0400 0.0397 0.0392 0.0385 0.0380	0 0.0811 0.1970 0.2980 0.5493 0.7102 0.8651 0.9413	0.9611 0.8796 0.7632 0.6620 0.4110 0.2506 0.0964 0.0207	0.6803 0.6682 0.6504 0.6357 0.5919 0.5680 0.5563 0.5519	0 0.0392 0.0958 0.1390 0.2563 0.3315 0.4037 0.4393 0.4491	0.3197 0.2925 0.2538 0.2253 0.1518 0.1005 0.0400 0.0088 0
	500	3.45	0.0674 0.0689 0.0707 0.0720 0.0739 0.0744 0.0745 0.0744 0.0744	0 0.0766 0.1908 0.2968 0.5201 0.6576 0.6761 0.8342 0.8455 0.9259	0.9326 0.8545 0.7385 0.6312 0.4050 0.2680 0.2494 0.0914 0.0801	0.7619 0.7483 0.7318 0.7190 0.6974 0.6868 0.6851 0.6740 0.6732 0.6686	0 0.0335 0.0797 0.1133 0.1886 0.2352 0.2422 0.2985 0.3023 0.3314	0.2381 0.2182 0.1885 0.1677 0.1140 0.0780 0.0727 0.0275 0.0245
99.82	800	5.52	0.1163 0.1281 0.1342 0.1366 0.1378 0.1381 0.1383 0.1384	0 0.1342 0.3074 0.4826 0.6556 0.7230 0.8313 0.8616	0.8837 0.7377 0.5584 0.3808 0.2066 0.1389 0.0304	0.7844 0.7708 0.7539 0.7398 0.7290 0.7256 0.7213 0.72795	0 0.0492 0.1099 0.1627 0.2120 0.2340 0.2693 0.2721	0.2156 0.1800 0.1362 0.0975 0.0590 0.0404 0.0094
	1100	7.58	0.1727 0.1860 0.2030 0.2074 0.2102 0.2114 0.2116	0 0.0717 0.3452 0.4995 0.6817 0.7611	0.8273 0.7423 0.4518 0.2931 0.1081 0.0275 0	0.7848 0.7760 0.7448 0.7317 0.7208 0.7181 0.7175	0 0.0257 0.1237 0.1790 0.2443 0.2727 0.2825	0.2152 0.1983 0.1315 0.0893 0.0349 0.0092
	1400	9.65	0.2399 0.2527 0.2662 0.2792 0.3001 0.3030	0 0.0663 0.1634 0.2965 0.6522 0.6970	0.7601 0.6810 0.5704 0.4243 0.0477	0.7739 0.7578 0.7357 0.7090 0.6565 0.6530	0 0.0330 0.0813 0.1476 0.3247 0.3470	0.2261 0.2092 0.1830 0.1434 0.0188
122.04	500	3.45	0.0449 0.0426 0.0395 0.0356 0.0332 0.0288 0.0261	0 0.1486 0.3279 0.5083 0.6088 0.8242 0.9739	0.9551 0.8094 0.6326 0.4561 0.3580 0.1470	0.2260 0.1974 0.1660 0.1357 0.1204 0.0945 0.0821	0 0.1395 0.3090 0.4791 0.5738 0.7768	0.7740 0.6631 0.5250 0.3852 0.3058 0.1287

# COMPONENTS:

- Hydrogen; H₂; [1333-74-0]
   Nitrogen; N₂; [7727-37-9]
   Carbon monoxide; CO; [630-08-0]

### ORIGINAL MEASUREMENTS:

Akers, W.W.; Eubanks, L.S. Adv. Cryogenic Engng. 1960, 3, 275-293.

EXPERIMENTAL VALUES:			Mole fractions in liquid			Mole fractions in vapor		
T/K	P/psia	P/MPa	ж _{Н 2}	x _{N₂}	^x co	у _{Н 2}	y _{N2}	y _{CO}
122.05	500	5.52	0.1382 0.1387 0.2256	0 0.1330 0.3550	0.8618 0.7283 0.4214**	0.3349 0.3095	0 0.1120	0.6651 0.5785

** Critical point.

# COMPONENTS: 1. Hydrogen; .H₂; [1333-74-0] Larson, A. T.; Black, C. A. 2. Nitrogen; N₂; [7727-37-9] Ind. Eng. Chem. 1925, 17, 715-6. VARIABLES: PREPARED BY: Temperature, pressure, composition C. L. Young

T/K $P_{\text{total}}$ /MPa $P_{\text{H}_2}$ /P $_{\text{N}_2}$ $P_{\text{H}_2}$ H ₂ 248.0 5.07 3.0 1.62	Ficients $^{\sharp}$ Mole f $^{\mathrm{N}_{2}}$ $^{x_{\mathrm{H}_{2}}}$ 0.73 0.00123	ractions*
total H ₂ H ₂ H ₂	N ₂	
248 0 5 07 3 0 1 62 0	0.00123	
254.7       1.90       0         263.2       2.07       0         270.2       2.35       1         273.2       2.61       1         275.7       2.70       1         292.2       3.19       1         248.2       10.13       3.30       1         253.2       3.66       1         258.7       3.85       1         263.2       4.43       1         268.0       4.84       2         273.2       5.28       2         295.2       7.54       3         251.2       15.20       4.70       1	0.84	0.00055 0.00064 0.00071 0.00082 0.00087 0.00090 0.00111 0.00102 0.00111 0.00124 0.00139 0.00153 0.00173 0.00243 0.00143
263.7     6.20     2       266.0     6.30     2       278.2     8.22     3	2.44 0.00469 2.58 0.00476 3.33 0.00621 3.61 0.00711	0.00185 0.00196 0.00252 0.00274

 $^{^{\}sharp}$  cm  3  of gas (measured at 101.325 kPa and 273.15 K) dissolved per gram of ammonia.  * 

# AUXILIARY INFORMATION

### METHOD /APPARATUS / PROCEDURE:

Static equilibrium cell. Pressure measured with Bourdon gauge.
Liquid samples taken and added to excess acid. Hydrogen and nitrogen estimated by volumetric method and combustion of hydrogen.

### SOURCE AND PURITY OF MATERIALS:

No details given except that nitrogen contained a trace of argon.

### ESTIMATED ERROR:

 $\begin{array}{lll} \delta \text{T/K} &=& \pm 0.2; & \delta^P_{\text{total}} / \text{MPa} &=& \pm 0.05; \\ \delta x_{\text{H}_2} &=& \delta y_{\text{N}_2} &=& \pm 1 \text{\% (estimated by compiler).} \end{array}$ 

REFERENCES.

calculated by compiler.

### SYSTEM INDEX

Underlined page numbers refer to evaluation text and those not underlined to compiled tables. All compounds are listed as in Chemical Abstracts. For example, toluene is listed as benzene, methyl— and dimethylsulfoxide is listed as methane, sulfinylbis—. Since hydrogen is usually one of the components it is omitted in the listing.

```
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Benzene, methyl-
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Benzene, 1,1-methylene bis- (ternary)
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Benzene, (1-methylethenyl) - (ternary)
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