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Volume 57

ETHENE

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SOLUBILITY DATA SERIES

Volume 57

ETHENE

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INTRODUCTION TO THE SOLUBILITY DATA SERIES

SOLUBILITY OF GASES IN LIQUIDS

NATURE OF THE PROJECT

The Solubility Data project (SDP) has as its aim a comprehensive review of published data for solubilities of gases, liquids and solids in liquids or solids. Data of suitable precision are compiled for each publication on data sheets in a uniform format. The data for each system are evaluated and, where data from independent sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

COMPILATIONS AND EVALUATIONS

The formats for the compilations and critical evaluations have been standardized for all volumes. A description of these formats follows.

Compilations

The format used for the compilations is, for the most part, self-explanatory. Normally, a compilation sheet is divided into boxes, with detailed contents described below.

Components: Each component is listed according to IUPAC name, formula, and Chemical Abstracts (CA) Registry Number. The Chemical Abstracts name is also included if this differs from the IUPAC name, as are trivial names if appropriate. IUPAC and common names are cross-referenced to Chemical Abstracts names in the System Index.

The formula is given either in terms of the IUPAC or Hill (1) system and the choice of formula is governed by what is usual for most current users: i.e., IUPAC for inorganic compounds, and Hill system for organic compounds. Components are ordered on a given compilation sheet according to:

(a) saturating components;
(b) non-saturating components according to chemical families; within carbon compounds, according to increasing carbon number;
(c) solvents according to chemical families; within carbon compounds, according to increasing carbon number.

In each class, ordering follows the 18-column IUPAC periodic table. The same order is followed in arranging the compilation sheets within a given volume.

Original Measurements: References are abbreviated in the forms given by Chemical Abstracts Service Source Index (CASSI). Names originally in other than Roman alphabets are given as transliterated by Chemical Abstracts. In the case of multiple entries (for example, translations) an asterisk indicates the publication used for compilation of the data.

Variables: Ranges of temperature, pressure, etc. are indicated here.

Prepared by: The names of all compilers are given here.

Experimental Values: Components are described as (1), (2), etc., as defined in the "Components" box. Data are reported in the units used in the original publication, with the exception that modern names for units and quantities are used; e.g., mass per cent for weight per cent; mol dm^{-3} for molar; etc. Usually, only one type of value (e.g., mass per cent) is found in the original paper, and the compiler has added the mole fractions from calculations based on 1989 atomic weights (2) and referenced sources of densities, where necessary. Temperatures are expressed as $t/°C$, $t/°F$ or T/K as in the original; if necessary, conversions to T/K are made, sometimes in the compilations, and always in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations (3) as far as possible.

Errors in calculations, fitting equations, etc. are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler" or by the compiler's name in parentheses or in a footnote. Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure and if the compiler finds that the equations are consistent with the data.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases, compilers note that numerical data have been obtained from published graphs using digitizing techniques. In these cases, the precision of the data can be determined by the quality of the original graph and the limitations of the digitizing technique.

Method: The apparatus and procedure are mentioned briefly. Abbreviations used in Chemical Abstracts are often used here to save space, reference being made to sources of further detail if these are cited in the original paper. Several reviews on experimental methods of determining gas solubilities are given in (4-10).

Source and Purity of Materials: For each component, referred to as (1), (2), etc., the following information (in this order and in abbreviated form) is provided if available in the original paper: source and specified method of preparation; properties; degree of purity. The solubility is usually more sensitive to impurities in the gaseous component than in the liquid component. However, the most important source of impurities is traces of unwanted gas dissolved in the liquid. Inadequate preliminary degassing of the absorbing liquid is probably the most often overlooked serious source of error in gas solubility measurements.

Estimated Error: If estimated errors were omitted by the original authors, and if relevant information is available, the compilers have attempted to estimate errors (identified by "compiler" or the compiler's name in parentheses or in a footnote) from the internal consistency of data and type of apparatus used. Methods used by the compilers for estimating and reporting errors are based on Ku and Eisenhart (11).

Comments and/or Additional Data: Compilations may include this section, in which short comments relevant to the general nature of the work or additional experimental and thermodynamic data are included which are judged by the compiler to be of value to the reader.

References: The format for these follows the format for the Original Measurements box, except that final page numbers are omitted. References (usually cited in the original paper) are given where relevant to interpretation of the compiled data, or where cross-reference can be made to other compilations.

Evaluations

The evaluator's task is to assess the reliability and quality of the data, to estimate errors where necessary, and to recommend "best" values. The evaluation takes the form of a summary in which all the data supplied by the compiler have been critically reviewed. There are only three boxes on a typical evaluation sheet, and these are described below.

Components: The format is the same as on the Compilation sheets.

Evaluator: Name and affiliation of the evaluator(s); date up to which the literature was checked.

Critical Evaluation:

(a) Critical text. The evaluator checks that the compiled data are correct, assesses their reliability and quality, estimates errors where necessary, and recommends numerical values based on all the published data (including theses, reports and patents) for each given system. Thus, the evaluator reviews the merits or shortcomings of the various data. Only published data are considered. Documented rejection of some published data may occur at this stage, and the corresponding compilations may be removed.

The solubilities in comparatively few systems are known with sufficient accuracy to enable a set of recommended values to be presented, either for measurements near atmospheric pressure or at high pressures. Although many systems have been studied by at least two independent groups of workers, the range of pressures or temperatures is often sufficiently different to make meaningful comparison impossible.

Occasionally, it is not clear why two groups of workers obtained very different but internally consistent sets of results at the same temperature and pressure, although both sets were obtained by reliable methods. In such cases, a decisive assessment may not be possible. In some cases, two or more sets of data have been classified as tentative even though 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 be regarded only as an "informed guess".

As well, many 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). As an example, it is difficult to determine coexisting liquid and vapor compositions near the critical point of a mixture using some common experimental techniques which yield accurate high pressure solubility data. As another example, conventional methods of analysis may give results with an expected error which would be regarded as sufficiently small for vapor-liquid equilibrium data but an order of magnitude too large for acceptable high pressure gas-liquid solubility.

Sometimes it is possible to judge the reliability of data for a particular gas-liquid system by testing whether the data are consistent with the behavior of homologous gases or liquids.

(b) Fitting equations. If the use of a smoothing equation is justifiable the evaluator may provide an equation representing the solubility as a function of the variables reported on all the compilation sheets, stating the limits within which it should be used.

(c) Graphical summary. In addition to (b) above, graphical summaries are often given.

(d) Recommended values. Data are recommended if the results of at least two independent groups are available and they are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the applied experimental and computational procedures. Data are reported as tentative if only one set of measurements is available, or if the evaluator considers some aspect of the computational or experimental method as mildly undesirable but estimates that it should cause only minor errors. Data are considered as doubtful if the evaluator considers some aspect of the computational or experimental method as undesirable but still considers the data to have some value where the order of magnitude of the solubility is needed. Data determined by an inadequate method or under ill-defined conditions are rejected. However, references to these data are included in the evaluation together with a comment by the evaluator as to the reason for their rejection.

(e) References. All pertinent references are given here, including all those publications appearing in the accompanying compilation sheets and those which, by virtue of their poor precision, have been rejected and not compiled.

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units (3) when the data can be accurately converted.

QUANTITIES AND UNITS USED IN COMPILATION AND EVALUATION OF SOLUBILITY DATA

Mixtures, Solutions and Solubilities

A *mixture* (12) describes a gaseous, liquid or solid phase containing more than one substance, where the substances are all treated in the same way.

A *solution* (12) describes a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the *solvent*, and may itself be a mixture, is treated differently than the other substances, which are called *solutes*. If the sum of the mole fractions of the solutes is small compared to unity, the solution is called a *dilute solution*.

The *solubility* of a solute 1 (solid, liquid or gas) is the analytical composition of a saturated solution, expressed in terms of the proportion of the designated solute in a designated solvent (13).

"Saturated" implies equilibrium with respect to the processes of dissolution and vaporization; the equilibrium may be stable or metastable. The solubility of a substance in metastable equilibrium is usually greater than that of the same substance in stable equilibrium. (Strictly speaking, it is the activity of the substance in metastable equilibrium that is greater.)

Either point of view, mixture or solution, may be taken in describing solubility. The two points of view find their expression in the reference states used for definition of activities, activity coefficients and osmotic coefficients. Note that the composition of a saturated mixture (or solution) can be described in terms of any suitable set of thermodynamic components.

For gases, the solubility is quoted, where possible, as mole fraction of the saturating gaseous component in the liquid phase at 1 bar partial pressure of gas. The distinction between vapor-liquid equilibria and the solubility of gases in liquids is arbitrary. It is generally accepted that the equilibrium at 300 K between a typical gas such as argon and a liquid such as water is gas liquid solubility whereas the equilibrium between hexane and cyclohexane at 350 K is an example of vapor-liquid equilibrium.

Physicochemical Quantities and Units

Solubilities of gases have been the subject of research for a long time, and have been expressed in a great many ways, as described below. In each case, specification of the temperature and either partial or total pressure of the saturating gaseous component is necessary. The nomenclature and units follow, where possible, ref. (3)

A note on nomenclature. In the IUPAC Green Book (3), the solute is component B and the solvent is component A. In compilations and evaluations, the first-named component (component 1) is the solute, and the second (component 2 for a two-component system) is the solvent. The reader should bear these distinctions in nomenclature in mind when comparing equations given here with those in the Green Book.

1. *Mole fraction* of substance 1, x_1 or $x(1)$:

$$x_1 = n_1 / \sum_{s=1}^{c} n_s \qquad [1]$$

where n_s is the amount of substance of s, and c is the number of distinct substances present (often the number of thermodynamic components in the system). *Mole per cent* of substance 1 is $100\,x_1$.

2. *Ionic mole fractions* of salt i, x_{i+}, x_{i-}:
For a mixture of s binary salts i, each of which ionizes completely into ν_{s+} cations and ν_{s-} anions, with $\nu_s = \nu_{s+} + \nu_{s-}$, and a mixture of p non-electrolytes j, of which some may be solvent components, a generalization of the definition in (14) gives:

$$x_{i+} = \frac{\nu_{i+} x_i}{1 + \sum_{i=1}^{s} (\nu_i - 1) x_s}, \qquad x_{i-} = \frac{\nu_{i-} x_{i+}}{\nu_{i+}}, \qquad i = 1 \ldots s \qquad [2]$$

$$x_j' = \frac{x_j}{1 + \sum_{i=1}^{s} (\nu_i - 1) x_i}, \qquad j = (s+1) \ldots p \qquad [3]$$

The sum of these mole fractions is unity, so that, with $c = s + p$,

$$\sum_{i=1}^{s} (x_{i+} + x_{i-}) + \sum_{i=s+1}^{c} x_i' = 1 \qquad [4]$$

General conversions to other units in multicomponent systems are complicated. For a three-component system containing non-electrolyte 1, electrolyte 2 and solvent 3,

$$x_1 = \frac{\nu_{2+} x_1'}{\nu_{2+} - (\nu_2 - 1) x_{2+}} \qquad x_2 = \frac{x_{2+}}{\nu_{2+} - (\nu_2 - 1) x_{2+}} \qquad [5]$$

These relations are used in solubility equations for salts, and for tabulation of salt effects on solubilities of gases (see below).

3. *Mass fraction* of substance 1, w_1 or $w(1)$:

$$w_1 = g_1 / \sum_{s=1}^{c} g_s \qquad [6]$$

where g_s is the mass of substance s. *Mass per cent* of substance 1 is $100\,w_1$. The equivalent terms *weight fraction*, *weight per cent* and *g (1)/100 g solution* are no longer used.

4. *Molality* of solute 1 in a solvent 2, m_1:

$$m_1 = n_1/n_2\ M_2 \qquad [7]$$

SI base units: mol kg^{-1}. Here, M_2 is the molar mass of the solvent. The equivalent term *weight solubility*, C_w, is no longer used.

5. *Amount concentration* of solute 1 in a solution of volume V, c_1:

$$c_1 = [\text{formula of solute}] = n_1/V \qquad [8]$$

SI base units: mol m^{-3}. The symbol c_1 is preferred to [formula of solute], but both are used. The old terms *molarity, molar* and *moles per unit volume* are no longer used.

6. *Mass concentration* of solute 1 in a solution of volume V, ρ_1 or γ_1:

$$\rho_1 = g_1/V \qquad [9]$$

SI base units: kg m^{-3}.

7. *Mole ratio*, $r_{n,12}$ (dimensionless)

$$r_{n,12} = n_1/n_2 \qquad [10]$$

Mass ratio, symbol $r_{g,12}$, may be defined analogously.

8. *Ionic strength*, I_m (molality basis), or I_c (concentration basis):

$$I_m = \frac{1}{2}\sum_i m_i z_i^2 \qquad I_c = \frac{1}{2}\sum_i c_i z_i^2 \qquad [11]$$

13

where z_i is the charge number of ion i. While these quantities are not used generally to express solubilities, they are used to express the compositions of non-saturating components. For a single salt i with ions of charges z_+, z_-,

$$I_m = |z_+z_-|\nu m_i, \quad I_c = |z_+z_-|\nu c_i \qquad [12]$$

14

Mole and mass fractions are appropriate to either the mixture or the solution point of view. The other quantities are appropriate to the solution point of view only. Conversions between some pairs of these quantities can be carried out using the equations given in Table 1 at the end of this Introduction. Other useful quantities will be defined in the prefaces to individual volumes or on specific data sheets.

In addition to these well-defined SI-based units, other units have been used to express the solubilities of gases. Units and nomenclature follow (4, 5, 7, 16), as modified by IUPAC recommendations (3). The equations describing Bunsen, Kuenen, Ostwald and absorption coefficients, as well as Henry's law constants, hold for ideal gases and perfect solutions only. Corrections for non-ideality should be made where possible. The corrections are less than 1 % for most gases near atmospheric pressure (5).

In much published data, the reference pressure is 1 atm = 0.101325 MPa rather than 1 bar = 0.1 MPa.

9. *Bunsen coefficient*, α (dimensionless):

The volume of saturating gas, V_1, reduced to $T^\circ = 273.15$ K, $p^\circ = 1$ bar, which is absorbed by unit volume V_2^* of pure solvent at the temperature of measurement and partial pressure $p^\circ = 1$ bar. If the gas is ideal, Henry's law (see below) holds, and the liquid is incompressible, then

$$\alpha = \frac{V_1^o}{V_2^*} = \left(\frac{V_1}{V_2^*}\right)\left(\frac{T^o}{T}\right) \qquad [13]$$

15

10. *Kuenen coefficient, S*:

The volume of saturating gas, V(g), reduced to T° = 273.15 K, p° = 1 bar, which is dissolved by unit mass of pure solvent at the temperature of measurement and partial pressure 1 bar. Thus,

$$S = \frac{V_1 T^o}{g_2 T} = \frac{\alpha V_{m,2}}{M_2} \qquad [14]$$

16

SI base units: $m^3\ kg^{-1}$. Here, M_2 is the molar mass of the solvent. The Kuenen coefficient is proportional to the molality of the dissolved gas.

11. *Ostwald coefficient, L* (dimensionless) (16):

The volume of saturating gas, V_1, absorbed by a volume V_2^* of pure solvent at the temperature and pressure of the measurement. Thus,

$$L = \frac{V_1}{V_2^*} = \left(\frac{\alpha T}{T^o}\right)\left(\frac{p^o}{p}\right) \qquad [15]$$

17

The Ostwald coefficient is equal to the ratio of the amount concentrations in the gas and in the liquid.

12. *Absorption coefficient, β* (dimensionless):

The most common of several definitions of absorption coefficient is the volume of gas, reduced to T° = 273.15 K, p° = 1 bar absorbed per unit volume of pure solvent at a total pressure of 1 bar. The absorption and Bunsen coefficients are therefore very similar, and are connected by

$$\beta = \alpha(1 - p_2/p^o) \qquad [16]$$

18

where p_2 is the partial pressure of the vapor of the solvent.

13. *Henry's Law constant, K_H*:

$$K_H = \lim_{x_1 \to 0}\left(\frac{p_1}{x_1}\right) \qquad [17]$$

19

SI base units: Pa. Unfortunately, the definition is used often at finite mole fractions, even though this is a limiting law. The following have also been defined as Henry's Law constants:

$$\begin{aligned} K_2 &= p_1/c_1 \\ K_c &= c_1^g/c_1 \end{aligned} \qquad [18]$$

20

where superscript g refers to the gas phase. K_2 has SI base units Pa $m^3\ mol^{-1}$, and K_c is dimensionless. The Henry's law constant has also been called the Henry coefficient and the Henry coefficient. Henry's law can be used, with great caution, to convert data from the experimental pressure to 1 bar if the mole fraction of the gas in the liquid is small, and the difference in pressures is small.

The relations between the mole fraction solubility and the various quantities given above are as follows. Note again that these relations hold for ideal gaseous and perfect solution phases only.

$$x_1 = \frac{1}{1+\dfrac{RT^o}{p_1^o V_{m,2}^* \alpha}} = \frac{1}{1+\dfrac{RT^o}{p_1^o M_2 S}} = \frac{1}{1+\dfrac{RT}{p_1 V_{m,2}^* L}} = \frac{1}{1+\dfrac{RT^o}{p^o V_{m,2}^* \beta}} \qquad [19]$$ 21

14. *Salt Effects on the Solubility of Gases* (17)

These are often reported as Sechenov (Setchenow, Setschenow) salt effect parameters k_{syz}, which are defined in various ways. The general semi-empirical Sechenov equation is

$$\log(z_1^o/z_1) = k_{syz}\, y \qquad [20]$$ 22

where solubility is expressed in quantities z, with superscript o designating pure solvent, and salt composition is expressed in quantities y. The quantities c_2, m_2, x_2', I_m and I_c are used for y, and the quantities c_1, m_1, x_{1+}, α, S and L for z, giving 30 definitions of k_{syz}. Here, components 1 and 2 are the gaseous solute and electrolyte, respectively. The ratios of z-values are the same for $z = c_1$, α and L and for m_1 and S, respectively, leaving 15 distinct definitions. If z is the same, the definitions of k_{syz} are related simply through 10 equations between pairs of c_2, m_2, x_2', I_m and I_c. Some relations among the definitions, in terms of k_{scc}, k_{smm} and k_{sxx}, are:

$$\begin{aligned}
k_{scc} &= k_{sc\alpha} = k_{scL} = \frac{m_2}{c_2}k_{smc} = \frac{x_2'}{c_2}k_{sxc} = \frac{I_c}{c_2}k_{sI_c c} \\
k_{smm} &= \frac{x_2'}{m_2}k_{sxm} = k_{smS} = \frac{c_2}{m_2}k_{scm} = \frac{I_m}{m_2}k_{sI_m m} \\
k_{sxx} &= \frac{c_2}{x_2'}k_{scx} = \frac{m_2}{x_2'}k_{smx} = \frac{I_m}{x_2'}k_{sI_m x} = \frac{I_c}{x_2'}k_{sI_c x}
\end{aligned} \qquad [21]$$ 23

These relations hold when a single salt is present; note that the relations between ionic strength and either molality or concentration are simple. If more than one salt is present, the ionic strength is the only practical quantity to be used for y.

Conversions between pairs of k_{scc}, k_{smm} and k_{sxx} are more complicated, and can be found using eqn [5] and Table 1 at the end of this Introduction. For example,

$$k_{sxx} = f(m)\left(\frac{k_{smm}}{\nu_{2+}} + \frac{1}{m_2}\log\frac{f(m)}{f(m^o)}\right) \qquad [22]$$ 24

where

$$f(m) = 1+(m_1+\nu_2 m_2)M_3 \qquad f(m^o) = 1+m_1^o M_3 \qquad [23]$$ 25

Errors in the salt effect parameters, as defined above, can be large. If the relative standard deviation in measurement of solubility is $s(c_1)/c_1$, then the relative standard deviation in k_{scc} is

$$\frac{s(k_{scc})}{k_{scc}} = \frac{\sqrt{2}}{c_2 k_{scc}\ln 10}\,\frac{s(c_1)}{c_1} \qquad [24]$$ [illegible]

For example, for $k_{scc} = 0.1$ and $c_2 = 0.01$ mol dm^{-3}, $s(k_{scc})/k_{scc}$ is 30 % when $s(c_1)/c_1 = 0.05$ % and 1200 % when $s(c_1)/c_1 = 2$ %. At $c_2 = 1$ mol dm^{-3}, the corresponding errors are 0.3 and 12 %, respectively.

If the solubility of a gas is greater than about $x = 0.01$ at partial pressure 1 bar, then several other factors must be taken into account, such as the density of the solution or the partial molar volume of the dissolved gas. In addition, corrections should be made for non-ideality of the gas. See (18) for details.

In addition, the following definitions concerning density are useful in conversions between concentrations and other quantities.

15. *Density*, ρ or γ:

$$\rho = g/V \qquad [25]$$ 27

SI base units: kg m^{-3}. Here g is the total mass of the system.

16. *Relative density*, $d = \rho/\rho^{\circ}$: the ratio of the density of a mixture at temperature t, pressure p to the density of a reference substance at temperature t', pressure p'. For liquid solutions, the reference substance is often water at 4° C, 1 bar. (In some cases 1 atm is used instead of 1 bar.) The term *specific gravity* is no longer used.

Thermodynamics of Solubility (18)

Thermodynamic analysis of solubility phenomena provides a rational basis for the construction of functions to represent solubility data, and thus aids in evaluation, and sometimes enables thermodynamic quantities to be extracted. Both these aims are often difficult to achieve because of a lack of experimental or theoretical activity coefficients. Where thermodynamic quantities can be found, they are not evaluated critically, since this task would involve examination of a large body of data that is not directly relevant to solubility. Where possible, procedures for evaluation are based on established thermodynamic methods. Specific procedures used in a particular volume will be described in the Preface to that volume.

Only one thermodynamic result is mentioned here: the temperature dependence of solubility. Sometimes it is possible to fit the mole fraction solubility at various temperatures using the equation

$$\ln x_1 = A + B(\mathrm{K}/T) + C\ln(T/\mathrm{K}) + D(T/\mathrm{K}) \qquad [26]$$ 28

where A, B, C and D are constants to be determined from least-squares fitting of the data. Sometimes, to avoid singular matrices of the least-squares normal equations, T is scaled; e.g., T is replaced by $T/100$.

If the gas and the solution of the dissolved gas are ideal, the coefficients can be used to find standard thermodynamic functions for transfer of the gas from the vapor to the liquid phase at the standard pressure (1 bar) and infinitely-dilute dissolved gas, as follows.

$$\Delta G^{o}_{m,1}/R = -A(T/\mathrm{K}) - B - C(T/\mathrm{K})\ln(T/\mathrm{K}) - D(T/\mathrm{K})^2 \qquad [27]$$ 29

$$\Delta S^{o}_{m,1}/R = A + C\ln(T/\mathrm{K}) + C + 2D(T/\mathrm{K}) \qquad [28]$$ 30

$$\Delta H^{o}_{m,1}/R = -B + C(T/\mathrm{K}) + D(T/\mathrm{K})^2 \qquad [29]$$ 31

$$\Delta C^{o}_{m,p}/R = C + 2D(T/\mathrm{K}) \qquad [30]$$ 32

Alternatively (but equivalently), the standard state of infinitely-dilute dissolved gas can be described as a hypothetical ideal dissolved gas at mole fraction $x_1 = 1$, $p = 1$ bar.

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Table 1. Interconversions between Quantities Used as Measures of Solubility
c-component Systems Containing c - 1 Solutes i and Single Solvent c

	x_i	w_i	m_i	c_i
$x_i =$	x_i	$\dfrac{1}{1+\dfrac{M_i}{M_c}\left(\dfrac{1}{w_i}-1+\sum\limits_{j\neq i}^{c-1}\left(\dfrac{M_c}{M_j}-1\right)\dfrac{w_j}{w_i}\right)}$	$\dfrac{1}{1+\dfrac{1}{m_iM_c}+\sum\limits_{j\neq i}^{c-1}\dfrac{m_j}{m_i}}$	$\dfrac{1}{1+\dfrac{1}{M_c}\left(\dfrac{\rho}{c_i}-M_i\right)+\sum\limits_{j\neq i}^{c-1}\dfrac{c_j}{c_i}\left(1-\dfrac{M_j}{M_c}\right)}$
$w_i =$	$\dfrac{1}{1+\dfrac{M_c}{M_i}\left(\dfrac{1}{x_i}-1+\sum\limits_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right)}$	w_i	$\dfrac{1}{1+\dfrac{1}{m_iM_i}\left(1+\sum\limits_{j\neq i}^{c-1}m_jM_j\right)}$	$\dfrac{c_iM_i}{\rho}$
$m_i =$	$\dfrac{1}{M_c\left(\dfrac{1}{x_i}-1-\sum\limits_{j\neq i}^{c-1}\dfrac{x_j}{x_i}\right)}$	$\dfrac{1}{M_i\left(\dfrac{1}{w_i}-1-\sum\limits_{j\neq i}^{c-1}\dfrac{w_j}{w_i}\right)}$	m_i	$\dfrac{1}{\dfrac{1}{c_i}\left(\rho-\sum\limits_{j\neq i}^{c-1}c_jM_j\right)-M_i}$
$c_i =$	$\dfrac{\rho}{M_i+M_c\left(\dfrac{1}{x_i}-1+\sum\limits_{j\neq i}^{c-1}\left(\dfrac{M_j}{M_c}-1\right)\dfrac{x_j}{x_i}\right)}$	$\dfrac{\rho w_i}{M_i}$	$\dfrac{\rho}{\dfrac{1}{m_i}\left(1+\sum\limits_{j\neq i}^{c-1}M_jm_j\right)+M_i}$	c_i

ρ - density of solution; M_i - molar masses of i. For relations for 2-component systems, set summations to 0.

PREFACE

Ethene is a chemical produced in large volumes both as a monomer for polymerization to produce poly(ethylene) as well as a reagent to produce a host of chemical intermediates. What is surprising is that in spite of the great commercial utilization of ethene, the published solubility data are, for the most part, scanty; only in a very few instances are the solubilities corroborated by two or more groups of researchers for any one solvent.

Ethene solubilities have been collected from technical publications up to the end of 1991 with the help of a number of IUPAC members from around the world; these data have since been compiled and critically evaluated in this *Solubility of Ethene volume.* It is anticipated that use will be made of these data in the development and operation of processes for the production and separation of ethene and products derived from it.

Certain phase equilibrium data involving high concentrations of ethene in the dense phase have been excluded from this volume. The exclusions are those at extremely low temperatures, generally termed vapor-liquid equilibria, as well as those at pressures above the critical pressure for ethene, termed the supercritical equilibrium region. The criteria for these fore-mentioned equilibria are considered to be outside the scope of this volume. Instead, this volume deals exclusively with the regular solubilities of the gas in pure solvents and mixed solvent solutions.

The physical and solution properties of ethene can be compared with those of ethane. Because of its lower molecular weight and lower normal boiling point, ethene is often less soluble in simple, non-polar solvents than ethane. On the other hand, because of its unsaturation or its higher chemical activity, ethene is often more soluble in polar and/or associating solvents than is ethane. Further, the molar volume of ethene gas differs from that of an ideal gas; the extent of the deviation is customarily expressed in terms of its second virial coefficient. Using the second virial coefficients from Dymond and Smith (1) an equation expressing the ethene molar volume as a function of temperature (from T = 240 K to T = 450 K) was developed.

For the second virial coefficient:

$$B = -3.083\ (10^7)\ (T/\mathrm{K})^{-2.162} \tag{1}$$

For molar volume:

$$V = 0.5\ C + 0.5\ [C^2 + 4BC]^{0.5} \tag{2}$$

In the above equations B,C and V are in cm^3/mol and $C = RT/P$.

The magnitude of the deviation from ideality is relatively small, ranging from 1.0% at 240 K to 0.1% at 450 K, but not negligible. As much as possible in this volume, where published solubilities are reported on a volumetric basis for the gas, the true gas molar volumes are used in converting the gas volumes to the number of moles of dissolved gas.

In the critical evaluations of the solubilities, two equations are used to describe the mole fraction solubilities as a function of the saturation temperature at constant gas partial pressure, and as a function of the gas partial pressure at constant temperature:

$$\log x = A + B\ (T/\mathrm{K})^{-1} + C\ \log(T/K) \tag{3}$$

$$\log x = D + E\ \log(p/\mathrm{MPa}) + F(p/\mathrm{MPa}) \tag{4}$$

In the above equations A-F are constants. For the simplest relation between solubility and temperature the constant C is equal to zero; however, in certain cases, the empirical correction term gives an improved representation of the solubility data. Similarly, if Henry's law applies, the first three terms of equation (4) represent another form of Henry's law and the constant D is related to Henry's constant while the constant E is equal to 1. For data which are not exactly described by Henry's law, the constant E varies somewhat from 1 and the constant F allows for some curvature of the log x - log p relation. A graph of log x versus log p is useful for solubilities obtained over a range of pressures because at the higher pressures the scale is compressed, but at lower pressures the scale is expanded while the linear relation between log x and log p is still maintained if Henry's law is obeyed. Therefore, it is possible to extrapolate high pressure solubility data to lower pressures and sometimes to 0.1013 MPa for comparison with solubilities obtained at this lower, atmospheric pressure. In some cases, this procedure serves as a consistency check for solubility data. A combined equation, a summation of equations (3) and (4), is also used to represent certain solubility data as a function of both temperature and gas partial pressure. The constants are evaluated by simple regression, or, if necessary by multivariate regression.

As the title page shows, this volume is the product of the efforts of a number of people: contributors, members of the Editorial Board past and present, and other members of the IUPAC Commission V8. I wish to acknowledge their combined contributions in their various capacities and to thank them for it. Finally, I wish to thank Francine Pétrin, and my wife, Bev, who did much of the word processing for the data sheets and critical evaluations.

Walter Hayduk
Ottawa, Canada
June 1994.

1. Dymond, J.H.; Smith, E.B. *The Virial Coefficients of Pure Gases and Mixtures*, Oxford Univ. Press, Oxford, 1980.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5]	Rubin Battino Department of Chemistry Wright State University Dayton, OH 45435 USA April, 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubility in Water for Pressures Less Than 0.2 MPa

Considering the importance of ethene industrially (mostly as a feedstock) it is surprising that there have been so few studies of its solubility in water. In fact, most of the measurements were made only at one temperature, with only Ref. 3,4, and 9 at more than one temperature. The best of the earlier data and those which cover the widest temperature range (287-346 K) are those of Morrison and Billett (3). The data of Wu et al. (10) and Orcutt and Seevers (2) are in reasonable accord with (3). An initial least squares fitting of the 14 points in (3) showed that the value at 294.25 K was significantly deviant. The remaining 13 points were fit to yield:

$$\ln x_1 = -66.9156 + 92.2101/\tau + 24.3792 \ln \tau \qquad (1)$$

In the above equation $\tau = T/100$ K and x_1 is for a gas partial pressure of 101.3 kPa. The standard deviation in $\ln x_1$ was 0.0036 and the standard deviation in x_1 was 2.5 E-7 for an average standard deviation of 0.39%. The compiler of the Morrison and Billett paper estimated the precision of the solubility measurements to be 2%. This is obviously the best of the older data.

Tentative values of solubility based on Eq. (1) expressed as Henry coefficient, $H_{1,2}$ (T, $P_{s,2}$), mole fraction at 101.325 kPa partial pressure of gas, x_1, and the Ostwald coefficient at infinite dilution, $L^{\infty}_{1,2}$, are given in Table 1.

This table also gives tentative values of changes in the cited thermodynamic functions on solution. The mole fraction was simply calculated as 101,325/$H_{1,2}$(T, $P_{s,2}$) since (11) shows that this results in an error of less than 0.15%. The thermodynamic functions were calculated in a straightforward manner (12).

Table 1: Tentative values for the solubility of ethene in water for a gas partial pressure of 0.1013 MPa

T/K	10^{-9} $H_{1,2}$/ Pa	10^5 x_1	$L^{\infty}_{1,2}$	ΔH_1^0/ kJ mol^{-1}	ΔS_1^0/ J mol^{-1} K^{-1}
278.15	0.6800	14.71	0.1863	-20.29	-146.3
283.15	0.7909	12.64	0.1630	-19.27	-142.7
288.15	0.9082	11.01	0.1444	-18.26	-139.1
293.15	1.031	9.70	0.1293	-17.25	-135.7
298.15	1.156	8.65	0.1171	-16.23	-132.2
303.15	1.284	7.79	0.1071	-15.22	-128.9
308.15	1.412	7.08	0.0988	-14.21	-125.5
313.15	1.537	6.50	0.0921	-13.19	-122.3
318.15	1.660	6.02	0.0865	-12.18	-119.1
323.15	1.777	5.63	0.0818	-11.17	-115.9

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

EVALUATOR:

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April, 1994

CRITICAL EVALUATION:

References

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12. Battino, R.; Argon, *Solubility Data Series*, Vol. 4. p. 1-3, Pergamon Press, Oxford, 1980.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Clever, H. L.; Baker, E. R.;
Hale, W. R.

J. Chem. Eng. Data 1970, *15*, 411-3.

VARIABLES:

T/K = 303.15
p_t/kPa = 101.3

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature $t/^{\circ}C$	Temperature T/K	Bunsen Coefficient α/ cm^3(STP) cm^{-3} atm^{-1}	Ostwald Coefficient L/cm^3 cm^{-3}	Mol Fraction 10^5x_1	Molality 10^3m_1/ mol kg^{-1}	Henry's Constant $10^{-6}K_H$/kPa
30.0	303.15	0.0982	0.1090	7.98	4.43	1.27

[a] All values except the Bunsen coefficient were calculated by the compiler. Values for 1 atm (101.3 kPa) assuming Henry's law.

The ethene molar volume at STP, V_1/cm mol^{-1} = 22,246.

Henry's constant, K_H/kPa = (p_1/kPa)/x_1

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and method were similar to those described by Markham and Kobe (ref 1).

The water was degassed by refluxing under partial vacuum, and transfered to the solubility apparatus without contact with atmospheric gases. The solubility of ethene at a total pressure of one atm (101.3 kPa) was measured by observing the volume of gas absorbed by 88.5 cm^3 of water at 30 $^{\circ}C$.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co., Inc. Stated to be 99.5 % minimum purity.

(2) Water. Distilled.

ESTIMATED ERROR:

$\delta T/K = \pm\ 0.05$
$\delta\alpha/\alpha = \pm\ 0.01$

REFERENCES:

1. Markham, A. E.; Kobe, K. A. *J. Am. Chem. Soc.* 1941, *63*, 449.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Wu, Z.; Zeck, S.; Langhorst, R.; Knapp, H.

Proc. Int. Conf. Coal Gas and Air, Beijing, China, 1985, *1*, 209-229.

VARIABLES: T/K = 298.15

P/kPa = 100 (1 bar)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Henry's Constants K/Bar	^1H/atm(mole fraction)$^{-1}$	Ostwald Coefficient ^1L/cm³ gas(cm³ solvent)$^{-1}$	^{2}Mole Fraction $10^5 x_1$
298.15	11490	11590	0.118	8.63

[1] Calculated by compiler.

[2] Calculated by compiler for a gas partial pressure of 101.325 kPa.

Values personally received from the first author for the gas and liquid phase compositions corresponding to a pressure of 1 bar were respectively: $y_1 = 0.968$, and $x_1 = 0.0000824$ mole fraction.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

Ethylene gas was stored in a glass burette equipped with an accurate manometer for measuring pressure and situated in a constant temperature air bath. A known quantity of completely degassed solvent was charged into an equilibrium cell immersed in a liquid bath. The volume of gas absorbed was measured after the gas was admitted into the cell. The solubility was determined from the quantities of gas and solvent used. The apparatus and procedure are described in detail in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.9 vol. percent.
2. Water was bidistilled and had a conductivity of 2 micromhos/cm.

ESTIMATED ERROR:

δP/kPa = ± 0.05
δT/K = ± 0.01
$\delta L/L$ = ± 0.01

REFERENCES:

1. Zeck, S. *Doctoral Dissertation*, Tech. Univ. Berlin, FRG, 1985.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Natarajan, G.S.;
Nageshwar, G.D.
Indian J. Technol. 1981, *19*,
298-299.

VARIABLES: T/K = 293.15-303.15

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Ethene Solubility s/g(10^6g water)$^{-1}$ [1]	[1] Ethene Mole Fraction, 10^5x_1	[1] Henry's Constant H/atm(mole fraction)$^{-1}$
20	293.15	143	9.40	10640
25	298.15	119	7.89	12670
30	303.15	104	6.97	14340

[1] Calculated by compiler. In the calculations it is assumed that the solubility as given is for a total pressure of one atmosphere. The mole fraction, x_1, is for a partial pressure of 101.325 kPa and H is based on the ethene partial pressure.

It was confirmed by private communication with Dr. Nageshwar that s was for a total pressure of one atmosphere.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. Water treatment not specified.

ESTIMATED ERROR:

$\delta s/s = \pm 3\%$

REFERENCES:

1. Dubois, H.D.; Skoog, D.A. *Anal. Chem.* 1948, *20*, 624.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Kidaka, T. Miyamoto, H.;
Murakami, T.
Proc. Soc. Chem. Engrs, Japan (Osaka),
Oct. 14, 1968, 89-90.

VARIABLES:

T/K = 298.15
P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1] T/K	Mole Fraction Ethene, $10^5\ x_1$ For: P = 101.325 kPa	$^2p_1$ = 101.325 kPa	[2] Ostwald Coefficient L /cm^{3}gas cm^{-3} solvent	[2] Henry's Constant H/atm (mole fraction)$^{-1}$
25.0	298.15	8.76	9.04	0.122	11060

[1] Calculated by compiler.

[2] Although not specifically stated in paper it was assumed by the compiler that the reported solubility was for a total pressure of 101.325 kPa; therefore, the solubility for a partial pressure of 101.325 kPa was calculated assuming Henry's law and an ethene molar volume of 24320 cm^3/mole at 298.15 K and 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.

SOURCE AND PURITY OF MATERIALS:

1. Source and purity not given.
2. Treatment not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm\ 0.03$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-1275.

VARIABLES: $T/K = 298.15 \pm 1.5$

$P/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Ethene Solubility s/g gas $(10^6$ g water$)^{-1}$	[1] Mole Fraction, 10^5x_1	[1] Henry s Constant H/atm(mole fraction$)^{-1}$
25.0	298.15	131 ± 10	8.41	11890

[1] Calculated by compiler. It is assumed that the solubility as given is for a gas partial pressure of 101.325 kPa.

The variation for s, as given, is from the original paper corresponding to a standard deviation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A bottle was three-fourths filled with distilled water. A gas pressure of 1 atm was maintained over the water from a rubber balloon reservoir in the line from the gas cylinder. The bottle was vigorously shaken for 5-10 min to establish equilibrium. The equilibrated solution was allowed to stand at least 30 min prior to analysis for separation of gas bubbles. Samples of aqueous solutions of 50 μl were injected into a U-tube desorber containing firebrick and Ascarite drying agent, heated to 100°C and through which helium carrier gas from a gas chromatograph was allowed to flow. The GC analyzer used a hydrogen flame ionization detector.

SOURCE AND PURITY OF MATERIALS:

1. Ethene minimum purity 99.0%.
2. Distilled water.

ESTIMATED ERROR:

$\delta s/s = \pm 8\%$ (Compiler)

$\delta T/K = \pm 1.5$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Truchard, A.M.; Harris, H.G.;
Himmelblau, D.M.

J. Phys. Chem. 1961, *65*, 575-576.

VARIABLES:

$T/K = 273.153$

$P/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

$^1T/K$	Henry's Constant H/atm(mole fraction)$^{-1}$	^{1}Mole Fraction Ethane, $(10^4)x_1$
273.15	5280	1.894

[1] Mole fraction ethene calculated by compiler for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two calibrated glass spheres, one larger than the other, immersed in a bath connected to a mercury manometer were used. Approximately 200 cm^3 of solvent was placed in the larger sphere and both were thoroughly evacuated. A supply of ethene was charged to the smaller flask to 2 atm pressure. Ethene was admitted to the flask containing the solvent and allowed to reach equilibrium by stirring. The pressures were read and material balances made to determine the solubility. Solubilities were measured for equilibrium pressures between 50 and 1300 mm of mercury pressure and Henry's law was found to apply in all cases.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. Water treatment not specified.

ESTIMATED ERROR:

$\delta H/H = \pm 0.02$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5]	Taft, R.W.; Purlee, E.L.; Riesz, P. *J. Amer. Chem. Soc.* 1955, *22*, 899-902.
VARIABLES: T/K = 293.15-303.15 P/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	Inverse of Henry's Constant, 10^3h/ moles (l atm)$^{-1}$	[2]Ethene Mole Fraction, 10^5x_1	[1]Henry's Constant H/atm (mole fraction)$^{-1}$
20.00	293.15	5.17	9.330	10718
25.00	298.15	4.66	8.419	11878
30.00	303.15	4.11	7.437	13447

[1] Calculated by compiler.

[2] Mole fraction solubility calculated by compiler for a partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 200 cm^3 glass flask was connected to a pressure-measuring manometer by means of a horizontally -mounted spiral tube. The spiral tube permitted the flask to be shaken with an amplitude of up to 2 cm for equilibration. The solvent (80-125 cm^3) was deaerated in the flask. The change in pressure of a known volume of gas was measured from which the solubility was determined. The total volume of the apparatus was initially determined by weighing the apparatus filled with distilled water. The "distribution constant", h, was determined for pressures below 101.325 kPa. Method described in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson, purity 99.5%.
2. Water was distilled.

ESTIMATED ERROR:

δT/K = ± 0.02

$\delta h/h$ = ± 0.01

REFERENCES:

1. Levy, J.B.; Taft, R.W.; Aaron, D.; Hammett, L.P.

   J. Amer. Chem.Soc. 1951, *73*,

   3792.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Morrison, T.J.; Billett, F.

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

VARIABLES:

$T/K = 286.9 - 346.0$

$P/kPa = 101.3$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

$t/°C$	T/K	[1]Solubility, s/ cm^3 (STP) kg^{-1}	[2]Mole Fraction $10^5\ x_1$	[2]Ostwald Coefficient L / cm^3 cm^{-3}	[2]Bunsen Coefficient α/ cm^3 (STP) cm^{-3}
13.8	286.95	140.9	11.40	0.1480	0.1409
17.8	290.25	128.8	10.42	0.1367	0.1287
20.5	293.65	118.0	9.54	0.1266	0.1178
21.1	294.25	115.1	9.31	0.1238	0.1149
25.0	298.15	107.2	8.67	0.1167	0.1069
30.3	303.45	95.5	7.72	0.1056	0.0951
35.2	308.35	87.3	7.05	0.0980	0.0868
40.0	313.15	81.1	6.55	0.0923	0.0805
44.6	317.75	75.2	6.07	0.0866	0.0745
49.0	322.15	70.5	5.69	0.0822	0.0697
54.9	328.05	65.5	5.29	0.0775	0.0646
60.2	333.35	62.2	5.02	0.0745	0.0611
65.0	338.15	59.2	4.78	0.0719	0.0581
72.9	346.05	56.1	4.53	0.0694	0.0548

[1] Original data expressed as cm^3 (STP) per 1000 g water at a total pressure of 101.3 kPa. A smoothing equation (ref. 1) is as follows:

$$\log_{10} s = -69.697 + 3900/T + 23.70 \log_{10}T \quad ; \ T/K$$

[2] Calculated by Compiler for a gas partial pressure of 101.3 kPa and using real gas molar volumes.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equipment consisted of a solvent degassing system, an absorption spiral and a gas burette for measuring the gas volume. Degassed solvent was allowed to flow down the absorption spiral containing the gas which was saturated with solvent vapor, at a total pressure of one atmosphere. The volume of gas absorbed was measured by means of the attached burette system. The volume of solution was also accumulated in a burette. Details were previously described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared from ethanol using phosphoric acid. Actual purity not determined.
2. Water degassed. No additional details given.

ESTIMATED ERROR:

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

$\delta\ s/s = \pm\ 0.02$ (Compiler)

REFERENCES:

1. Morrison, T.J.
J. Chem. Soc. 1952, 3814.

2. Morrison, T.J.
J. Chem. Soc. 1948, 2033.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Orcutt, F.S.; Seevers, M.H.

J. Biol. Chem. 1937, *117*, 501-507.

VARIABLES:

T/K = 298.15

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	T/K	α/ Bunsen Coefficient cm^3 gas(STP) cm^{-3} solvent	[1]Ostwald Coefficient L/ cm^3 gas cm^{-3} solvent	[1]Mole Fraction $x_1 \cdot 10^5$	[1]Henry's Constant/ atm (mole fraction)$^{-1}$
25	298.15	0.108	0.118	8.771	11400

[1] Calculated by Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The liquid is saturated by ordinary tonometer methods. It is then transferred to a manometric extraction chamber (which was previously evacuated) by a modified Ostwald pipette as described in reference 1. The gas is then extracted and by comparing the manometer reading after extraction to the reading obtained using a "blank" determination, the volume of gas is determined.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not specified.
2. Water is deaerated by bubbling with ethene.

ESTIMATED ERROR:

$\delta\alpha/\alpha = \pm\ 0.02$(Compiler)

REFERENCES:

1. Van Slyke, D.D,; Neill, J.M. *J. Biol. Chem.* 1924, *61* , 523.

1/

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Grollman, A.

J. Biol. Chem. 1929, *82*, 317-325.

VARIABLES:

$T/K = 298.15$ (25.0°C)

$p/kPa = 73.3-133.3$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Ethene Partial Pressure p/mm mercury	[1]p/kPa	Ostwald Coefficient L/cm^3 gas$(\text{cm}^3 \text{ solvent})^{-1}$	[2]Mole fraction, $10^5 x_1$
550	73.33	0.112	
600	80.0	0.113	
650	86.7	0.113	
700	93.3	0.112	
750	100.0	0.113	
800	106.7	0.113	
850	113.3	0.113	
900	112.0	0.114	
950	126.7	0.113	
1000	133.3	0.113	
Average:	--	0.1129	8.39

[1] Calculated by compiler.

[2] Mole fraction solubility for a gas partial pressure of 101.325 kPa and based on the average value for the Ostwald coefficient calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass bubbling-type of saturator immersed in a constant temperature bath was used. A known volume of saturated solution was transferred over mercury into a Van Slyke desorption apparatus. Gas removed in three evacuations was transferred to a sample tube where the volume was determined and a sample of the gas was analyzed. Solubilities were determined at several pressures below atmospheric and above atmospheric and expressed as Ostwald coefficients.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. Water distilled.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$

$\delta L/L = \pm 4\%$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Grollman, A.

J. Biol. Chem. 1929, *82*, 317-325.

VARIABLES:

T/K = 310.65 (37.5°C)

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Bunsen Coefficient β/cm^3 gas NTP cm^{-3} solvent	[1]Ostwald Coefficient L/cm^3 gas (cm^3 solvent)$^{-1}$	[2]Solubility Mole fraction, 10^5x_1
37.5	310.65	0.078	0.0887	6.34

[1]Calculated by compiler.

[2]Calculated by compiler using a gas molar volume at a temperature of 310.65 K and a pressure of 101.325 kPa of 25360 cm^3/mole.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass bubbling-type of saturator immersed in a constant temperature bath was used. The gas was presaturated with water vapor. A known volume of saturated solution was transferred over mercury into a Van Slyke desorption apparatus. Gas removed in three evacuations was transferred to a sample tube where the volume was determined and a sample of the gas was analyzed. The solubilities were expressed as the Bunsen coefficients.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. Water distilled.

ESTIMATED ERROR:

$\delta\beta/\beta$ = ± 0.04 (Compiler)

δT/K = ± 0.05

REFERENCES:

13

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5]	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, Ontario Canada K1N 6N5 June 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubility in Water for Pressures greater than 0.2 MPa (2 atm)

Ethene solubilities in water at elevated pressures have been reported in 6 publications (1-6) for temperatures ranging from 298 K to 573 K and pressures to 86 MPa. Data for the solubilities of mixtures of ethane and ethene in water at elevated pressures have also been reported (6). Since the solubility measurements were made at widely differing pressures and temperatures, ethene partial pressure data were needed for a meaningful evaluation. These partial pressures were calculated based on the gas phase compositions where reported or they were evaluated from the vapour pressure of water assuming Raoult's law applies for water. Both approaches gave very similar results.

Values of log x versus log p were plotted for each set of data. A linear relationship usually suggests a satisfactory consistency in the data but such a test is not rigorous and, in general, deviations from linearity are to be expected at high pressures. These plots were used to extrapolate the solubilities to obtain a value at a partial pressure of 0.1013 MPa. The procedure for the extrapolation was to give preference to the data for the lowest pressures available, and to extrapolate these values to a pressure of 0.1013 MPa assuming a direct relationship between log x and log p. It appears likely that Henry's law will be best obeyed at the lowest pressures and if it is, as data are extrapolated to low pressures, the slope of the log x - log p line will be equal to one. It is noted that at elevated pressures the log x - log p line is often somewhat curved and the slope is often less than one.

Solubilities which have been extrapolated to an effective gas partial pressure of 0.1013 MPa are compared with those actually measured at a partial pressure of 0.1013 MPa where possible, in Table 1 and Figure 1. The source of the oxygen solubilities in water for Figure 1 is the Solubility Data Series volume on Oxygen (7). From Figure 1 it is evident that all the six sources of data when extrapolated using Henry's law are relatively consistent, agreeing with one another, agreeing with the low pressure solubilities of ethene in water, and having a similar temperature effect on solubility as that for oxygen dissolving in water. Although certain individual extrapolated values show deviations of as much as 20% from a line representing the data, such deviations are probably mostly the result of extrapolations over large pressure ranges, rather than of errors in the experimental results themselves. The data of Anthony and McKetta (6) and Davis and McKetta (2) appear to be the most consistent of the data. It is apparent that the solubility of ethene in water has a minimum, as does the solubility of oxygen in water, at a temperature near the normal boiling temperature of water (T_{nbp}). It is also apparent that the high pressure solubilities for ethene in water are accurate only to about ± 5%. It is clear, therefore, that experimental work of higher accuracy and for a larger range of pressures and for higher temperatures is required to fully define the solubility relationship for ethene in water.

The data of Bradbury et al. (1), Davis and McKetta (2), Anthony and McKetta (3,6), Sanchez and Lentz (4) and Sokolov and Konshin (5) are all classified as tentative.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Water; H_2O; [7732-18-5]

EVALUATOR:

Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, Ontario
Canada K1N 6N5

June 1994

CRITICAL EVALUATION:

Table 1 Comparison of extrapolated high pressure solubilities with those measured at 0.1013 MPa pressure for various temperatures.

T/K	$10^5\ x_1$ For 0.1013 MPa pressure	$10^5\ x_1$ Extrapolated to 0.1013 MPa	Difference %	Reference
298.15	8.70	10.4	+19.5	(5)
308.15	7.08	6.85	-3.4	(1)
310.93	6.75	6.90	+2.2	(2)
310.93	6.75	6.30	-7.1	(6)
327.59	5.32	4.95	-7.5	(2)
328.15	5.29	6.05	+14.4	(1)
344.26	4.49	4.32	-3.9	(3)
344.26	4.49	4.52	+0.7	(6)
348.15	4.34	4.73	+9.0	(1)
360.93	4.10	4.80	+17.1	(2)

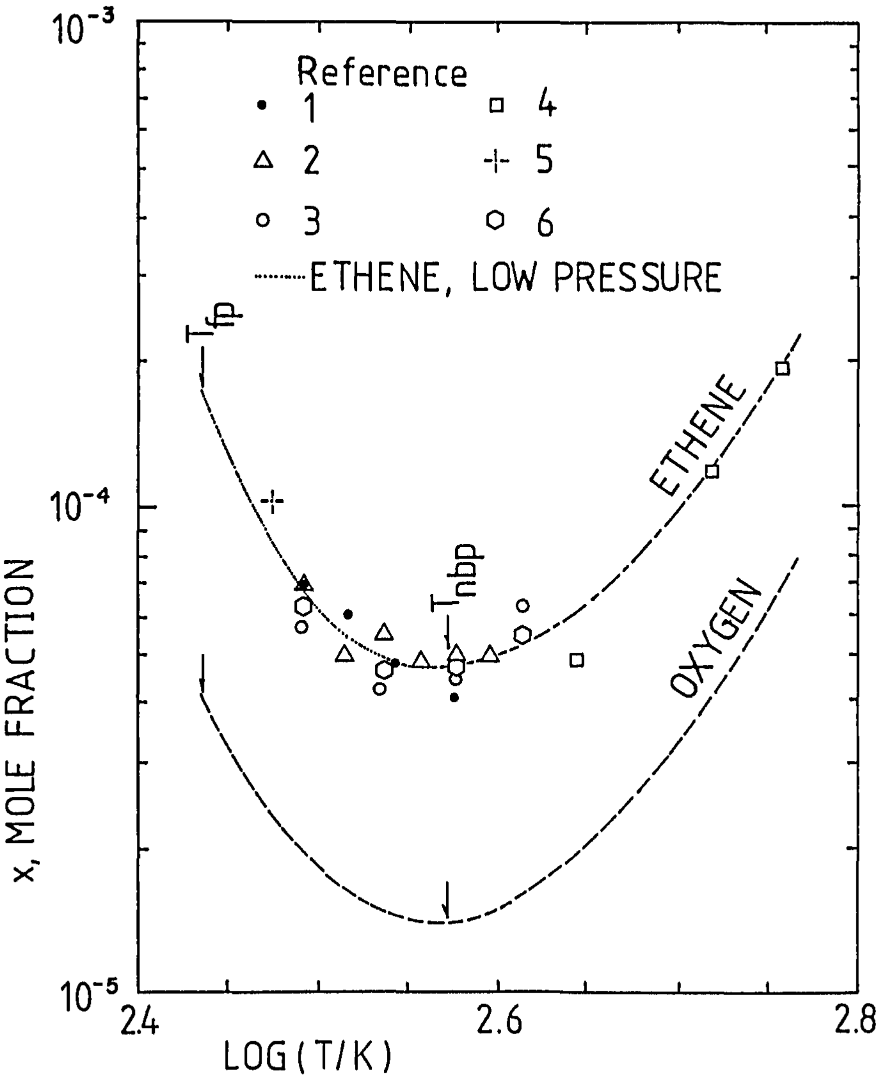

Figure 1 Mole fraction ethene and oxygen solubility in water extrapolated to 0.1013 MPa partial pressure.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5]	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, Ontario Canada K1N 6N5 June 1994

CRITICAL EVALUATION:

Ethane; C_2H_6; [74-84-0] and Ethene; C_2H_4; [74-85-1] Gas mixtures.

This system has been investigated by Anthony and McKetta (6). It is of interest that Henry's law is obeyed for both gas components even up to the high pressures utilized in this work. From these solubilities it is possible to estimate solubilities for lower pressures. These results are entirely consistent with those involving only two components. No comparable data are available for comparison.

The results of Anthony and McKetta (6) are classified as tentative.

References

1. Bradbury, E.J.; McNulty, D.; Savage, R.L.; McSweeny, E.E.; *Ind. Eng. Chem.*, 1952, *44*, 211-212.
2. Davis, J.E.; McKetta, J.J.; *J. Chem. Eng. Data*, 1960, *5*, 374-375.
3. Anthony, R.G.; McKetta, J.J., *J. Chem. Eng. Data*, 1967, *12*, 17-20.
4. Sanchez, M.; Lentz, H.; *High Temp. High Press.*, 1973, *5*, 689-699.
5. Sokolov, Yu. P.; Konshin, A.I.; *Zh. Prikl. Khim.*, 1990, *63*, 710-713.
6. Anthony, R.G.; McKetta, J.J.; *J. Chem. Eng. Data*, 1967, *12*, 21-28.
7. Battino, R. Oxygen and Ozone, *IUPAC Solubility Data Series*, Vol. 7, Pergamon Press, Oxford, 1981.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sokolov, Yu. P.; Konshin, A.I.

Zh. Prikl. Khim. <u>1990</u>, *63*, 710-713.

VARIABLES:

T/K = 298.15
P/MPa = 0.20 - 1.11

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	T/K	P/MPa	Solubility C_1/mM	Solubility [1]x_1, mol fraction	[2]Distribution Constant, K_d	[3]Henry's Constant H/MPa (mol fraction)$^{-1}$
25.0	298.15	0.20	11.6	0.000210	0.143 ± 0.005	950 ± 50
		0.31	18.0	0.000325		
		0.51	29.6	0.000535		
		0.71	41.8	0.000755		
		0.91	52.8	0.000954		
		1.11	64.4	0.001164		

[1] Calculated by Compiler with C_1 taken to mean millimolar or millimoles per litre.

[2] Distribution constant $K_d = C_l/C_g$ where C_l = mole/litre in liquid and C_g = mole /litre in gas.

[3] Stated by authors to be $\lim_{x_1 \to 0} (p_1/x_1)$ for p_1 = partial pressure of gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubilities were measured using a stirred reactor with a magnetic drive having a volume of 250 cm^3 and equipped with a pressure gauge and a surrounding jacket for temperature control. Gas and sample handling systems were attached. A volume of 100-200 cm^3 of deaerated solvent was charged to the reactor and equilibrated. A small liquid sample chamber was used to confine a known volume of saturated solution. The sample was then completely evaporated into a much larger vessel. Helium carrier gas was used to increase the pressure of the vapor-gas mixture to about 0.12 MPa. The sample was then analyzed by gas chromatography. Details are in Ref. 1.

SOURCE AND PURITY OF MATERIALS:

No information about gas or solvent source or purity was supplied.

ESTIMATED ERROR:

$\delta x/x = \pm 5\%$ (Compiler)

REFERENCES:

1. Sokolov, Yu. A.; Konshin, A.I. *Zh. Prikl. Khim.* <u>1987</u>, *60*, 2720.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanchez, M.; Lentz, H.

High Temp. - High Press. 1973, *5*, 689-699.

VARIABLES:

T/K = 439.15 - 573.15

P/MPa = 10.0 - 94.5

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	[1]T/K	Pressure bar	Pressure [1]MPa	Mole Fraction Ethene in Gas, y_1	Mole Fraction Ethene in Liquid, x_1	[1]Partial Pressure Ethene, p_1/MPa
166	439.15	100	10	0.860	0.004	8.60
		150	15	0.890	0.005	13.35
		635	63.5	0.959	0.010	60.90
		945	94.5	0.910	(0.008)[2]	86.00
250	523.15	190	19.0	0.630	0.014	11.97
		240	24.0	0.688	0.018	16.51
		375	37.5	0.766	0.026	28.73
		570	57.0	0.750	0.034	42.75
		730	73.0	0.810	0.040	59.13
300	573.15	240	24.0	0.516	0.024	12.38
		380	38.0	0.597	0.036	22.69
		550	55.0	0.550	0.047	30.25

[1] Calculated by compiler.

[2] Brackets as in original paper.

Smoothed values as obtained by extrapolation and interpolation are also available in this paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a high pressure piston pump, Bourdon pressure gauges, a stainless steel capillary tube equilibrium cell 4.7 mm in inside diameter, a tubular storage chamber for the gas, as well as an associated temperature sensing element, sampling probes and valves. The apparatus was mounted in a constant temperature chamber. The equilibrium cell was charged with a known quantity of solvent by rotating it to a horizontal position. The quantity of gas was determined by material balance and the PV relation in the gas supply tube.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was specified to be 99.99%.
2. Water was double distilled.

ESTIMATED ERROR:

$\delta T/K = \pm 0.5$

$\delta x_1/x_1 = \pm 0.05$ or $\pm 5\%$ (Compiler)

REFERENCES:

16

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Anthony, R.G.; McKetta, J.J.

J. Chem. Eng. Data <u>1967</u>, *12*, 17-20.

VARIABLES:

T/K = 310.9-410.9

P/MPa = 3.43-34.40

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/F(^1T/K)	Total Pressure P/psia	Total Pressure ^1P/MPa	^{1,2}Partial Pressure p/MPa	Partial Pressure p_1/MPa	Mole Fraction Ethene in Liquid, $10^3 x_1$	Mole Fraction Water in Vapor, $10^3 y_1$
99.9(310.87)	497.2	3.428	3.422	3.420	2.012	2.363
	1000.2	6.896	6.890	6.886	2.854	1.485
	1012.2	6.979	6.972	6.969	3.146	1.416
100.0(310.93)	1483.2	10.23	10.22	10.21	3.388	1.495
100.1(310.98)	513.2	3.538	3.532	3.530	1.907	2.374
	1000.2	6.896	6.890	6.886	3.134	1.532
	1002.2	6.910	6.903	6.899	2.854	1.542
	2075.2	14.31	14.30	14.29	3.685	1.533
	3067.2	21.15	21.14	21.11	3.720	1.579
	4029.7	27.78	27.78	27.74	3.855	1.622
	4724.2	32.57	32.57	32.52	4.125	1.545
159.9(344.21)	2007.7	13.84	13.81	13.77	3.209	5.086
	2887.2	19.91	19.87	19.81	4.134	4.971
160.0(344.26)	517.7	3.569	3.537	3.530	1.555	10.955
	1505.2	10.35	10.32	10.29	2.921	5.374

[1] Calculated by compiler. [2] Partial pressure p is calculated from the vapor pressure of water and p_1 from the composition of the vapor y_1.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The high pressure apparatus is described in reference 1. It consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer (Meeco Model W) was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the Orsat gas burette at constant temperature, and then the gas volume and pressure was determined. The minimum accuracy of the liquid sampling and analysis method was stated to be ± 5% as described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was Phillips pure grade.
2. Water was distilled and deaerated.

ESTIMATED ERROR:

δT/K = ± 0.1　　$\delta P/P$ = ± 0.001

$\delta x_1/x_1$ = ± 5% (Reference 2)

REFERENCES:

1. Wehe, A.H.; McKetta, J.J. *J. Chem. Eng. Data* <u>1961</u>, *6*, 167.
2. Wehe, A.H.; McKetta, J.J. *Anal. Chem.* <u>1961</u>, *33*, 291.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5]	Anthony, R.G.; McKetta, J.J. *J. Chem. Eng. Data* 1967, *12*, 17-20.
VARIABLES: T/K = 310.9-410.9 P/MPa = 3.43-34.40	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/F(^1T/K)	Total Pressure P/psia	^1P/MPa	^{1,2} Partial Pressure p/MPa	p_1/MPa	Mole Fraction Ethene in Liquid, 10^3x_1	Mole Fraction Water in Vapor, 10^3y_1
160.0(344.26)	3064.7	21.13	21.10	21.02	3.576	5.124
	4079.7	28.13	28.10	27.98	3.826	--
160.1(344.32)	1074.7	7.410	7.377	7.363	2.319	6.325
	4289.7	29.58	29.54	29.43	3.945	5.110
	4989.2	34.40	34.37	34.22	4.124	5.115
219.9(377.54)	1526.2	10.52	10.41	10.34	3.010	17.26
	2102.2	14.49	14.38	14.28	3.368	14.86
	4099.7	28.27	28.15	27.89	4.589	13.24
220.0(377.59)	1018.2	7.020	6.904	6.860	2.240	22.79
220.1(377.65)	534.2	3.683	3.565	3.546	1.329	37.37
220.2(377.71)	3144.7	21.68	21.56	21.38	3.937	13.71
279.7(410.76)	616.7	4.252	3.911	3.844	1.540	95.98

[1] Calculated by compiler. [2] Partial pressure p is calculated from the vapor pressure of water and p_1 from the composition of the vapor y_1.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The high pressure apparatus is described in reference 1. It consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer (Meeco Model W) was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the Orsat gas burette at constant temperature, and then the gas volume and pressure was determined. The minimum accuracy of the liquid sampling and analysis method was stated to be ± 5% as described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was Phillips pure grade.
2. Water was distilled and deaerated.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$ $\delta P/P = \pm 0.001$

$\delta x_1/x_1 = \pm 5\%$ (Reference 2)

REFERENCES:

1. Wehe, A.H.; McKetta, J.J. *J. Chem. Eng. Data* 1961, *6*, 167.
2. Wehe, A.H.; McKetta, J.J. *Anal. Chem.* 1961, *33*, 291.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5]	Anthony, R.G.; McKetta, J.J. *J. Chem. Eng. Data* 1967, *12*, 17-20.
VARIABLES: T/K = 310.9-410.9 P/MPa = 3.43-34.40	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/F(^{1} T/K)	Total Pressure P/psia	Total Pressure ^1P/MPa	Partial Pressure[1,2] p/MPa	Partial Pressure[1,2] p_1/MPa	Mole Fraction Ethene in Liquid, 10^3x_1	Mole Fraction Water in Vapor, 10^3y_1
279.8(410.82)	529.7	3.652	3.311	3.615	1.329	10.18
	1032.2	7.117	6.776	6.684	2.475	60.77
	3874.7	26.71	26.38	25.92	5.631	29.83
279.9(410.87)	1556.2	10.73	10.39	10.25	3.375	44.43
	4005.2	27.61	27.28	26.77	5.602	30.47
280.0(410.93)	1339.2	9.233	8.893	8.784	--	48.66
	3002.2	20.70	20.36	20.02	4.728	32.93
280.1(410.98)	2018.2	13.91	13.57	13.38	4.019	38.25
280.2(411.04)	1499.2	10.34	9.996	9.799	3.264	51.98

[1] Calculated by compiler. [2] Partial pressure p is calculated from the vapor pressure of water and p_1 from the composition of the vapor y_1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The high pressure apparatus is described in reference 1. It consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer (Meeco Model W) was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the Orsat gas burette at constant temperature, and then the gas volume and pressure was determined. The minimum accuracy of the liquid sampling and analysis method was stated to be ±5% as described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was Phillips pure grade.
2. Water was distilled and deaerated.

ESTIMATED ERROR:

$\delta T/K = \pm\ 0.1$ $\delta P/P = \pm\ 0.001$

$\delta x_1/x_1 = \pm 5\%$ (Reference 2)

REFERENCES:

1. Wehe, A.H.; McKetta, J.J. *J. Chem. Eng. Data* 1961, *6*, 167.
2. Wehe, A.H.; McKetta, J.J. *Anal. Chem.* 1961, *33*, 291.

16

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Anthony, R.G.; McKetta, J.J.

J. Chem. Eng. Data 1967, *12*, 17-20.

VARIABLES:

T/K = 310.9-410.9

P/MPa = 1.38-34.47

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

	Total Pressure		Partial Pressure[1,2]		Mole Fraction Ethene in	Mole Fraction Water in
t/F ([1]T/K)	P/psia	[1]P/MPa	p/MPa	p_1/MPa	Liquid, $10^3\ x_1$	Vapor, $10^3\ y_1$
100 (310.93)	200	1.379	1.372	1.372	0.838	5.126
	400	2.758	2.751	2.750	1.557	2.824
	500	3.447	3.441	3.439	1.875	2.400
	1000	6.895	6.888	6.883	2.955	1.661
	1500	10.34	10.34	10.33	3.351	1.519
	2000	13.79	13.78	13.77	3.574	1.535
	2500	17.24	17.23	17.21	3.732	1.543
	3000	20.68	20.68	20.65	3.830	1.550
	3500	24.13	24.12	24.09	3.905	1.557
	4000	27.58	27.57	27.54	3.954	1.559
	4500	31.03	31.02	30.98	3.982	1.561
	5000	34.47	34.47	34.42	3.999	1.563
160 (344.26)	200	1.379	1.346	1.344	0.585	25.22
	400	2.758	2.725	2.721	1.112	13.42
	500	3.447	3.415	3.409	1.344	11.18
	1000	6.895	6.862	6.849	2.355	6.675

[1] Calculated by compiler.

[2] Partial pressure p is calculated from the vapor pressure of water and p_1 from the composition of the vapor y_1.

The data above are *smoothed* data as listed in the paper.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The high pressure apparatus is described in reference 1. It consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer (Meeco Model W) was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the Orsat gas burette at constant temperature, and then the gas volume and pressure was determined. The minimum accuracy of the liquid sampling and analysis method was stated to be ± 5% as described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was Phillips pure grade.
2. Water was distilled and deaerated.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm\ 0.1 \qquad \delta P/P = \pm\ 0.001$

$\delta x_1/x_1 = \pm\ 5\%$ (Reference 2)

REFERENCES:

1. Wehe, A.H.; McKetta, J.J. *J. Chem. Eng. Data* 1961, *6*, 167.
2. Wehe, A.H.; McKetta, J.J. *Anal. Chem.* 1961, *33*, 291.

16

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Anthony, R.G.; McKetta, J.J.

J. Chem. Eng. Data 1967, *12*, 17-20.

VARIABLES:

T/K = 310.9-410.9

P/MPa = 1.38-34.47

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

...continued

	Total Pressure		Partial Pressure[1,2]		Mole Fraction Ethene in Liquid	Mole Fraction Water in Vapor
t/F ([1]T/K)	P/psia	[1]P/MPa	p/MPa	p_1/MPa	Liquid, $10^3 x_1$	Vapor, $10^3 y_1$
160 (344.26)	1500	10.34	10.31	10.29	2.858	5.452
	2000	13.79	13.76	13.72	3.159	5.037
	2500	17.24	17.20	17.15	3.369	4.909
	3000	20.68	20.65	20.58	3.545	4.910
	3500	24.13	24.10	24.01	3.702	4.909
	4000	27.58	27.55	27.44	3.840	4.900
	4500	31.03	30.99	30.87	3.961	4.900
	5000	34.47	34.44	34.30	4.085	4.900
220 (377.59)	200	1.379	1.262	1.260	0.567	86.36
	400	2.758	2.641	2.626	1.100	47.69
	500	3.447	3.331	3.312	1.346	39.20
	1000	6.895	6.778	6.739	2.281	22.60
	1500	10.34	10.23	10.16	2.941	17.59
	2000	13.79	13.67	13.58	3.351	15.47
	2500	17.24	17.12	16.99	3.628	14.37

[1] Calculated by compiler.

[2] Partial pressure p is calculated from the vapor pressure of water and p_1 from the composition of the vapor y_1.

The data above are *smoothed* data as listed in the paper.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The high pressure apparatus is described in reference 1. It consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer (Meeco Model W) was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the Orsat gas burette at constant temperature, and then the gas volume and pressure was determined. The minimum accuracy of the liquid sampling and analysis method was stated to be ±5% as described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was Phillips pure grade.
2. Water was distilled and deaerated.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$ $\delta P/P = \pm 0.001$

$\delta x_1/x_1 = \pm 5\%$ (Reference 2)

REFERENCES:

1. Wehe, A.H.; McKetta, J.J. *J. Chem. Eng. Data* 1961, *6*, 167.
2. Wehe, A.H.; McKetta, J.J. *Anal. Chem.* 1961, *33*, 291.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Anthony, R.G.; McKetta, J.J.

J. Chem. Eng. Data 1967, *12*, 17-20.

VARIABLES: $T/K = 310.9\text{-}410.9$

$P/MPa = 1.38\text{-}34.47$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/F ($^1T/K$)	Total Pressure P/psia	^1P/MPa	^{1,2}Partial Pressure p/MPa	p_1/MPa	Mole Fraction Ethene in Liquid, $10^3\ x_1$	Mole Fraction Water in Vapor, $10^3\ y_1$
220 (377.59)	3000	20.68	20.57	20.40	3.872	13.83
	3500	24.13	24.02	23.81	4.107	13.50
	4000	27.58	27.46	27.21	4.333	13.32
	4500	31.03	30.91	30.62	4.545	13.18
	5000	34.47	34.36	34.02	4.751	13.10
280 (410.93)	200	1.379	1.038	1.031	0.545	252.53
	400	2.758	2.417	2.399	1.079	130.20
	500	3.447	3.106	3.078	1.320	107.00
	1000	6.895	6.554	6.481	2.455	60.03
	1500	10.34	10.00	9.867	3.352	45.89
	2000	13.79	13.45	13.26	3.970	38.62
	2500	17.24	16.90	16.63	4.435	34.93
	3000	20.68	20.34	20.01	4.836	32.59
	3500	24.13	23.79	23.38	5.105	31.01
	4000	27.58	27.24	26.75	5.535	29.94
	4500	31.03	30.69	30.11	5.852	29.58
	5000	34.47	34.13	33.47	6.180	29.08

[1] Calculated by compiler.

[2] Partial pressure p is calculated from the vapor pressure of water and p_1 from the composition of the vapor y_1.

The data above are *smoothed* data as listed in the paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The high pressure apparatus is described in reference 1. It consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer (Meeco Model W) was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the Orsat gas burette at constant temperature, and then the gas volume and pressure was determined. The minimum accuracy of the liquid sampling and analysis method was stated to be ± 5% as described in reference 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was Phillips pure grade.

2. Water was distilled and deaerated.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$ $\delta P/P = \pm 0.001$

$\delta x_1/x_1 = \pm 5\%$ (Reference 2)

REFERENCES:

1. Wehe, A.H.; McKetta, J.J. *J. Chem. Eng. Data* 1961, *6*, 167.

2. Wehe, A.H.; McKetta, J.J. *Anal. Chem.* 1961, *33*, 291.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Davis, J.E.; McKetta, J.J.

J. Chem. Eng. Data 1960, *5* , 374-375.

VARIABLES: $T/K = 310.9-394.3$

$P/MPa = 0.12-3.74$, (1.16-36.9 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/F	$^1T/K$	Total Pressure P/psia	Total Pressure $^1P/MPa$	Partial Pressure $^1p_1/MPa$	Ethene Mole Fraction, $10^4 x_1$
100	310.93	47	0.3241	0.3175	2.3
		89	0.6136	0.6071	4.1
		145	0.9997	0.9932	6.1
		197	1.358	1.352	7.71
		257	1.772	1.765	10.2
		340	2.344	2.338	13.8
		461	3.179	3.172	17.8
		481	3.316	3.310	18.0
		497	3.427	3.420	18.6
130	327.59	32	0.2206	0.2053	0.91
		91	0.6274	0.6121	2.82
		147	1.014	0.9982	4.71
		291	2.006	1.991	9.23
		355	2.448	2.432	11.0
		409	2.820	2.805	12.9
		452	3.116	3.101	14.2
		521	3.592	3.577	15.5

[1] Calculated by compiler.
Henry's law is not obeyed.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave was used in which the cell was charged with ethylene and water and rocked for 45 min at constant temperature. The cell was kept at rest for 15 min to allow for phase separation. The water solution was sampled and the sample was fed into an analytical train. A 50 cm^3 sample was fed into an evacuated, jacketed flask. After equilibrium was established in the flask the pressure was measured by a mercury manometer. The vapor was completely displaced into a second flask by using mercury. A second stripping operation was obtained by draining the mercury from the first flask. The solubility was based on the sum of the two stripped quantities.

SOURCE AND PURITY OF MATERIALS:

1. Ethene analyzed as 99.2% pure with nitrogen the major impurity.
2. Water was distilled and degassed.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$ at high pressures

$\delta x_1/x_1 = \pm 4\%$ at the lowest pressure (compiler)

REFERENCES:

17

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Davis, J.E.; McKetta, J.J.

J. Chem. Eng. Data 1960, *5*, 374-375.

VARIABLES: T/K = 310.9-394.3

P/MPa = 0.12-3.74, (1.16-36.9 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

t /F	[1]T/K	Total Pressure P/psia	Total Pressure [1]P/MPa	Partial Pressure [1]p_1/MPa	Ethene Mole Fraction, $10^4\ x_1$
160	344.26	17	0.1172	0.0846	0.27
		74	0.5102	0.4776	1.90
		114	0.7860	0.7533	2.85
		184	1.269	1.236	5.19
		210	1.448	1.415	5.27
		333	2.296	2.263	8.23
		345	2.379	2.346	9.00
		491	3.385	3.353	12.2
		504	3.475	3.442	12.5
190	360.93	75	0.5171	0.4527	2.00
		185	1.276	1.211	5.29
		219	1.510	1.445	6.30
		289	1.993	1.928	7.94
		331	2.282	2.218	9.06
		412	2.841	2.776	11.4
		506	3.489	3.424	13.7

[1] Calculated by compiler.

Henry's law is not obeyed.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave was used in which the cell was charged with ethylene and water and rocked for 45 min at constant temperature. The cell was kept at rest for 15 min to allow for phase separation. The water solution was sampled and the sample was fed into an analytical train. A 50 cm^3 sample was fed into an evacuated, jacketed flask. After equilibrium was established in the flask the pressure was measured by a mercury manometer. The vapor was completely displaced into a second flask by using mercury. A second stripping operation was obtained by draining the mercury from the first flask. The solubility was based on the sum of the two stripped quantities.

SOURCE AND PURITY OF MATERIALS:

1. Ethene analyzed as 99.2% pure with nitrogen the major impurity.
2. Water was distilled and degassed.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 2% at high pressures

$\delta x_1/x_1$ = ± 4% at the lowest pressure (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Davis, J.E.; McKetta, J.J.

J. Chem. Eng. Data 1960, *5*, 374-375.

VARIABLES: T/K = 310.9-394.3

P/MPa = 0.12-3.74, (1.16-36.9 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

		Total Pressure		Partial Pressure	Ethene Mole
t/F	^1T/K	P/psia	^1P/MPa	$^1p_1$/MPa	Fraction, 10^4x_1
220	377.59	59	0.4068	0.2901	1.28
		130	0.8963	0.7797	3.61
		198	1.365	1.249	5.41
		229	1.579	1.462	6.47
		269	1.855	1.738	7.49
		416	2.868	2.752	12.0
		527	3.634	3.519	14.9
250	394.26	116	0.7998	0.5950	2.68
		195	1.344	1.140	5.14
		276	1.903	1.698	8.10
		354	2.441	2.236	10.3
		367	2.530	2.326	10.3
		543	3.744	3.539	15.6

[1] Calculated by compiler.

Henry's law is not obeyed.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave was used in which the cell was charged with ethylene and water and rocked for 45 min at constant temperature. The cell was kept at rest for 15 min to allow for phase separation. The water solution was sampled and the sample was fed into an analytical train. A 50 cm^3 sample was fed into an evacuated, jacketed flask. After equilibrium was established in the flask the pressure was measured by a mercury manometer. The vapor was completely displaced into a second flask by using mercury. A second stripping operation was obtained by draining the mercury from the first flask. The solubility was based on the sum of the two stripped quantities.

SOURCE AND PURITY OF MATERIALS:

1. Ethene analyzed as 99.2% pure with nitrogen the major impurity.

2. Water was distilled and degassed.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 2% at high pressures

$\delta x_1/x_1$ = ± 4% at the lowest pressure (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Davis, J.E.; McKetta, J.J.

J. Chem. Eng. Data 1960, *5* , 374-375.

VARIABLES: T/K = 310.9-394.3

P/kPa = 101.3, 344.6

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/F	[1]T/K	Total Pressure P/psia	 [1]P/kPa	[1]Partial Pressure p_1/kPa	Ethene Mole Fraction, $10^4 x_1$
100	310.93	14.7	101.325	94.77	0.64
130	327.59	14.7	101.325	86.03	0.42
160	344.26	14.7	101.325	68.67	0.37
190	360.93	14.7	101.325	36.88	0.18
100	310.93	50	344.65	338.09	2.30
130	327.93	50	344.65	329.35	1.65
160	344.26	50	344.65	311.99	1.35
190	360.93	50	344.65	280.20	1.30
220	377.59	50	344.65	227.98	1.10
250	394.26	50	344.65	139.75	0.70

[1]Calculated by compiler.

These *smoothed* data have been taken directly from the paper; additional smoothed data also available at higher pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave was used in which the cell was charged with ethylene and water and rocked for 45 min at constant temperature. The cell was kept at rest for 15 min to allow for phase separation. The water solution was sampled and the sample was fed into an analytical train. A 50 cm^3 sample was fed into an evacuated, jacketed flask. After equilibrium was established in the flask the pressure was measured by a mercury manometer. The vapor was completely displaced into a second flask by using mercury. A second stripping operation was obtained by draining the mercury from the first flask. The solubility was based on the sum of the two stripped quantities.

SOURCE AND PURITY OF MATERIALS:

1. Ethene analyzed as 99.2% pure with nitrogen the major impurity.
2. Water was distilled and degassed.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

17

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bradbury, E.J.; McNulty, D.;
Savage, R.L.; McSweeney, E.E.
Ind. Eng. Chem. 1952, *44*, 211-212.

VARIABLES: T/K = 308.15-379.15
P/MPa = 0.46-53.1, (4.55-524 atm)

PREPARED BY:
W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Total Pressure P/atm	[1]P/MPa	[2]Ethene Partial Pressure, p_1/MPa	Solubility s/g(100g)$^{-1}$	Ethene Mole Fraction, x_1
35	308.15	8.3	0.841	0.835	0.084	0.000539
		8.8	0.902	0.896	0.093	0.000597
		20.4	2.07	2.06	0.197	0.00126
		35.0	3.55	3.54	0.307	0.00197
		35.6	3.61	3.60	0.321	0.00206
		69.0	6.99	6.99	0.460	0.00295
		69.0	6.99	6.99	0.475	0.00304
		147.0	14.9	14.9	0.542	0.00347
		194.0	19.7	19.7	0.593	0.00379
		220.0	22.3	22.3	0.607	0.00388
		236.0	23.9	23.9	0.621	0.00397
		265.0	26.9	26.8	0.637	0.00407
		272.0	27.6	27.6	0.647	0.00414
		293.0	29.7	29.7	0.651	0.00416
		297.0	30.1	30.1	0.654	0.00418
		318.0	32.2	32.2	0.665	0.00425
		349.0	35.4	35.4	0.668	0.00427
		392.0	39.7	39.7	0.696	0.00445

[1] Calculated by compiler.

[2] Ethene partial pressure was calculated by compiler based on the vapor pressure of water.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave equipped with a temperature controller, pressure tester and burette system for measuring the volumes of gas and solvent was used. A mercury pump provided pressure as required. Ethylene was compressed in a storage reservoir and supplied to the autoclave through a needle valve. After equilibration in the autoclave a saturated sample was depressured to atmospheric pressure and 298.15 K. Volumes of gas and liquid were obtained. Corrections were made for the residual ethene in the water and non-ideality of the gas. The Solubility is reported as a mass of gas.

SOURCE AND PURITY OF MATERIALS:

1. Ethene from Ohio Chemical Company was of 99.5% purity.
2. Water was distilled, and boiled for deaeration.

ESTIMATED ERROR:

δT/K = ± 0.1
$\delta P/P$ = ± 0.25%
$\delta s/s$ = ± 2%

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bradbury, E.J.; McNulty, D.;

Savage, R.L.; McSweeney, E.E.

Ind. Eng. Chem. 1952, *44*, 211-212.

VARIABLES: T/K = 308.15-379.15

P/MPa = 0.46-53.1, (4.55-524 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/C	T/K	Total Pressure P/atm	[1]P/MPa	[2]Ethene Partial Pressure, p_1/MPa	Solubility s/g $(100g)^{-1}$	Ethene Mole Fraction, x_1
35	308.15	448.0	45.4	45.4	0.720	0.00460
		510.0	51.7	51.7	0.740	0.00473
55	328.15	4.75	0.481	0.466	0.043	0.000276
		7.9	0.800	0.785	0.063	0.000404
		14.8	1.50	1.48	0.111	0.000712
		28.9	2.93	2.91	0.209	0.00134
		55.4	5.61	5.60	0.339	0.00217
		112.0	11.3	11.3	0.460	0.00295
		169.0	17.1	17.1	0.527	0.00337
		219.0	22.2	22.2	0.563	0.00360
		344.0	34.9	34.8	0.622	0.00398
		404.0	40.9	40.9	0.660	0.00422
		443.0	44.9	44.9	0.688	0.00440
		490.0	49.6	49.6	0.695	0.00444
		524.0	53.1	53.1	0.713	0.00456
75	348.15	4.55	0.461	0.422	0.032	0.000205

[1] Calculated by compiler.

[2] Ethene partial pressure was calculated by compiler based on the vapor pressure of water.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave equipped with a temperature controller, pressure tester and burette system for measuring the volumes of gas and solvent was used. A mercury pump provided pressure as required. Ethylene was compressed in a storage reservoir and supplied to the autoclave through a needle valve. After equilibration in the autoclave a saturated sample was depressured to atmospheric pressure and 298.15 K. Volumes of gas and liquid were obtained. Corrections were made for the residual ethene in the water and non-ideality of the gas. The Solubility is reported as a mass of gas.

SOURCE AND PURITY OF MATERIALS:

1. Ethene from Ohio Chemical Company was of 99.5% purity.
2. Water was distilled, and boiled for deaeration.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta P/P$ = ± 0.25%

$\delta s/s$ = ± 2%

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bradbury, E.J.; McNulty, D.;

Savage, R.L.; McSweeney, E.E.

Ind. Eng. Chem., 1952, *44*, 211-212.

VARIABLES: T/K = 308.15-379.15

P/MPa = 0.46-53.1, (4.55-524 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/C	T/K	Total Pressure P/atm	Total Pressure [1]P/MPa	[2]Ethene Partial Pressure, p_1/MPa	Solubility s/g (100g)$^{-1}$	Ethene Mole Fraction, x_1
75	348.15	15.7	1.59	1.55	0.099	0.000635
		28.6	2.90	2.86	0.178	0.00114
		55.8	5.65	5.62	0.302	0.00194
		111.0	11.2	11.2	0.455	0.00291
		121.0	12.3	12.2	0.467	0.00299
		122.0	12.4	12.3	0.472	0.00302
		174.0	17.6	17.6	0.527	0.00337
		228.0	23.1	23.1	0.566	0.00362
		310.0	31.4	31.4	0.628	0.00402
		382.0	38.7	38.7	0.667	0.00426
		440.0	44.6	44.5	0.700	0.00448
		518.0	52.5	52.4	0.728	0.00465
104	377.15	27.7	2.81	2.69	0.160	0.00103
101	374.15	75.0	7.60	7.49	0.410	0.00263
104	377.15	149.0	15.1	15.0	0.536	0.00343
106	379.15	256.0	25.9	25.8	0.632	0.00404
102	375.15	362.0	36.7	36.6	0.678	0.00434
102	375.15	433.0	43.9	43.8	0.707	0.00452

[1] Calculated by compiler.

[2] Ethene partial pressure was calculated by compiler based on the vapor pressure of water.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A rocking autoclave equipped with a temperature controller, pressure tester and burette system for measuring the volumes of gas and solvent was used. A mercury pump provided pressure as required. Ethylene was compressed in a storage reservoir and supplied to the autoclave through a needle valve. After equilibration in the autoclave a saturated sample was depressured to atmospheric pressure and 298.15 K. Volumes of gas and liquid were obtained. Corrections were made for the residual ethene in the water and non-ideality of the gas. The Solubility is reported as a mass of gas.

SOURCE AND PURITY OF MATERIALS:

1. Ethene from Ohio Chemical Company was of 99.5% purity.
2. Water was distilled, and boiled for deaeration.

ESTIMATED ERROR:

δT/K = ± 0.1
$\delta P/P$ = ± 0.25%
$\delta s/s$ = ± 2%

REFERENCES:

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COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Ethane; C_2H_6; [74-84-0]

3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Anthony, R.G.; McKetta, J.J.

J. Chem. Eng. Data 1967, *12*,

21-28.

VARIABLES:

T/K = 310.9 - 410.9
P/MPa = 3.47 - 34.60
y_1/mole fraction = 0 - 1

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Temp.	Pressure		Gas Phase Mole Fraction			Liquid Phase Mole Fraction	
			Hydrocarbon Dry Basis		Water in	Ethane	Ethene
°F, (^{1}K)	psia	^{1}MPa	Ethane, y_2	Ethene, y_1	Gas, 10^3 y_3	10^3 x_2	10^3 x_1
100 ± 0.1 (310.93 ± 0.06)	503.2	3.469	0.2741	0.7251	2.320	0.1993	1.2756
	503.2	3.469	0.4033	0.5967	2.139	0.2520	1.0820
	504.2	3.476	0.4517	0.5483	2.159	0.2905	0.9493
	503.7	3.429	0.8154	0.1845	1.817	0.5616	0.3692
	995.7	6.865	0.7308	0.2692	0.7846	0.589	0.8030
	1000.7	6.900	0.9205	0.0792	0.6778	0.761	0.2007
	1000.7	6.900	0.2387	0.7613	1.264	0.238	2.162
220 ± 0.3 (377.59 ± 0.17)	503.9	3.474	0.2201	0.7799	39.19	0.0980	0.9790
	503.2	3.469	0.2115	0.7885	37.75	0.0920	0.9090
	500.7	3.452	0.3284	0.6716	40.58	0.1289	0.7982
	501.7	3.459	0.5122	0.4878	38.89	0.2194	0.5666
	504.7	3.480	0.8921	0.1079	37.59	0.3723	0.1269
	1002.2	6.910	0.6066	0.3934	20.49	0.425	0.9597
	1005.2	6.931	0.8357	0.1643	20.32	0.5783	0.3698
	1499.2	10.337	0.4925	0.5075	15.15	0.4396	1.4684
	1004.2	6.924	0.6068	0.3932	20.17	0.3593	0.9107
	1491.2	10.281	0.6525	0.3475	14.77	0.5653	0.9977
	1008.7	6.995	0.1481	0.8519	22.07	0.1122	1.852
	1499.2	10.337	0.1943	0.8057	16.44	0.1901	2.3379

[1] Calculated by Compiler.
It was shown that Henry's law was obeyed for both gas components for the complete pressure range to 4000 psia.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a high pressure cell mounted in a thermostat and equipped for mixing and pressure measurement. A water analyzer was used for the water vapor content of the vapor phase. The water phase was sampled and analyzed by means of an absolute manometer and an Orsat gas burette. To maintain equilibrium in the cell during sampling, a volume of mercury was injected into the cell equal to that of the saturated solution withdrawn. The hydrocarbon was desorbed at low pressure in the gas burette at constant temperature, and then the gas volume and pressure was determined. The gas was also analyzed.

Details are given in Ref. 1 and 2.

SOURCE AND PURITY OF MATERIALS:

1. Ethene minimum purity 99.3%.
2. Ethane minimum purity 99.1%.
3. Water was distilled and deaerated.

ESTIMATED ERROR:

δT/K = ± 0.1
$\delta P/P$ = ± 0.2%
$\delta x/x$ = ± 5% (Authors)
$\delta y/y$ = ± 2% - 5%

REFERENCES:

1. Wehe, A.H.; McKetta, J.J.
   J. Chem. Eng. Data 1961, *6*, 167.

2. Wehe, A.H.; McKetta, J.J.
   Anal. Chem. 1961, *33*, 291.

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COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Ethane; C_2H_6; [74-84-0] 3. Water; H_2O; [7732-18-5]	Anthony, R.G.; McKetta, J.J. *J. Chem. Eng. Data* 1967, *12*, 21-28.
VARIABLES:	**PREPARED BY:**
T/K = 310.9 - 410.9 P/MPa = 3.47 - 34.60 y_1/mole fraction = 0 - 1	W. Hayduk

EXPERIMENTAL VALUES:

...continued

Temp.	Pressure		Gas Phase Mole Fraction			Liquid Phase Mole Fraction	
			Hydrocarbon Dry Basis		Water in	Ethane	Ethene
°F, ([1]K)	psia	[1]MPa	Ethane, y_2'	Ethene, y_1'	Gas, $10^3\ y_3$	$10^3\ x_2$	$10^3\ x_1$
100 ± 0.1	1080.2	7.448	0.9906	0.0094	0.7017	0.8810	0.0030
(310.93	1503.2	10.364	0.9460	0.0540	0.6809	0.7531	0.2452
± 0.06)	1486.2	10.247	0.8676	0.2324	0.7886	0.7663	0.4087
	1521.2	10.488	0.6560	0.3440	0.9710	0.5472	1.1368
	1505.2	10.378	0.2423	0.7577	1.383	0.2517	2.417
	1994.2	13.749	0.2570	0.7430	1.201	0.2550	2.4870
	1513.2	10.433	0.2701	0.7299	1.215	0.2463	2.417
	1992.2	13.736	0.2639	0.7361	1.154	0.2932	2.5018
	1992.2	13.784	0.4227	0.5773	0.8641	0.4275	1.9589
	1975.2	13.618	0.8491	0.1509	0.6238	0.7694	0.5006
	3001.7	20.696	0.8324	0.1676	0.644	1.099	0.6561
160 ± 0.2	2010.2	13.860	0.7958	0.2042	3.171	0.676	0.6556
(344.26	1519.2	10.474	0.7860	0.2140	3.429	0.651	0.6098
± 0.11)	2010.2	13.860	0.7830	0.2170	5.108	0.5644	0.4624
	502.2	3.463	0.7740	0.2260	10.24	0.3508	0.2671
	2015.2	13.894	0.5472	0.4528	3.820	0.468	1.4237
	1504.2	10.371	0.5268	0.4732	4.393	0.437	1.2906
	997.7	6.879	0.5350	0.4650	5.727	0.3645	1.105
	502.2	3.463	0.5281	0.4719	0.916	0.2386	0.6212
	1999.2	13.784	0.2975	0.7025	3.832	0.271	2.1715
	1514.2	10.440	0.3103	0.6897	4.937	0.474	2.3429
	995.7	6.865	0.3011	0.6989	6.050	0.2353	1.5887
	504.8	3.480	0.6917	0.3083	10.55	0.1494	0.9686
	1494.2	10.302	0.6781	0.3219	3.992	0.547	0.8966
	1990.2	13.722	0.8950	0.1050	2.641	0.788	0.2930
	1514.2	10.440	0.8996	0.1004	3.390	0.710	0.2809
	995.7	6.865	0.8933	0.1067	4.709	0.698	0.2252
	298.2	2.056	0.8851	0.1149	10.13	0.331	0.1144
279.5	504.7	3.480	0.2830	0.7170	109.4	0.1274	0.9286
(410.65)							
280 ± 0.1	1009.2	6.958	0.7560	0.2440	57.76	0.6166	0.6304
(410.93	503.7	3.473	0.7370	0.2630	108.01	0.3485	0.3275
± 0.06)	1500.2	10.343	0.5447	0.4553	43.44	0.6923	1.4217
	1002.2	6.910	0.5617	0.4383	58.66	0.4530	1.0230
	512.2	3.531	0.5490	0.4510	105.50	0.2718	0.5422
	1496.2	10.316	0.2732	0.7268	38.19	0.2889	2.3140
	1009.2	6.958	0.2651	0.7349	61.45	0.2405	1.7225
	1494.2	10.302	0.7540	0.2460	40.75	0.8060	0.8261
	1996.2	13.763	0.7496	0.2504	33.14	0.8862	0.9168

[1] Calculated by Compiler.

continued...

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COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethane; C_2H_6; [74-84-0]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Anthony, R.G.; McKetta, J.J.

J. Chem. Eng. Data 1967, *12*, 21-28.

VARIABLES:

T/K = 310.9 - 410.9
P/MPa = 3.47 - 34.60
y_1/mole fraction = 0 - 1

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

...continued

Temp.	Pressure		Gas Phase Mole Fraction			Liquid Phase Mole Fraction	
			Hydrocarbon Dry Basis		Water in	Ethane	Ethene
°F, (¹K)	psia	¹MPa	Ethane, y_2'	Ethene, y_1'	Gas, 10^3 y_3	10^3 x_2	10^3 x_1
100 ± 0.1 (310.93 ± 0.06)	5019.7	34.609	0.5488	0.4512	1.131	0.6492	1.9548
	4004.7	27.611	0.5588	0.4412	1.180	0.5823	1.7366
	3007.7	20.737	0.5655	0.4345	1.175	0.5748	1.5942
	5004.7	34.506	0.7414	0.2586	0.778	0.8257	1.0773
	4004.7	27.611	0.7485	0.2515	0.718	0.7635	1.0084
	3001.5	20.694	0.7441	0.2559	0.849	0.7061	0.9739
	5022.7	34.630	0.3731	0.6269	1.141	0.4198	2.6492
	4002.2	27.594	0.3653	0.6347	1.162	0.4133	2.4916
	3014.7	20.786	0.3636	0.6364	1.293	0.3804	2.3585
	5004.7	34.506	0.2696	0.7304	1.312	0.3236	3.0824
	3999.7	27.577	0.2687	0.7313	1.383	0.2927	3.0453
	3007.2	20.734	0.2729	0.7261	1.299	0.2588	2.7411
160 ± 0.2 (344.26 ± 0.11)	5008.7	34.534	0.2711	0.7289	3.976	0.3126	2.981
	4010.7	27.653	0.2658	0.7342	4.079	0.2900	2.7889
	3014.7	20.786	0.2697	0.7303	4.174	0.2781	2.5599
	5000.7	34.479	0.6779	0.3221	2.752	0.7477	1.155
	4004.7	34.506	0.6922	0.3078	2.736	0.7003	1.1637
	3008.7	20.744	0.7011	0.2989	3.004	0.6413	1.0637
	4998.7	34.465	0.8162	0.1838	2.643	0.8778	0.6710
	4002.7	27.598	0.8144	0.1856	2.580	0.8188	0.6822
	3007.7	20.737	0.8185	0.1815	2.623	0.7336	0.6163
	5000.0	34.474	0.9169	0.0831	2.442	0.9484	0.2627
	4009.7	27.646	0.9186	0.0814	2.325	0.9120	0.3120
	3004.7	20.717	0.9225	0.0775	2.518	0.8529	0.2771
219.9 ± 0.1 (377.54 ± 0.06)	4015.7	27.687	0.7270	0.2730	6.937	0.9076	1.2314
	3004.7	20.717	0.7247	0.2753	10.16	0.8025	1.0655
	2012.2	13.874	0.7245	0.2755	12.90	0.7052	0.8968
	4009.7	27.646	0.4401	0.5599	9.377	0.5428	2.4124
	3012.7	20.772	0.4392	0.5608	11.65	0.5067	2.1783
	2010.2	13.860	0.4374	0.5626	13.28	0.4499	1.856
	3997.7	27.563	0.2637	0.7363	11.22	0.3586	3.1954
	3008.7	20.744	0.2608	0.7392	12.44	0.3384	2.9466
	2012.2	13.874	0.2587	0.7413	14.10	0.2545	2.4448
	4014.7	27.680	0.9053	0.0947	7.568	1.093	0.3900
	3010.7	20.758	0.9112	0.0888	9.297	1.012	0.3680
	2011.2	13.867	0.9040	0.0960	11.10	0.9072	0.2998
280 ± 0.1 (410.93 ± 0.06)	3009.7	20.751	0.8325	0.1675	22.29	1.237	0.7372
	2009.2	13.853	0.8477	0.1523	27.31	1.0313	0.5967
	1503.2	10.364	0.8336	0.1664	34.88	0.8897	0.4923
	2993.7	20.641	0.5762	0.4238	27.17	0.8337	2.0783
	2000.2	13.791	0.5628	0.4372	32.11	0.7022	1.6548
	1506.7	10.388	0.5608	0.4392	41.20	0.5970	1.3830
	3002.2	20.699	0.3753	0.6247	29.43	0.5504	2.9936
	1999.2	13.784	0.3662	0.6338	35.84	0.4523	2.3747
	1504.7	10.375	0.3606	0.6393	44.13	0.3820	1.9190

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[1] Calculated by Compiler.

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COMPONENTS:	EVALUATOR:
(1) Ethene; C_2H_4; [74-85-1] (2) Electrolyte (3) Water; H_2O; [7732-18-5]	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA USA August 1992

CRITICAL EVALUATION:

AN EVALUATION OF THE SOLUBILITY OF ETHENE IN AQUEOUS ELECTROLYTE SOLUTIONS.

The solubility of a gas in an aqueous electrolyte solution often approximates the behavior pointed out by Sechenov over 100 years ago. It obeys the equation, $(1/c_2)\log(S^\circ/S) = k_{scc}$, where S°, S represent the solubility of the gas in pure water and in the aqueous electrolyte solution, respectively, c_2 is the concentration of the electrolyte, and k_{scc}, the Sechenov salt effect parameter when both the gas and electrolyte concentrations are in volume units.

Other gas and electrolyte measures lead to slightly different values of the salt effect parameter. The commonly used forms are:

$$k_{scc}/\mathrm{L\ mol^{-1}} = (1/(c_2/\mathrm{mol\ L^{-1}}))\ \log\ (c_1^\circ/\mathrm{mol\ L^{-1}})/(c_1/\mathrm{mol\ L^{-1}})$$

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

$$k_{scx}/\mathrm{L\ mol^{-1}} = (1/(c_2/\mathrm{mol\ L^{-1}}))\ \log\ (x_1^\circ/x_1)$$

$$k_{cmx}/\mathrm{kg\ mol^{-1}} = (1/(m_2/\mathrm{mol\ kg^{-1}}))\ \log\ (x_1^\circ/x_1)$$

where subscript 1 represents the non-electrolyte gas and subscript 2 the electrolyte.

The gas solubility ratio in pure water and electrolyte solution, c_1°/c_1 will be numerically the same using the Bunsen coefficient ratio, α°/α, or the Ostwald coefficient ratio, L°/L, as well as the mol L^{-1} ratio. The molality ratio, m_1°/m_1, is the same as the Kuenen coefficient ratio, S°/S, or the solvomolaity ratio, A°/A. The mole fraction ratio, x°/x, is the same as the inverse Henry's constant ratio, H/H°, when the Henry's constant is of the form, $(H/\mathrm{kPa}) = (p_1/\mathrm{kPa})/x_1$. The gas mol fractions are usually calculated treating each electrolyte ion as an entity. A more detailed description of these units and the interconversions among them is in Solubility Series volume 10, *NITROGEN*, pp. xxix - xliii.

A useful graphical test of salt effect data of either a particular worker or to compare different workers data is to put the Sechenov equation in the form:

$$\log S = \log S^\circ - k_s\ c_2$$

and plot log S *vs.* C_2, the linear slope will be the negative of the salt effect parameter in what ever set of units is used for S and c_2. Several such figures follow in this evaluation.

Two groups of workers have measured the solubility of ethene in several of the same aqueous electrolyte solutions. Unfortunately the two report values of the solubility of ethene in water at 298 K which differ by 2.6 percent. The difference makes for some difficulty in comparing their results by a plot of log L *vs.* c_2 as we have used here. There are data on 18 single electrolyte systems and 8 systems containing mixtures of two or three electrolytes. In general the data for ethene solubility in aqueous electrolyte solutions show better consistency than the data for less soluble gases reviewed in previous *Solubility Series* volumes.

Many workers use electrolyte ionic strength instead of volume concentration, and the salt effect parameter is given in electrolyte ionic strength. There are valid reasons to do this; however, we have used the electrolyte volume concentration in all of the single electrolyte solutions evaluations. The conversion to ionic strength basis requires dividing our result by the small whole number of one for 1-1 electrolytes, three for 1-2 and 2-1 electrolytes, four for 2-2 electrolytes and six for 1-3 and 3-1 electrolytes. The solubilities in the mixed electrolyte solutions are plotted as a function of ionic strength. The salt effect parameters in ionic strength are symbolized $k_{sI(c)c}$ and $k_{sI(m)m}$ for ionic strength in volume concentration and molality units, respectively.

The systems containing a single electrolyte are given in the order of the standard arrangement for inorganic compounds used by the U. S. National Institute of Science and Technology. The number before each system is the standard order number for the electrolyte cation.

I. Systems with a single electrolyte component.

There are problems with ethene that one does not see with less reactive or inert gases. Ethene may form complexes with some cations, e.g. silver, and the reaction of ethene with water may be catalyzed by certain cations, e.g. mercury. With the exception of silver nitrate we do not believe this to be a problem with the systems and temperatures reviewed here.

2(1) Ethene + Hydrochloric acid [7647-01-0] + Water

Yano, Suetaka, Umehara and Horiuchi (7) measured the solubility of ethene in water and four concentrations of HCl up to 1.520 mol L^{-1}. Their data (fig 1A) shows a slope of -0.046 with a standard deviation of the slope of 0.003. Thus, we take as the tentative salt effect parameter, k_{scc} = 0.046 L mol^{-1}.

2(2) Ethene + Perchloric acid [7601-90-3] + Water

Purlee and Taft (3) measured the solubility of ethene in water and six perchloric acid solutions up to 9.36 mol L^{-1} at 303 K. We have converted their Henry's constants to Ostwald coefficients and the results are in figure 1B. There is little doubt the acid salts out more at concentrations greater than 6.0 mol L^{-1} perchloric acid than at lower concentrations. The slope of -0.018 fits the data well up to 6.0 mol L^{-1} if one treats the value at 3.90 mol L^{-1} as an error. The tentative value is k_{scc} = 0.018 at 303.15 K.

2(3) Ethene + Sulfuric acid [7664-93-9] + Water

Yano *et al.* (7) measured the solubility of ethene in water and in sulfuric acid solutions of 0.258, 0.516 and 0.786 mol L^{-1} sulfuric acid at 298.15 K. The data are plotted in figure 1A. The slope of -0.123 with standard deviation of the slope of 0.002 gives the tentative salt effect parameter, k_{scc} = 0.123. In ionic strength this would be $k_{sI(c)c}$ = 0.041.

2(4) Ethene + nitric acid [7697-37-2] + Water

Both Yano, Suetaka, Umehara and Horiuchi (7) and Onda, Sada, Kobayashi, Kito and Ito (5) have studied this system at 298.15 K and 1 atm up to 1.81 mol L^{-1} nitric acid. Although their solubility values differ by only 2 - 3 percent, statistically their data do not accord well. The Onda *et al.* data has a slope of -0.003 with a standard deviation of 0.002, the Yano *et al.* data has a slope of -0.004 with a standard deviation of 0.004, and the combined data set has a slope of -0.002 with a standard deviation of 0.005. We choose as the tentative salt effect

COMPONENTS:	EVALUATOR:
(1) Ethene; C_2H_4; [74-85-1] (2) Electrolyte (3) Water; H_2O; [7732-18-5]	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA USA August 1992

CRITICAL EVALUATION:

parameter, k_{scc} = 0.002 at 298 K (fig 1A). One could use a salt effect parameter of zero and not be in any appreciable error over the 0 - 2 mol L^{-1} nitric acid concentration range at 298 K.

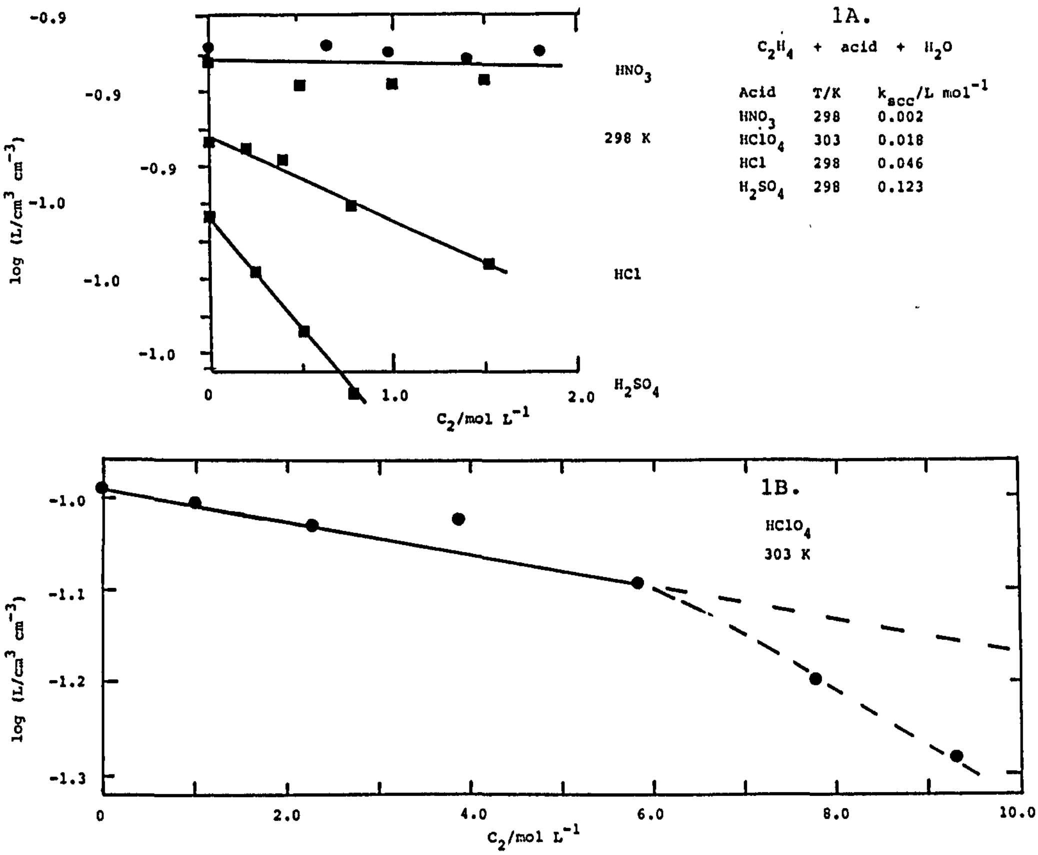

Figure 1. Log Ostwald *vs*. Electrolyte Concentration. C_2H_4 + Strong Acids + H_2O.

18(1) Ethene + Ammonium Nitrate [6484-52-2] + Water

Onda *et al*. (4) measured the solubility of ethene in water and five ammonium nitrate concentrations up to 3.8 mol L^{-1} at 1 atm (101.3 kPa) and 298 K. A plot of log *L* *vs*. c_2 is linear with slope -0.0513 and standard deviation 0.0005. The tentative salt effect parameter, k_{scc} = 0.0513 L mol^{-1} at 298.15 K.

36(1) Ethene + Copper chloride [7477-39-4] + Water

Yano *et al*. (7) measured the solubility of ethene in water and solutions of 0.500, 1.500 and 3.000 mol L^{-1} $CuCl_2$ at 298 K and 1 atm (101.3 kPa). The Sechenov plot is linear with slope -0.207 and standard deviation 0.002. The tentative salt effect parameter is k_{scc} = 0.207 L mol^{-1} at 298.15 K. As a function of ionic strength it is $k_{sI(c)c}$ = 0.069.

37(1) Ethene + Silver nitrate [7761-88-8] + Water

Clever, Baker and Hale (6) measured the solubility of ethene in dilute silver nitrate solution at 303.15 K and 95.75 kPa partial pressure. The system appears to strongly salt in because of formation of a silver-ethene complex. No salt effect parameter was calculated. Instead the authors estimated the aqueous solution concentration of free ethene from the solubility in potassium nitrate solutions of the same concentration, and assumed the remainder of the ethene in solution was in the form of the silver complex. The data treatment gives an equilibrium constant, K_{assn} = 76 L mol^{-1} for the reaction $Ag^+(aq) + C_2H_4(aq) \rightleftharpoons (C_2H_4)Ag^+(aq)$.

76(1) Ethene + Lanthanum chloride [10099-58-8] + Water

Morrison and Billett (2) measured the solubility of ethene in water and in 1.0 mol kg^{-1} $LaCl_3$ solutions at temperatures of 285.75, 303.15, 322.45 and 344.85 K. They did not report the solubility in the lanthanum chloride solution, but gave the salt effect parameters. They are:

T/K	285.75	303.15	322.55	344.85
k_{smm}/kg mol^{-1}	0.336	0.300	0.315	0.285
$k_{sI(m)m}$	0.056	0.050	0.053	0.048

One would expect a steady decrease in the salt effect parameter as temperature increases, thus one must question the values at 303.15 and 322.55 K which show the opposite trend. The results are classed as tentative, but use with caution.

96(1) Ethene + Barium chloride [14832-99-6] + Water

Onda *et al.* (4) measured the solubility of ethene in water and at nine concentrations of $BaCl_2$ up to 1.741 mol L^{-1} at 298.15 K and 1 atm (101.3 kPa) partial pressure. The Sechenov plot is linear with slope -0.273 and standard deviation 0.003. The tentative salt effect parameter is k_{scc} = 0.273 L mol^{-1} and in ionic strength $k_{sI(c)c}$ = 0.091.

98(1) Ethene + Lithium chloride [7447-41-8] + Water

Morrison and Billett (2) measured the solubility of ethene in pure water and in 1 molal LiCl solutions at four temperatures. They report the solubility in water and the salt effect parameter in molal units. Yano *et al.* (7) report the ethene solubility at concentrations of 0.500, 1.000 and 1.500 mol L^{-1} LiCl at 298.15 K. The Sechenov plot of their data is linear with slope -0.119 and standard deviation 0.006. The Morrison and Billett results were converted by the evaluator to volume units and are compared with the Yano *et al.* results below.

T/K	285.75	298.15	303.15	322.55	344.85
k_{scc} /L mol^{-1}	0.114	0.119	0.099	0.093	0.092
k_{smm} /kg mol^{-1}	0.104	0.108	0.089	0.082	0.083
k_{smx} /kg mol^{-1}	0.119	0.123	0.104	0.097	0.098

The two groups did not report any results at a common temperature. Their results do not lie on a smooth curve as a function of temperature. The Yano *et al.* value is based on more measurements so might be considered more reliable, but their data do scatter as shown by a standard deviation that is 5 per cent of the slope.

99(1) Ethene + Sodium chloride [7647-18-5] + Water

Onda *et al.* (4) measured the solubility of ethene in pure water and in seven NaCl solutions ranging up to 4.224 mol L^{-1} at 298.15 K, Yano *et al.* (7) measured the solubility in water and in three NaCl solutions up to 1.500 mol L^{-1} at 298.15 K and Morrison and Billett (2) measured the solubility in water and in 1 molal NaCl at temperatures of 285.75, 303.15, 322.55 and 344.85 K. The Sechenov plot of the Onda *et al.* data was linear with slope -0.139 and standard deviation 0.001, the Yano *et al.* data was linear and of slope 0.154 and standard deviation 0.003, the combined data set was linear with slope 0.137 and standard deviation 0.003. The evaluator has arbitrarily chosen the Onda *et al.* slope to represent the salt effect parameter (fig 2). The Morrison and Billett values were converted to volume units and are compared in the table below. Other representations of the salt effect parameter are also compared.

COMPONENTS:	EVALUATOR:
(1) Ethene; C_2H_4; [74-85-1] (2) Electrolyte (3) Water; H_2O; [7732-18-5]	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA USA August 1992

CRITICAL EVALUATION:

T/K	285.75	298.15	303.15	322.55	344.85
k_{scc}/L mol^{-1}	0.150	0.139	0.138	0.123	0.114
k_{smm}/kg mol^{-1}	0.140		0.127	0.114	0.101
k_{smx}/kg mol^{-1}	0.155		0.142	0.129	0.116

The agreement among the data sets is reasonable and the salt effect parameters are classed as tentative.

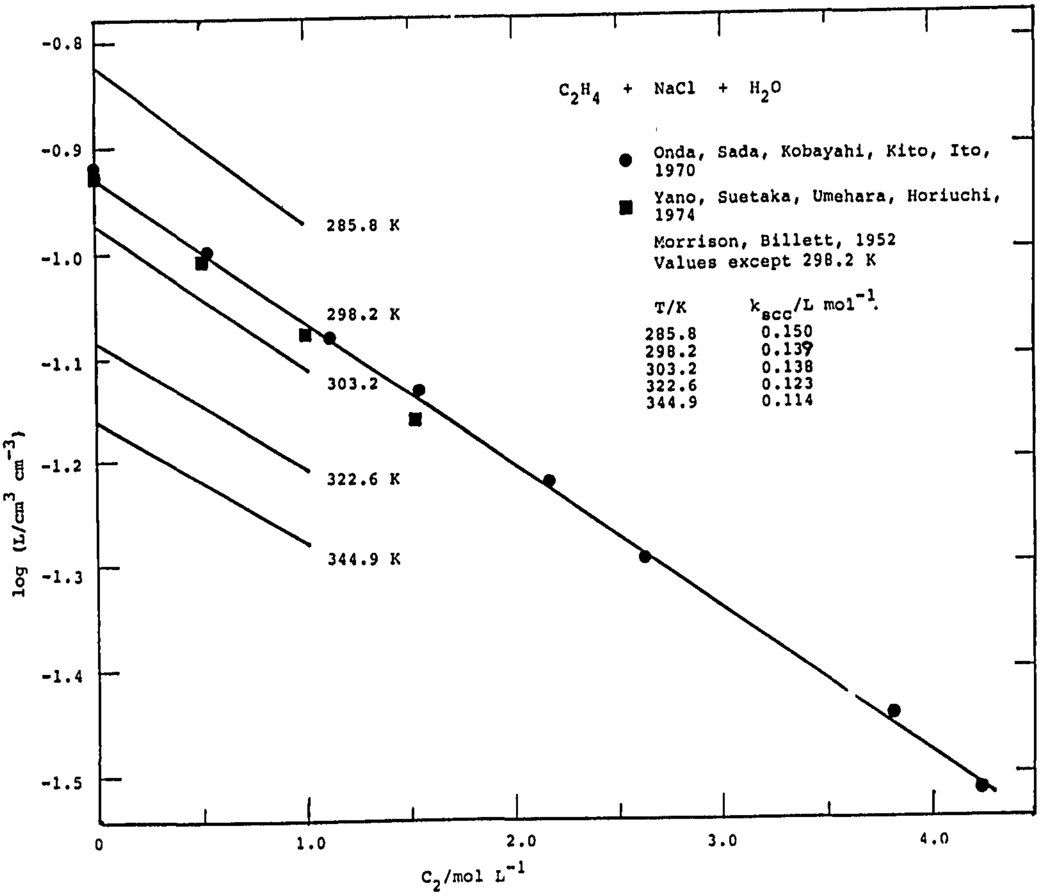

Figure 2. Log Ostwald *vs.* NaCl Concentration at Several Temperatures. The Morrison and Billett (2) lines are based on only two points, the solubility in water and in one mol L^{-1} NaCl (The compiler converted the author's molality value).

99(2) Ethene + Sodium bromide [7647-15-6] + Water

Yano *et al.* (7) measured the solubility of ethene in water and at 0.500, 1.000 and 1.500 mol L^{-1} NaBr at 298.15 K and 1 atm (101.3 kPa) partial pressure. The Sechenov plot is linear with a slope of -0.132 and standard deviation of 0.002. The tentative salt effect parameter is k_{scc} = 0.132 L mol^{-1}

99(3) Ethene + Sodium sulfite [7757-83-7] + Water

Two groups report data on this system. Onda *et al.* (4) report the solubility of ethene in water and five solutions up to 0.818 mol L^{-1} Na_2SO_3 at 298.15 K and 1 atm (101.3 kPa) partial pressure. The Sechenov plot is linear with slope -0.353 and standard deviation 0.013. Yano *et al.* (7) report the ethene solubility in water and three solutions up to 1.500 mol L^{-1} Na_2SO_3. The Sechenov plot is linear with slope -0.416 and standard deviation 0.002. The combined data sets have a slope of -0.416 and a standard deviation of 0.020. We have made the arbitrary decision to average the slopes of the two groups giving a weight of one to the slope of larger standard deviation and a weight of two to the other slope. Thus, the tentative salt effect parameter becomes k_{scc} = 0.395 L mol^{-1}. In terms of ionic strength this would be $k_{sI(c)c}$ = 0.132.

99(4) Ethene + Sodium sulfate [7732-18-5] + Water

Onda *et al.* (4) measured the solubility in water and five solutions up to 1.139 mol L^{-1} Na_2SO_4 at 298.15 K and 1 atm (101.3 kPa) partial pressure ethene. The Sechenov plot is linear with slope -0.394 and a standard deviation of 0.004. The tentative salt effect parameter is k_{scc} = 0.394 L mol^{-1} and in ionic strength its $k_{sI(c)c}$ = 0.132.

100(1) Ethene + Potassium chloride [7747-40-7] + Water

Yano *et al.* (7) measured the solubility of ethene in water and in 0.500, 1.000 and 1.500 mol L^{-1} KCl at 298.15 K at 1 atm (101.3 kPa) partial pressure. The Sechenov plot is linear with slope -0.136 and standard deviation 0.001. The tentative salt effect parameter is k_{scc} = 0.136 L mol^{-1}.

100(2) Ethene + Potassium bromide [7758-02-3] + Water

Yano *et al.* (7) measured the solubility of ethene in water and in 0.500, 1.000 and 1.500 mol L^{-1} KBr at 298.15 K at 1 atm (101.3 kPa) partial pressure. The Sechenov plot is linear with slope -0.118 and standard deviation 0.002. The tentative salt effect parameter is k_{scc} = 0.118 L mol^{-1}.

100(3) Ethene + Potassium iodide [7681-11-0] + Water

Morrison and Billett (2) measured the solubility of ethene in water and in 1 mol kg^{-1} KI at four temperatures. They report only the solubility in water and the salt effect parameter k_{smm}. The evaluator has converted the author's parameter to volume and mole fraction units. The results are summarized below. The 298.15 K values were interpolated from the author's data by the evaluator.

T/K	285.75	298.15	303.15	322.25	344.85
k_{scc} /L mol^{-1}	0.093	0.088	0.085	0.072	0.060
k_{smm} /kg mol^{-1}	0.070	0.064	0.061	0.050	0.036
k_{smx} /kg mol^{-1}	0.085	0.079	0.076	0.065	0.051

The values are classed as tentative.

100(4) Ethene + Potassium nitrate [7757-79-1] + Water

Clever, Baker and Hale (6) measured the solubility of ethene in water and aqueous KNO_3 at six concentrations up to 1.080 mol L^{-1}. Four of the measurements were made at concentrations of 0.115 mol L^{-1} or less. They show a much larger than normal salting out. Similar claims for unusual salt effects at low salt concentrations have been made by others, see *SDS Oxygen* volume (v. 10) salt effect evaluation for several examples. So far none of these claims have been substantiated. The unusual effect may be true, but for the present we suspect some systematic error. A small error in the solubility can cause a large error in the salt effect parameter at low salt concentrations. The solubility in water and in the 1.080 mol L^{-1} KNO_3 solution give a salt effect parameter of 0.133. It is a doubtful value.

II. Systems with multi-electrolyte components

These systems have been studied as a function of total ionic strength. In most of the systems a constant mole ratio between or among the electrolytes components is maintained at each total ionic strength. The evaluator has used the single electrolyte "ionic strength" salt effect

COMPONENTS:	EVALUATOR:
(1) Ethene; C_2H_4; [74-85-1] (2) Electrolyte (3) Water; H_2O; [7732-18-5]	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 August 1992

CRITICAL EVALUATION:

parameters to predict the mixed electrolyte parameter. The sum of the fraction of ionic strength from each electrolyte times its ionic strength salt effect parameter is the predicted salt effect parameter for the mixed electrolyte.

Ethene + Nitric acid [7697-37-2]
+ Sodium chloride [7647-14-5] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in four solutions containing a $NaCl/HNO_3$ ionic strength ratio of 0.615/0.385. A Sechenov plot of log *L vs. I* (*I* = ionic strength, mol L^{-1}) is linear and of slope -0.083 and standard deviation 0.003 (fig 3, line 2). The predicted salt effect parameter is (0.615)(0.139) + (0.385)(0.002) = 0.086 which is within a standard deviation of the observed constant. The data are classed as tentative.

Ethene + Ammonium Nitrate [6484-52-2]
+ Sodium chloride [7647-14-5] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in four solutions containing $NaCl/NH_4NO_3$ at an ionic strength ratio of 0.482/0.518. A Sechenov plot of log *L vs. I* (*I* = ionic strength, molality) is linear and of slope -0.090 and standard deviation 0.0009 (fig 3, line 3). The predicted salt effect parameter is (0.482)(0.139) + (0.518)(0.051) = 0.094 which is within 5 percent of the observed constant. The data are classed as tentative.

Ethene + Ammonium nitrate [6484-52-2]
+ Barium chloride [14832-99-6] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in four solutions containing $BaCl_2/NH_4NO_3$ at an ionic strength ratio of 0.540/0.460. A Sechenov plot of log *L vs. I* (*I* = ionic strength, mol L^{-1}) is linear and of slope -0.078 and standard deviation 0.005 (fig 3, line 1). The predicted salt effect parameter is (0.540)(0.091) + (0.460)(0.051) = 0.072 which is just over one standard deviation of the observed constant. The data are classed as tentative.

Ethene + Ammonium nitrate [6484-52-2] + Barium chloride [14832-99-6]
+ Sodium chloride [7647-14-5] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in four solutions containing $NH_4NO_3/BaCl_2/NaCl$ at an ionic strength ratio of 0.333/0.333/0.333. A Sechenov plot of log *L vs. I* (*I* = ionic strength, mol L^{-1}) is linear and of slope -0.089 and standard deviation 0.002 (fig 3, line 5). The predicted salt effect parameter is (0.333)(0.051) + (0.333)(0.091) + (0.333)(0.139) = 0.094 which is 5.6 percent larger than the observed constant. The data are classed as tentative.

Ethene + Sulfuric acid [7664-93-9]
+ Sodium sulfate [7757-82-6] + Water

Kobe and Kenton (1) report one measurement of the solubility of ethene in a mixture of 0.90 molal H_2SO_4 and 1.76 molal Na_2SO_4. The solution has a total ionic strength of 7.98 in molal units. The evaluator used an accepted solubility in water to calculate an ionic strength salt effect parameter, $k_{\mathrm{sI(m)m}}$ = 0.088. The value is classed tentative.

Ethene + Ammonium nitrate [6484-52-2]
+ Sodium sulfate [7757-82-6] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in seven solutions containing NH_4NO_3/Na_2SO_4 at an ionic strength ratio of 0.613/0.387. A Sechenov plot of log *L vs. I* (*I* = ionic strength, mol L^{-1}) is linear and of slope -0.079 and standard deviation 0.004 (fig 3, line 4). The predicted salt effect parameter is (0.613)(0.051) + (0.387)(0.132) = 0.082 which is within one standard deviation of the observed constant. The data are classed as tentative.

Ethene + Sodium hydrogen carbonate [144-55-8]
+ Sodium carbonate [497-19-8] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in three solutions containing $NaHCO_3/Na_2CO_3$ at an ionic strength ratio of 0.822/0.178. A Sechenov plot of log *L* *vs*. *I* (*I* = ionic strength, mol L^{-1}) is linear and of slope -0.195 and standard deviation 0.008 (fig 3, line 7). The single electrolyte salt effect parameters are not available to predict the constant. The result is classed as tentative.

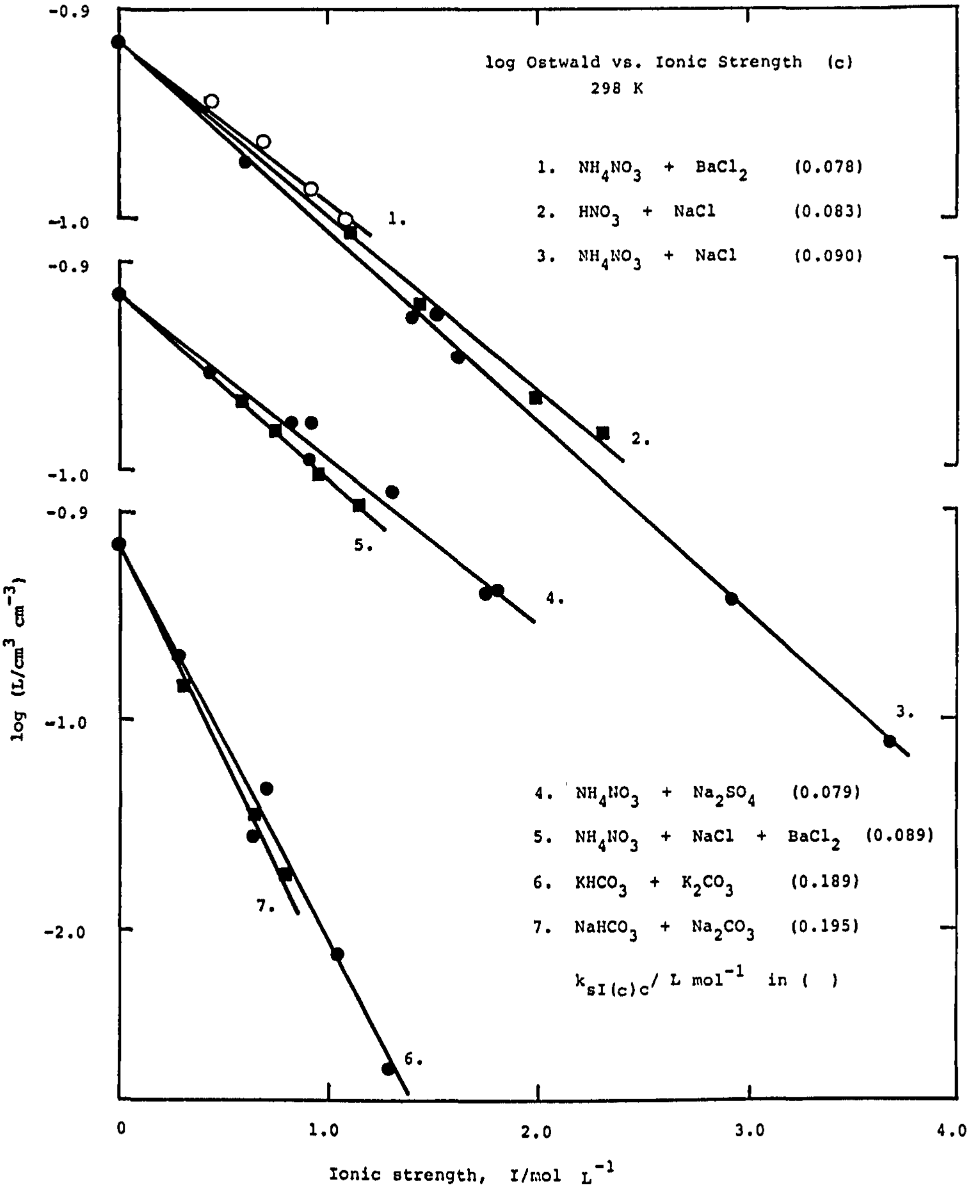

Figure 3. Log Ostwald *vs*. Ionic Strength, mol L^{-1}, 298.2 K. Mixed electrolytes. The electrolytes are kept at a constant ionic strength ratio in each set of measurements. In most cases the salt effect parameter calculated from the individual electrolyte parameters is within a standard deviation of the experimental parameter for the mixed electrolyte.

COMPONENTS: (1) Ethene; C_2H_4; [74-85-1] (2) Electrolyte (3) Water; H_2O; [7732-18-5]	EVALUATOR: H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 August 1992

CRITICAL EVALUATION:

Ethene + Potassium hydrogen carbonate [298-14-6]
+ Potassium carbonate [584-08-7] + Water

Onda, Sada, Kobayashi, Kito and Ito (5) measured the solubility of ethene in water and in five solutions containing $KHCO_3/K_2CO_3$ at an ionic strength ratio of 0.834/0.166. A Sechenov plot of log L *vs.* I (I = ionic strength, mol L^{-1}) is linear and of slope -0.189 and standard deviation 0.011 (fig 3, line 6). The single electrolyte salt effect parameters are not available to predict the constant. The result is classed as tentative.

REFERENCES

1. Kobe, K. A.; Kenton, F. H. *Ind. Eng. Chem., Anal. Ed.* 1938, *10*, 76.
2. Morrison, T. J.; Billett, F. *J. Chem. Soc.* 1952, 3819-22.
3. Purlee, E. I.; Taft, R. W. *J. Am. Chem. Soc.* 1956, *78*, 5811-12.
4. Onda, K.; Sada, E.; Kobayahi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 18-24.
5. Onda, K.; Sada, E.; Kobayahi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 137-42.
6. Clever, H. L.; Baker, E. R.; Hale, W. R. *J. Chem. Eng. Data* 1970, *15*, 411-13.
7. Yano, T.; Suetaka, T.; Umehara, T.; Horiuchi, A. *Kagaku Kogaku* 1974, *38*, 320-23.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Hydrochloric acid, nitric acid or sulfuric acid
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Suetaka, T.;
Umehara, T.; Horiuchi, A.

Kagaku Kogaku,

1974, *38*, 320-323.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Concentration of electrolyte /mol L^{-1}	Solubility of ethene /mmol L^{-1}
Hydrochloric acid; HCl; [7647-01-0]	
0.000	4.83
0.200	4.79
0.400	4.72
0.770	4.46
1.520	4.15
Nitric acid; HNO_3; [7697-37-2]	
0.500	4.72
1.061	4.72
1.520	4.75
Sulfuric acid; H_2SO_4; [7664-93-9]	
0.258	4.51
0.516	4.19
0.786	3.87

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus. Salt solution allowed to enter stirred absorption chamber. Pressure within absorption chamber adjusted to be as near atmospheric pressure as possible. Details in source and ref. 1.

SOURCE AND PURITY OF MATERIALS:

1. High purity sample, purity better than 99.5 mole per cent.
2. Special grade.
3. Distilled.

ESTIMATED ERROR:

Solubility = ±2% (Compiler)

REFERENCES:

1. Yano, T.; Suetaka, T.; Umehara, T.

   Nippon Kagaku Kaishi

   1972, *11*, 2194.

) -/

COMPONENTS:

1. Ethene, (Ethylene); C_2H_4; [74-85-1]
2. Nitric acid; HNO_3; [7697-37-2]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K.

J. Chem. Eng. Jpn. 1970, *3*, 137-142.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Concentration of nitric acid / mol l^{-1}	Ionic Strength* / mol l^{-1}	Bunsen coefficient,* α
298.15	0.646	0.646	0.1114
	0.657	0.657	0.1113
	0.979	0.979	0.1103
	1.408	1.408	0.1096
	1.810	1.810	0.1105

* quoted in original paper.

Pressure = 1 atmosphere = 1.01325×10^5Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Concentrated solution prepared by weighing, less concentrated solutions prepared by subsequent dilution. Concentration of acid estimated by titration. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, purity 99.6 mole per cent.
2. Analytical grade sample.
3. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.2$; $\delta\alpha = \pm 2\%$.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, Y.
   J. Chem. Eng. Jpn. 1970, *3*, 18.

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COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Perchloric acid; $HClO_4$; [7601-90-3]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Purlee, E.L.; Taft, R.W.

J. Amer. Chem. Soc. 1956, *78*, 5811-5812.

VARIABLES:

T/K = 303.15
P/kPa = 101.325
M_2/moles/l = 0-9.36

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Perchloric acid Conc. in Water w/mass%	M_2/mol dm^{-3}	Ethene Solubility expressed as Inverse of Henry's Constant $10^3 h$/mol (1 atm)$^{-1}$
30.0	303.15	0.0	0.0	4.11
		9.75	1.027	3.97
		20.80	2.34	3.74
		32.01	3.90	3.79
		43.60	5.85	3.24
		53.73	7.80	2.54
		60.71	9.36	2.10

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 200 cm^3 glass flask was connected to a pressure-measuring manometer by means of a horizontally -mounted spiral tube. The spiral tube permitted the flask to be shaken with an amplitude of up to 2 cm for equilibration. The solvent (80-125 cm^3) was deaerated in the flask. The change in pressure of a known volume of gas was measured from which the solubility was determined. The total volume of the apparatus was initially determined by weighing the apparatus filled with distilled water. The "distribution constant", h, was determined for pressures below 101.325 kPa. Method described in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson, purity 99.5%.
2. Perchloric acid was from Baker and was the CP grade.

ESTIMATED ERROR:

δT/K = ± 0.01

$\delta h / h$ = ± 0.02

REFERENCES:

1. Levy, J.B.; Taft, R.W.; Aaron, D.; Hammett, L.P. *J. Amer. Chem. Soc.* 1951, *73*, 3792.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Lanthanum chloride; $LaCl_3$; [10099-58-8]

(3) Water; H_2O; [7732-18-5]

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:

Temperature			Salt Effect Parameters		
t/°C	T/K	1/(T/K)	(1/c)log(S°/S)[1]	(1/m)log(S°/S)	(1/m)log(x°/x)
12.6	285.75	0.0035	0.112	0.336	0.359
30.0	303.15	0.0033	0.100	0.300	0.323
49.4	322.55	0.0031	0.105	0.315	0.338
71.7	344.85	0.0029	0.095	0.285	0.308

[1] For the 1-3 electrolyte the compiler changed to m = c/3 for m_2/mol kg^{-1} in the salt effect parameter.

The salt effect parameters were calculated from two measurements. The solubility of ethene in water, S°, and in the one molal salt solution, S. Only the solubility of the ethene 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.

Note that the first salt effect parameter above uses the author's notation with c in gram equivalents per kg water. The author's c would be better represented as $m_2((1/3)LaCl_3)$/mol kg^{-1} = 3 $m_2(LaCl_3)$/mol kg^{-1}, that is, it would have been better if the author had expressed the salt effect parameter in terms of moles of $LaCl_3$ per kg water rather than equivalents of $LaCl_3$ per kg water.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The degassed solvent flows in a thin film down an absorption helix containing the ethene 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) Ethene. Prepared from ethanol and phosphoric acid.

(2) Lanthanum chloride. "AnalaR" material.

(3) Water. No information given.

ESTIMATED ERROR:

$\delta k/kg^{-1}$ mol = 0.010

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene or ethylene; C_2H_4; [74-85-1] (2) Lithium chloride; LiCl; [7447-41-8] (3) Water; H_2O; [7732-18-5]	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:

Temperature			Salt Effect Parameters	
t/°C	T/K	1/(T/K)	$(1/m_2)\log(S°/S)$[1]	$(1/m_2)\log(x°/x)$
12.6	285.75	0.0035	0.104	0.119
30.0	303.15	0.0033	0.089	0.104
49.4	322.55	0.0031	0.082	0.097
71.7	344.85	0.0029	0.083	0.098

[1] The authors used (1/c)log(S°/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_2/mol kg^{-1}. The ethene solubility S is cm^3(STP) kg^{-1}.

The salt effect parameters were calculated from two measurements. The solubility of ethene in water, S°, and in the one molal salt solution, S. Only the solubility of the ethene 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 complier 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 ethene 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) Ethene. Prepared from ethanol and phosphoric acid.

(2) Lithium chloride. "AnalaR" material.

(3) Water. No information given.

ESTIMATED ERROR:

$\delta k/\text{kg}^{-1}\text{ mol} = 0.010$

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene, (Ethylene); C_2H_4; [74-85-1] 2. Sodium chloride; NaCl; [7647-14-5] 3. Water; H_2O; [7732-18-5]	Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 18-24.
VARIABLES: T/K = 298.15 P/kPa = 101.3	PREPARED BY: C.L. Young.

EXPERIMENTAL VALUES:

T/K	Conc. of salt / mol l^{-1}	Bunsen coefficient, α
298.15	0.524	0.0925
	1.123	0.0759
	1.538	0.0674
	2.170	0.0552
	2.619	0.0467
	3.805	0.0331
	4.224	0.0284

Pressure = 1 atmosphere = 1.01325 x 10^5Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solutions made up by weight and density measured but not reported in paper. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.6 mole per cent.
2. Analytical grade.
3. Distilled and degassed.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%.

(estimated by compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene or ethylene; C_2H_4; [74-85-1] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	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:

Temperature			Salt Effect Parameters	
t/°C	T/K	1/(T/K)	$(1/m_2)\log(S°/S)$[1]	$(1/m_2)\log(x°/x)$
12.6	285.75	0.0035	0.140	0.155
30.0	303.15	0.0033	0.127	0.142
49.4	322.55	0.0031	0.114	0.129
71.7	344.85	0.0029	0.101	0.116

[1] The authors used (1/c)log(S°/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_2/mol kg^{-1}. The ethene solubility S is cm^3(STP) kg^{-1}.

The salt effect parameters were calculated from two measurements. The solubility of ethene in water, S°, and in the one molal salt solution, S. Only the solubility of the ethene 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 ethene 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) Ethene. Prepared from ethanol and phosphoric acid.

(2) Sodium chloride. "AnalaR" material.

(3) Water. No information given.

ESTIMATED ERROR:

$\delta k/kg^{-1}$ mol = 0.010

REFERENCES:

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

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Lithium chloride, sodium chloride, sodium bromide or sodium sulfite
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Suetaka, T.;
Umehara, T.; Horiuchi, A.

Kagaku Kogaku,

<u>1974</u>, *38*, 320-323.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Concentration of electrolyte /mol L^{-1}	Solubility of ethene /mmol L^{-1}
Lithium chloride; LiCl; [7447-41-8]	
0.000	4.83
0.500	4.29
1.000	3.75
1.500	3.20
Sodium chloride; NaCl; [7647-14-5]	
0.500	4.01
1.000	3.41
1.500	2.83
Sodium bromide; NaBr; [7647-15-6]	
0.500	4.19
1.000	3.57
1.500	3.07
Sodium sulfite; Na_2SO_3; [7757-83-7]	
0.500	3.02
1.000	1.87
1.500	3.07

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus. Salt solution allowed to enter stirred absorption chamber. Pressure within absorption chamber adjusted to be as near atmospheric pressure as possible. Details in source and ref. 1.

SOURCE AND PURITY OF MATERIALS:

1. High purity sample, purity better than 99.5 mole per cent.
2. Special grade.
3. Distilled.

ESTIMATED ERROR:

Solubility = ±2% (Compiler)

REFERENCES:

1. Yano, T.; Suetaka, T.; Umehara, T.

   Nippon Kagaku Kaishi

   <u>1972</u>, *11*, 2194.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ammonium nitrate, sodium sulfite or sodium sulfate
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Onda, K.; Sada, E.;Kobayashi, T.; Kito, S.; Ito, K.

J. Chem. Eng. Jpn.

1970, *3*, 18-24.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Nitric acid, ammonium salt (Ammonium nitrate); NH_4NO_3; [6484-52-2]

Concentration of salt /mol L^{-1}	Bunsen coefficient, α
0.537	0.1050
1.937	0.0879
2.426	0.0839
2.793	0.0798
3.793	0.0713

Sulfurous acid, disodium salt (Sodium sulfite); Na_2SO_3; [7757-83-7]

Concentration of salt /mol L^{-1}	Bunsen coefficient, α
0.141	0.1011
0.267	0.0932
0.455	0.0770
0.747	0.0600
0.818	0.0592

Sulfuric acid, disodium salt (Sodium sulfate); Na_2SO_4; [7757-82-6]

Concentration of salt /mol L^{-1}	Bunsen coefficient, α
0.206	0.0916
0.448	0.0734
0.718	0.0587
0.944	0.0471
1.139	0.0392

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solutions made up by weight and density measured but not reported in paper. Equilibrium established betweem a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.6 mole per cert.
2. Analytical grade.
3. Distilled and degassed.

ESTIMATED ERROR:

$\delta T/K = \pm 0.2$; $\delta\alpha = \pm 2\%$.

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Potassium bromide, potassium chloride or copper chloride
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Suetaka, T.; Umehara, T.; Horiuchi, A.

Kagaku Kogaku,

1974, *38*, 320-323.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

Concentration of electrolyte /mol L^{-1}	Solubility of ethene /mmol L^{-1}
Potassium bromide; KBr; [7758-02-3]	
0.000	4.83
0.500	4.24
1.000	3.71
1.500	3.21
Potassium choride; KCl; [7747-40-7]	
0.500	4.14
1.000	3.52
1.500	3.03
Copper chloride; $CuCl_2$; [7477-39-4]	
0.500	3.73
1.000	2.33
3.000	1.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus. Salt solution allowed to enter stirred absorption chamber. Pressure within absorption chamber adjusted to be as near atmospheric pressure as possible. Details in source and ref. 1.

SOURCE AND PURITY OF MATERIALS:

1. High purity sample, purity better than 99.5 mole per cent.
2. Special grade.
3. Distilled.

ESTIMATED ERROR:

Solubility = ±2% (Compiler)

REFERENCES:

1. Yano, T.; Suetaka, T.; Umehara, T.

Nippon Kagaku Kaishi

1972, *11*, 2194.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene or ethylene; C_2H_4; [74-85-1] (2) Potassium iodide; KI; [7681-11-0] (3) Water; H_2O; [7732-18-5]	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:

Temperature			Salt Effect Parameters	
t/°C	T/K	1/(T/K)	$(1/m_2)\log(S°/S)$[1]	$(1/m_2)\log(x°/x)$
12.6	285.75	0.0035	0.070	0.085
30.0	303.15	0.0033	0.061	0.076
49.4	322.55	0.0031	0.050	0.065
71.7	344.85	0.0029	0.036	0.051

[1] The authors used (1/c)log(S°/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_2/mol kg^{-1}. The ethene solubility S is cm^3(STP) kg^{-1}.

The salt effect parameters were calculated from two measurements. The solubility of ethene in water, S°, and in the one molal salt solution, S. Only the solubility of the ethene 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 ethene 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) Ethene. Prepared from ethanol and phosphoric acid.

(2) Potassium iodide. "AnalaR" material.

(3) Water. No information given.

ESTIMATED ERROR:

$\delta k/\text{kg}^{-1}\,\text{mol} = 0.010$

REFERENCES:

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

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) Potassium nitrate; KNO_3; [7757-79-1]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Clever, H. L.; Baker, E. R.; Hale, W. R.

J. Chem. Eng. Data 1970, *15*, 411-3.

VARIABLES:

$T/T = 303.15$
$p_1/\text{kPa} = 101.3$
$c_2/\text{mol dm}^{-3} = 0 - 1.08$

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Potassium Nitrate	Ethene Solubility at 101.3 kPa		Solubility Ratio[b]
$t/^0\text{C}$	T/K^a	$c_2/$ mol dm^{-3}	$c_1/$ cm^3(STP) cm^{-3}	$10^3c_1/$ mol dm^{-3} [a]	c_1^0/c_1
30.0	303.15	0	98.2 ± 0.5 (5)	4.41	1.000
		0.0084	96.2 (1)	4.32	1.021
		0.0173	92.7 ± 1.0 (2)	4.17	1.059
		0.0280	89.6 ± 3.0 (2)	4.03	1.096
		0.115	84.2 ± 2.5 (3)	3.79	1.166
		0.525	73.0 ± 5.2 (4)	3.28	1.343
		1.08	71.0 ± 1.6 (3)	3.19	1.383

[a] Calculated by the compiler. Molar volume STP, $V/\text{cm}^3\ \text{mol}^{-1} = 22,246$.

[b] The solubility ratios give salt effect parameters, $k_{scc}/\text{dm}^3\ \text{mol}^{-1} = (1/(c_2/\text{mol dm}^{-3}))\log(c_1^0/c_1)$, that range from 1.43 at low KNO_3 concentration to 0.13 at high KNO_3 concentration. The values at low KNO_3 concentrations should be used with caution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and method were similar to that described by Markham and Kobe (ref 1).

Aqueous solutions of potassium nitrate were prepared, degassed by refuxing under reduced pressure, and transfered to the solubility apparatus without contact with atmospheric gases. The solubility of ethene at a total pressure of one atm (101.3 kPa) was measured by observing the volume of gas, saturated with water vapor, absorbed by an 88.5 cm^3 sample of degassed solution at 30 °C.

The solubilities were calculated for one atm partial pressure ethene assuming Henry's law.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co., Inc. Stated to have 99.5 % minimum purity.

(2) Potassium nitrate. Source not given. Reagent grade.

(3) Water. Distilled.

ESTIMATED ERROR:

$\delta T/\text{K} = \pm 0.05$
$\delta c_1/c_1 = \pm 0.01$

REFERENCES:

1. Markham, A. E.; Kobe, K. A. *J. Am. Chem. Soc.* 1941, *63*, 449.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) Silver nitrate; $AgNO_3$; [7761-88-8]

(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Clever, H. L.; Baker, E. R.; Hale, W. R.

J. Chem. Eng. Data 1970, *15*, 411-3.

VARIABLES:

$T/K = 303.15$
$p_1/kPa = 95.75$
$c_2/mol\ dm^{-3} = 0 - 0.0338$

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Silver Nitrate	Ethene Solubility at 0.945 atm (95.75 kPa)	
$t/^{0}C$	T/K^{a}	$c_2/$ mol dm^{-3}	$c_1/cm^3(STP)\ dm^{-3}$	$10^3c_1/mol\ dm^{-3a}$
30.0	303.15	0	92.8 ± 0.5 (5)	4.17
		0.0011	99.2 ± 0.2 (2)	4.46
		0.0028	104 ± 0.0 (2)	4.68
		0.0056	119 ± 2.0 (2)	5.35
		0.0113	149 ± 2.0 (2)	6.70
		0.0226	200 ± 2.0 (2)	8.99
		0.0338	242 (1)	10.88

[a] Calculated by the compiler. Molar volume STP, $V/cm^3\ mol^{-1} = 22,246$

The numbers in ( ) are the number of determinations.

Henry's constant for pure water is

$$C_2H_4(aq,\ c_1) \rightleftarrows C_2H_4(g,\ p_1) \qquad K_H = (p_1/kPa)/(c_1/mol\ dm^{-3}) = 23130$$

The authors combined the data above with other information to calculate the silver ion + ethene association constant

$$Ag^{+}(aq) + C_2H_4(aq) \rightleftarrows C_2H_4\text{-}Ag^{+}(aq) \qquad K_1 = 76.$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and method were similar to that described by Markham and Kobe (ref 1).

Aqueous solutions of Silver nitrate were prepared, degassed by refluxing under vacuum, and transfered to the solubility apparatus without contact with atmospheric gases. The solubility of ethene at a partial pressure of 0.945 atm (95.75 kPa) was measured by observing the volume of gas, saturated with water vapor, absorbed by an 88.5 cm^3 sample of degassed solution at 30.0 ^{0}C and a total pressure of 1 atm (101.3 kPa).

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co., Inc. Stated to have 99.5 % minimum purity.

(2) Silver nitrate. Reagent grade.

(3) Water. Distilled.

ESTIMATED ERROR:

$\delta T/K = \pm\ 0.05$
$\delta c_1/c_1 = \pm\ 0.01$

REFERENCES:

1. Markham, A. E.; Kobe, K. A. *J. Am. Chem. Soc.* 1941, *63*, 449.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene, (Ethylene); C_2H_4; [74-85-1] 2. Nitric acid; HNO_3; [7697-37-2] 3. Sodium chloride; NaCl; [7647-14-5] 4. Water; H_2O; [7732-18-5]	Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 137-142.
VARIABLES:	PREPARED BY:
T/K = 298.15 P/kPa = 101.3	C.L. Young

EXPERIMENTAL VALUES:

T/K	Concentration$^+$ of sodium chloride / mol l^{-1}	Concentration$^+$ of nitric acid / mol l^{-1}	Ionic * Strength / mol l^{-1}	Bunsen * coefficient, α
298.15	0.678	0.424	1.102	0.0903
	0.875	0.546	1.421	0.0834
	1.224	0.744	1.988	0.0754
	1.421	0.887	2.308	0.0722

* quoted in original paper.

\+ calculated from ionic strength and statement in paper that ratio of ionic strength of sodium chloride to total ionic strength was 1:0.6156.

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Concentrated solution prepared by weighing, less concentrated solutions prepared by dilution. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source and ref.(1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, purity 99.6 mole per cent.
2. Analytical grade sample.
3. Analytical grade sample.
4. No information given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.2$; $\delta\alpha = \pm 2\%$.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, Y.
J. Chem. Eng. Jpn. 1970, *3*, 18.

COMPONENTS:

1. Ethene, (Ethylene); C_2H_4; [74-85-1]
2. Carbonic acid, monosodium salt; (Sodium bicarbonate); $NaHCO_3$; [144-55-8]
3. Carbonic acid disodium salt; Na_2CO_3; [497-19-8]
4. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K.

J. Chem. Eng. Jpn. 1970, *3*, 137-142.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	Conc of sodium bicarbonate /mol l^{-1} $^+$	Conc of sodium carbonate /mol l^{-1} $^+$	Ionic strength* / mol l^{-1}	Bunsen coefficient, α^*
298.15	0.248	0.018	0.302	0.0951
	0.530	0.038	0.645	0.0824
	0.657	0.047	0.799	0.0774

* quoted in original paper.

\+ calculated from ionic strength and ratio of ionic strengths due to the two salts given in paper.

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Concentrated solution prepared by weighing, less concentrated solutions prepared by subsequent dilution. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, purity 99.6 mole per cent.
2. Analytical grade sample.
3. Analytical grade sample.
4. No information given.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, Y.

J. Chem. Eng. Jpn. 1970, *3*, 18.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) Sulfuric acid; H_2SO_4; [7664-93-9]

(3) Sodium sulfate; Na_2SO_4; [7757-82-6]

(4) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K: 298.15
p_1/kPa: 101.325 (1 atm)

PREPARED BY:

P. L. Long
H. L. Clever

EXPERIMENTAL VALUES:

Temperature t/°C	Temperature T/K	Solvent Volume V/cm^3	Ethene Volume Absorbed v_1/cm	Bunsen Coefficient $\alpha/\text{cm}^3\,(\text{STP})\,\text{cm}^{-3}\,\text{atm}^{-1}$	Ostwald Coefficient $L/\text{cm}^3\,\text{cm}^{-3}$
25	298.15	49.54	1.19		
		49.54	1.19	0.022	0.024

The solvent is a mixture of 800 g H_2O
200 g Na_2SO_4 (anhydrous)
40 ml H_2SO_4 (Conc., 36 normal)

Thus the molality of the solution is

$m_2/\text{mol kg}^{-1} = 0.90$ (H_2SO_4)

$m_3/\text{mol kg}^{-1} = 1.76$ (Na_2SO_4)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is described in detail in an earlier paper (1). The apparatus consists of a gas buret, a pressure compensator, and a 200 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 absorption bulb. The bulb is shaken until equilibrium is reached. The remaining gas is returned to the buret. The difference in the final and initial volumes is taken as the volume of gas absorbed.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Source not given. Purity stated to be 99+ per cent.

(2, 3) Sulfuric acid and sodium sulfate. Sources not given. Analytical grade.

(4) Water. Distilled.

ESTIMATED ERROR:

$\delta\alpha/\text{cm}^3 = \pm 0.001$ (authors)

REFERENCES:

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

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Sodium chloride, barium chloride or sodium sulfate
3. Nitric acid, ammonium salt (ammonium nitrate); NH_4NO_3; [6484-52-2]
4. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Onda, K.; Sada, E.;Kobayashi, T.; Kito, S.; Ito, K.

J. Chem. Eng. Jpn.

1970, *3*, 137-142.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

[1] Concentration of component 2 /mol L^{-1}	[1] Concentration of ammonium nitrate /mol L^{-1}	[2] Ionic strength /mol L^{-1}	[2] Bunsen coefficient, α /mole L^{-1}
Component 2:	sodium chloride; NaCl; [7647-14-5]		
0.298	0.193	0.600	0.0973
0.662	0.482	1.373	0.0824
0.777	0.834	1.611	0.0784
1.411	1.515	2.926	0.0603
1.777	1.909	3.686	0.0514
Component 2:	barium chloride; $BaCl_2$; [14832-99-6]		
0.077	0.198	0.430	0.1046
0.124	0.318	0.691	0.0998
0.164	0.419	0.911	0.0948
0.195	0.500	1.086	0.0915
Component2:	sodium sulfate; Na_2SO_4; [7757-82-6]		
0.055	0.261	0.425	0.1020
0.105	0.502	0.818	0.0965
0.117	0.554	0.904	0.0926
0.118	0.561	0.915	0.0964
0.168	0.801	1.306	0.0894
0.226	1.072	1.749	0.0798

[1] Calculated by compiler from ionic strength and ratio of ionic strength due to the two salts as given in paper.

[2] Quoted in original paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Concentrated solution prepared by weighing, less concentrated solutions prepared by dilution. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, purity 99.6 mole per cent.
2. Analytical grade sample.
3. Analytical grade sample.
4. No information given.

ESTIMATED ERROR:

δ*T*/K = ±0.2; δα = ±2%.

(estimated by compiler)

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, Y.

J. Chem Eng. Jpn. 1970, *3*, 18.

COMPONENTS:

1. Ethene, (Ethylene); C_2H_4; [74-85-1]
2. Carbonic acid, monopotassium salt, (Potassium bicarbonate); $KHCO_3$; [298-14-6]
3. Carbonic acid, dipotassium salt, (Potassium carbonate); K_2CO_3; [584-08-7]
4. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K.

   J. Chem. Eng. Jpn. 1970, *3*, 137-142.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	Conc of $^+$ potassium bicarbonate / mol l^{-1}	Conc of $^+$ potassium carbonate / mol l^{-1}	Ionic strength* / mol l^{-1}	Bunsen * coefficient α^*
298.15	0.239	0.016	0.286	0.0983
	0.538	0.036	0.645	0.0805
	0.587	0.039	0.704	0.0848
	0.873	0.058	1.046	0.0709
	1.084	0.072	1.299	0.0627

* quoted in original paper.

\+ calculated from ionic strength and ratio of ionic strengths due to the two salts given in paper.

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Concentrated solution prepared by weighing, less concentrated solutions prepared by subsequent dilution. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, purity 99.6 mole per cent.
2. Analytical grade sample.
3. Analytical grade sample.
4. No information given.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, Y.

   J. Chem. Eng. Jpn. 1970, *3*, 18.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene, (Ethylene); C_2H_4; [74-85-1] 2. Sodium chloride; NaCl; [7647-14-5] 3. Barium chloride; $BaCl_2$; [14832-99-6] 4. Nitric acid, ammonium salt, (ammonium nitrate); NH_4NO_3; [6484-52-2]. 5. Water; H_2O; [7732-18-5]	Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 137-142.
VARIABLES:	PREPARED BY:
Composition	C.L. Young.

EXPERIMENTAL VALUES:

T/K	Concentration⁺ of sodium chloride / mol l^{-1}	Concentration⁺ of barium chloride / mol l^{-1}	Concentration⁺ of ammonium nitrate / mol l^{-1}	Ionic * Strength / mol l^{-1}	Bunsen * coefficient, α
298.15	0.195	0.065	0.195	0.584	0.0985
	0.249	0.083	0.249	0.748	0.0955
	0.317	0.106	0.317	0.952	0.0911
	0.383	0.127	0.382	1.145	0.0881

* quoted in original paper.

\+ calculated from ionic strength and statement in paper that the ratio of ionic strength of three salts was 1:1:1

Pressure = 1 atmosphere = 1.01325×10^5Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Concentrated solution prepared by weighing, less concentrated solutions prepared by subsequent dilution. Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Details in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, purity 99.6 mole per cent.
2. Analytical grade sample.
3. Analytical grade sample.
4. Analytical grade sample.
5. No information given.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%.

(estimated by compiler).

REFERENCES:

Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, Y.

J. Chem. Eng. Jpn. 1970, *3*, 18.

COMPONENTS:	EVALUATOR:
(1) Ethene; C_2H_4; [74-85-1] (2) Organic Nonelectrolyte (3) Water; H_2O; [7732-18-5]	H. Lawrence Clever Department of Chemistry Emory University Atlanta, GA 30322 USA August 1992

CRITICAL EVALUATION:

AN EVALUATION OF THE SOLUBILITY OF ETHENE IN AQUEOUS ORGANIC NONELECTROLYTE SOLUTIONS.

Seven papers report ethene solubility data in eleven aqueous organic nonelectrolyte solutions. Most of the data were collected at 298 K and 1 atm (101.3 kPa) partial pressure of ethene. Only one system has been studied by more than one laboratory. There is no reliable way to evaluate these data. They are classed as tentative until confirmed by further experimental work.

Ethene + Methanol [57-56-1] + Water

Ethene + Ethanol [64-17-1] + Water

Ethene + 1-Propanol [71-23-8] + Water

Yano, Kidaka, Miyamoto and Murakami (3) measured the solubility of ethene in water, the pure alcohol and four mixtures of 0.2, 0.4, 0.6 and 0.8 mole fraction alcohol at 298.15 K by a volumetric method for each of the three systems. The solubility values in water and in the pure alcohols agree well with other data. The data sets are classed tentative.

Ethene + 2-Butanone [74-18-5] + Water

Yorizane, Masuoka, Ida and Ideda (1) measured the solubility of ethene in both phases of the two phase liquid formed by mixing 2-butanone, $CH_3COCH_2CH_3$ (methyl ethylketone), and water. The gas phase was stated to be greater than 99 percent ethene. Measuremenets are reported at five temperatures between 281 and 298 K and at ethene pressures between 1.013 and 5.238 MPa (10 - 51.7 atm). Ethene hydrates were observed to form at temperatures < 284 K and pressures > 1.175 MPa. The data are classed as tentative.

Ethene + 2-Amino-ethanol [141-43-5] + Water

Sada and Kito (4) report the solubility of ethene in 0 to 3.83 mol L^{-1} $H_2NCH_2CH_2OH$ at 288.15 K and 0 to 5.70 mol L^{-1} organic component at 298.15 K. The 2-amino-ethanol has little effect on the solubility of ethene in water. The Bunsen coefficient increases about 10 % as the organic component increases from 0 to 5.70 mol L^{-1} at 298.15 K. The data are classed as tentative.

Ethene + 2,2'-Iminobis-ethanol [111-42-2] + Water

Sada, Kumazawa and Butt (5) measured the solubility of ethene in 0 to 3.123 mol L^{-1} $(HOCH_2CH_2)_2NH$ at 298.15 K. The solubility (Bunsen coefficient) appears to go through a small maximum at 2.038 mol L^{-1} amine, but the change is only a percent or two more than experimental error. The data are classed tentative.

Ethene + 2,2',2''-Nitrilotris-ethanol [102-71-6] + Water

Sada *et al.* (5) Measured the solubility of ethene in 0 to 2.624 mol L^{-1} $(HOCH_2CH_2)_3N$ at 298.15 K. There appears to be a small increase in solubility (Bunsen coefficient) as the amine concenration increases, but the increase is only about twice the estimated error of the measurement. The data are classed as tentative.

Ethene + 1-Amino-2-propanol [78-96-6] + Water

Sada *et al.* (6) measured the solubility of ethene in 0 to 3.240 mol L^{-1} $CH_3CHOHCH_2NH_2$ at 298.15 K. The solubility (Bunsen coefficient) may go through a small maximum as the amine concentration increases, but the change is only about twice the magnitude of the estimated error of the measurement. The data are classed as tentative.

Ethene + 1,2-Ethanediamine [107-15-3] + Water

Sada *et al.* (5) measured the solubility of ethene in 0 to 3.683 mol L^{-1} $H_2NCH_2CH_2NH_2$ at 298.15 K. The solubility (Bunsen coefficient) appears to go through a small but definite maximum as the amine concentration increases. The data are classed as tenetative.

Ethene + 1,1'Iminobis-2-propanol [110-97-4] + Water

Sada *et al.* (6) measured the solubility of ethene in 0 to 2.982 mol L^{-1} $(CH_3CHOHCH_2)_2NH$ at 298.15 K. The solubility (Bunsen coefficient) appears to go through a small maximum as the amine concentration increases. The data are classed as tentative.

Ethene + 1-Methyl-2-pyrrolidione [872-50-4] + Water

Shenderei and Ivanovskii (2) report ethene solubilities at 273, 278, 288 and 293 K and 13.3 - 101.3 kPa in mixed solvents of 0 to 0.557 mole fraction water. Wu, Zeck, Langhorst and Knapp (7) report ethene solubility at 298.15 K and 1 bar in mixed solvent of 0.083 to 0.960 mole fraction water. Limited comparison can be made between the Henry's constants calculated by the compiler in atm/mol fraction for the two studies. The results are of similar magnitude, but the Wu *et al.* Henry constants appears to be larger at 0.544-0.557 mole fraction water and smaller at 0.083-0.104 mole fraction water than expected from the trends shown by the Shenderei and Ivanovskii values. There is no way to say which data set is the more reliable, both data sets are classed as tentative.

REFERENCES

1. Yorizane, M.; Masuoka, H.; Ida, S.; Ideda, T. *J. Chem Eng. Jpn.* 1947, *7*, 379-80.
2. Shenderei, E. R.; Ivanovskii, F. P. *Gaz. Prom.* 1962, *7*, 11 - 17.; *Khim. Prom.* 1963, *10*, 91-97.
3. Yano, T.; Kidaka, T.; Miyamoto, H.; Murakami, T. *Proc. Soc. Chem. Engrs. Japan (Osaka)* Oct 14, 1968, 89-90.
4. Sada, E.; Kito, S. *Kagaku Kogaku* 1972, *36*, 218-20.
5. Sada, E.; Kumazawa, H.; Butt, M. A. *J. Chem. Eng. Data* 1977, *22*, 277-78.
6. Sada, E. Kumazawa, H.; Butt, M. A. *J. Chem. Eng. Data* 1978, *23*, 161-63.
7. Wu, Z.; Zeck, S.; Langhorst, R.; Knapp, H. *Proc. Int. Conf. Coal, Gas and Air, Beijing, China* 1985, *1*, 209-19.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Methanol; CH_4O; [57-56-1]

3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Kidaka, T. Miyamoto, H.;

Murakami, T.

Proc. Soc. Chem. Engrs. Japan (Osaka),
Oct. 14, 1968, 89-90.

VARIABLES:

T/K = 298.15
P/kPa = 101.325
Mole Fraction Alcohol, x'_2 = 0-1

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	Mole Fraction Alcohol in Mixed Solvent/x'_2	Ethene solubility, x_1, for ^1P=101.325	$^2p_1$=101.325^1	^{2} Ostwald Coefficient L /cm^3 gas(cm^3 solvent)$^{-1}$
25.0	0.0 (water)	0.0000876	0.0000904	0.122
	0.2	0.000175	0.000186	0.200
	0.4	0.000416	0.000454	0.408
	0.6	0.000954	0.001074	0.825
	0.8	0.00219	0.00254	1.711
	1.0 (alcohol)	0.00408	0.00488	2.93

[1] Although not specifically stated in the paper, it is assumed that the mole fraction solubility, x, is for a total pressure of 101.325 kPa.

[2] The solubility corresponding to a gas partial pressure of 101.325 kPa was calculated by the compiler; Raoult's law was assumed to apply to the mixed solvent solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not given.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm\ 0.03$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethanol; C_2H_6O; [64-17-1]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Kidaka, T. Miyamoto, H.;
Murakami, T.
Proc. Soc. Chem. Engrs. Japan (Osaka),
Oct. 14, 1968, 89-90.

VARIABLES:

T/K = 298.15
P/kPa = 101.325
Mole Fraction Alcohol, $x_2' = 0\text{-}1$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	Mole Fraction Alcohol in Mixed Solvent, x_2'	Ethene solubility for: ^1P=101.325, x	Ethene solubility for: ^2p=101.325, x_1	^{2}Ostwald Coefficient L/cm^{3}gas cm^{-3}solvent
25.0	0.0 (water)	0.0000876	0.0000904	0.122
	0.2	0.000279	0.000291	0.270
	0.4	0.000847	0.000892	0.633
	0.6	0.00199	0.00212	1.22
	0.8	0.00351	0.00373	2.15
	1.0 (alcohol)	0.00558	0.00605	2.52

[1] Although not specifically stated in the paper, it is assumed that the mole fraction solubility, x, is for a total pressure of 101.325 kPa.

[2] The solubility corresponding to a gas partial pressure of 101.325 kPa was calculated by the compiler; Raoult's law was assumed to apply to the mixed solvent solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not given.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.03$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Propanol; C_3H_8O; [71-23-8]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Kidaka, T. Miyamoto, H.;
Murakami, T.
Proc. Soc. Chem. Engrs. Japan (Osaka),
Oct. 14, 1968, 89-90.

VARIABLES:

T/K = 298.15
P/kPa = 101.325
Mole Fraction Alcohol, x'_2 = 0-1

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	Mole Fraction Alcohol in Mixed Solvent, x'_2	Ethene solubility for: ^1P=101.325, x	^2p =101.325, x_1	^{2}Ostwald Coefficient L /cm^{3}gas(cm^3 solvent)$^{-1}$
25.0	0.0 (water)	0.0000876	0.0000904	0.122
	0.2	0.000603	0.000622	0.513
	0.4	0.00174	0.00179	1.068
	0.6	0.00323	0.00333	1.55
	0.8	0.00495	0.00509	1.95
	1.0 (alcohol)	0.00697	0.00717	2.36

[1] Although not specifically stated in the paper, it is assumed that the mole fraction solubility, x, is for a total pressure of 101.325 kPa.

[2] The solubility corresponding to a gas partial pressure of 101.325 kPa was calculated by the compiler; Raoult's law was assumed to apply to the mixed solvent solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not given.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.03$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Butanone (methyl ethylketone); C_4H_8O; [74-18-5]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yorizane, M.; Masuoka, H.;
Ida, S.; Ideda, T.

J. Chem. Eng. (Japan) <u>1947</u>, *7*, 379-380.

VARIABLES:

T/K = 281.15 - 298.15

P/MPa = 1.013 - 5.238

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Pressure		[1] Mole Percent Top Liquid Phase			[1] Mole Percent Bottom Liquid Phase		
t /C	[2]T/K	Atm	MPa	Ethene	MEK	Water	Ethene	MEK	Water
8.0	281.15	15.0	1.520	18.36	71.50	10.14	0.22	7.05	92.73
10.8	283.05	10.0	1.013	13.22	70.68	16.10	0.21	7.22	92.57
10.8	283.95	20.0	2.026	26.47	65.26	8.27	0.30	5.82	93.88
10.8	283.95	48.5	4.914	98.10	1.90	0	0.26	2.62	97.12
14.8	287.95	10.0	1.013	10.46	71.94	17.60	0.20	7.87	91.93
14.8	287.95	20.0	2.026	23.99	66.71	9.30	0.26	6.00	93.47
14.8	287.95	30.0	3.040	40.02	53.23	6.75	0.30	4.26	95.44
14.8	287.95	35.0	3.546	52.52	45.14	2.34	0.21	3.72	96.07
14.8	287.95	40.0	4.053	62.61	35.40	1.99	0.41	3.81	95.78
14.8	287.95	45.0	4.560	74.03	25.97	0	0.47	3.59	95.94
15.0	288.15	51.0	5.168	91.15	5.99	2.86	0.03	3.23	96.47

[1] This solubility is between a gas (ethene) phase, stated to be greater than 99% ethene and two separate, immiscible liquid phases with the compositions expressed as mole percent.

[2] Calculated by compiler.

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was described earlier (ref.1). The equilibrium cell was a Jerguson gauge of stainless steel with glass windows having an internal volume of 90 ml. Equilibrium was achieved by means of a gas recirculation pump. Samples of each phase were analyzed by means of a Shimadzu GC equipped with a peak integrator and a Porapack Q column. The concentrations of water vapor in the ethene were so low that they could not be detected.

At low temperatures (less than 11 °C) and high pressures (greater than 11.6 atm) ethylene hydrates were observed to form.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Specified purity 99.95%.
2. 2-Butanone. Specified purity 99.6%.
3. Water. Distilled.

ESTIMATED ERROR:

Accuracy: Not specified.

REFERENCES:

1. Yorizane, M.; Yoshimura, S.; Masuoka, H.

   Bull. Japan Petrol. Inst. <u>1972</u>, *14*, 105.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Butanone (methyl ethylketone); C_4H_8O; [74-18-5]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Yorizane, M.; Masuoka, H.;
Ida, S.; Ideda, T.

J. Chem. Eng. (Japan) 1947, *7*, 379-380.

VARIABLES:

T/K = 281.15 - 298.15

P/MPa = 1.013 - 5.238

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ....continued

		Pressure		[1] Mole Percent Top Liquid Phase			[1] Mole Percent Bottom Liquid Phase		
t/C	[2] T/K	Atm	MPa	Ethene	MEK	Water	Ethene	MEK	Water
20	293.15	10	1.013	8.80	70.39	20.81	0.15	7.07	92.78
20		20	2.026	18.72	68.38	12.90	0.21	5.92	93.87
20		30	3.040	36.66	56.73	6.61	0.35	4.90	94.75
20		35	3.546	44.08	50.69	5.23	0.39	4.41	95.20
20		40	4.053	55.78	39.69	4.53	0.38	3.98	95.64
20		45	4.560	52.25	44.80	2.95	0.41	3.49	96.10
20		50	5.066	75.76	22.65	1.59	0.39	3.04	96.57
25	298.15	20	2.026	20.16	64.63	15.21	0.27	6.13	93.60
25		35	3.546	36.76	54.42	8.82	0.30	4.06	95.64
25		40	4.053	47.93	47.42	4.65	0.33	3.65	96.02
25		45	4.560	51.97	43.86	4.17	0.33	3.62	96.05
25		51.7	5.238	71.52	26.90	1.58	0.36	3.35	96.29

[1] This solubility is between a gas (ethene) phase, stated to be greater than 99% ethene and two separate, immiscible liquid phases with the compositions expressed as mole percent.

[2] Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was described earlier (ref.1). The equilibrium cell was a Jerguson gauge of stainless steel with glass windows having an internal volume of 90 ml. Equilibrium was achieved by means of a gas recirculation pump. Samples of each phase were analyzed by means of a Shimadzu GC equipped with a peak integrator and a Porapack Q column. The concentrations of water vapor in the ethene were so low that they could not be detected.

At low temperatures (less than 11 °C) and high pressures (greater than 11.6 atm) ethylene hydrates were observed to form.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Specified purity 99.95%.
2. 2-Butanone. Specified purity 99.6%.
3. Water. Distilled.

ESTIMATED ERROR:

Accuracy: Not specified.

REFERENCES:

1. Yorizane, M.; Yoshimura, S.; Masuoka, H.

   Bull. Japan Petrol. Inst. 1972, *14*, 105.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene (Ethylene); C_2H_4; 2. 2-Aminoethanol, (monoethanolamine); C_2H_7NO; [141-43-5] 3. Water; H_2O; [7732-18-5]	Sada, E.; Kito, S. *Kagaku Kogaku* 1972, *36*, 218-20.
VARIABLES: T/K = 288.15, 298.15 P/kPa = 101.3	PREPARED BY: C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of monoethanolamine / mol l^{-1} (soln).	Bunsen coefficient,
288.15	0.0	0.1432
	0.9679	0.1450
	2.2273	0.1432
	2.8605	0.1437
	3.8283	0.1408
298.15	0.0	0.1111
	1.0049	0.1149
	1.9091	0.1161
	2.8337	0.1187
	4.2082	0.1218
	5.7019	0.1244

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium established between measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Concentration of amine determined by titration. Details in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.6 mole per cent.

2/3. Of satisfactory purity.

ESTIMATED ERROR:

$\delta T/K = \pm 0.2$; $\delta\alpha = \pm 2\%$.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.
J. Chem. Eng. Japan 1970, *3*, 18 and 137.

COMPONENTS:

1. Ethene (Ethylene); C_2H_4; [74-85-1]
2. 1,2-Ethanediamine, (Ethyldiamine); $C_2H_8N_2$; [107-15-3]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sada, E.; Kumazawa, H.; Butt, M.A.

J. Chem. Eng. Data 1977, *22*, 277-278.

VARIABLES:

$T/K = 293.15$

$P/kPa = 101.3$

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	Conc. of amine / mol l^{-1}	Bunsen coefficient, α
293.15	0.0	0.1111
	0.561	0.1153
	1.049	0.1184
	1.596	0.1196
	2.023	0.1187
	2.091	0.1199
	2.890	0.1186
	2.929	0.1185
	3.464	0.1145
	3.683	0.1124

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Concentration of amine determined by titration. Details in source and ref.(1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.8 mole per cent.
2. Reagent grade of guaranteed quality.
3. Distilled and degassed.

ESTIMATED ERROR:

$\delta T/K = \pm 0.2$; $\delta\alpha = \pm 2\%$.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 18.

COMPONENTS:

1. Ethene (Ethylene); C_2H_4; [74-85-1]
2. Ethanol, 2,2'-iminobis-, (Diethanolamine); $C_4H_{11}NO_2$; [111-42-2]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sada, E.; Kumazawa, H.; Butt, M.A.

J. Chem. Eng. Data 1977, *22*, 277-278.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of amine / mol l^{-1}	Bunsen coefficient α
298.15	0.00	0.1111
	0.949	0.1131
	1.540	0.1141
	2.038	0.1156
	2.442	0.1136
	2.895	0.1121
	2.977	0.1115
	3.123	0.1104

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Concentration of amine determined by titration. Details in source and ref.(1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.6 mole per cent.
2. Reagent grade of guaranteed quality.
3. Distilled and degassed.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K.

   J. Chem. Eng. Jpn. 1970, *3*, 18.

COMPONENTS:

1. Ethene (Ethylene); C_2H_4; [74-85-1]
2. Ethanol, 2,2',2''-nitrilotris-, (Triethanolamine); $C_6H_{15}NO_3$; [102-71-6]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sada, E.; Kumazawa, H.; Butt, M.A.;

J. Chem. Eng. Data 1977, *22*, 277-278.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.3$

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	Conc. of amine / mol l^{-1}	Bunsen coefficient, α
298.15	0.00	0.1111
	0.193	0.1131
	0.443	0.1138
	0.599	0.1156
	0.707	0.1161
	0.889	0.1165
	1.148	0.1163
	1.557	0.1150
	2.277	0.1100
	2.624	0.1053

Pressure = 1 atmosphere = 1.01325×10^5 Pa

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium established between a measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Concentration of amine determined by titration. Details in source and ref.(1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.6 mole per cent.
2. Reagent grade of guaranteed quality.
3. Distilled and degassed.

ESTIMATED ERROR:

$\delta T/K = \pm 0.2$; $\delta\alpha = \pm 2\%$.

(estimated by compiler).

REFERENCES:

1. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K.
J. Chem. Eng. Jpn. 1970, *3*, 18.

COMPONENTS:

1. Ethene (Ethylene); C_2H_4; [74-85-1]
2. 2-Propanol, 1-amino-, (Isopropanolamine); C_3H_9NO; [78-96-6]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sada, E.; Kumazawa, H.; Butt, M.A.

J. Chem. Eng. Data 1978, *23*, 161-163.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	Conc. of amine /mol l^{-1}	Bunsen coefficient, α
298.15	0.0	0.1111
	0.279	0.1145
	0.819	0.1155
	0.1319	0.1145
	2.175	0.1124
	2.301	0.1123
	2.802	0.1122
	3.240	0.1100

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium established between measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Concentration of amine determined by titration. Details in source and refs.(1) and (2).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.6 mole per cent.
2. Reagent grade of guaranteed quality.
3. Distilled and degassed.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%.

(estimated by compiler).

REFERENCES:

1. Sada, E.; Kumazawa, H.; Butt, M.A. *J.Chem.Eng. Data* 1977,*22*,277.
2. Onda, K.; Sada, E.; Kobayashi,T.; Kito, S.; Ito, K. *J.Chem.Eng. Jpn.* 1970, *3*, 18.

COMPONENTS:

1. Ethene (Ethylene); C_2H_4; [74-85-1]
2. 2-Propanol, 1,1′-aminobis- (Diisopropanolamine); $C_6H_{15}NO_2$; [110-97-4]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sada, E.; Kumazawa, H.; Butt, M.A.

J. Chem. Eng. Data 1978, *23*, 161-163.

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Conc. of amine / mol l^{-1}	Bunsen coefficient, α
298.15	0.0	0.1111
	0.236	0.1131
	0.290	0.1125
	0.550	0.1120
	1.048	0.1105
	1.467	0.1077
	2.127	0.1030
	2.982	0.1001

Pressure = 1 atmosphere = 1.01325×10^5 Pa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium established between measured volume of gas and a measured amount of gas-free liquid in a cell fitted with a magnetic stirrer. Amount of gas absorbed estimated from change in volume of gas. Concentration of amine determined by titration. Details in source and refs. (1) and (2).

SOURCE AND PURITY OF MATERIALS:

1. Commercial sample, minimum purity 99.6 mole per cent.
2. Reagent grade of guaranteed quality.
3. Distilled and degassed.

ESTIMATED ERROR:

δT/K = ±0.2; $\delta\alpha$ = ±2%

(estimated by compiler).

REFERENCES:

1. Sada, E.; Kumazawa, H.; Butt, M.A. *J. Chem. Eng. Data* 1977, *22*, 277.
2. Onda, K.; Sada, E.; Kobayashi, T.; Kito, S.; Ito, K. *J. Chem. Eng. Jpn.* 1970, *3*, 18.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4 ; [74-85-1] 2. 2-Pyrrolidinone, 1-methyl-, (N-methylpyrrolidinone); C_5H_9NO; [872-50-4] 3. Water; H_2O; [7732-18-5]	Shenderei, E.R.; Ivanovskii, F.P. *Gaz. Prom.* 1962, *7* , 11-17. Same paper also in: *Khim. Prom.* 1963, *10*,91-97.
VARIABLES: $T/K = 273-288$ $P/kPa = 101.3$ (1 atm) Water conc./mole fraction = 0-0.56	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

			Henry's constant		
t/C	T^1/K	water content in solvent, mole fraction	K/mm mercury (mole fraction)$^{-1}$	H^1/atm (mole fraction)$^{-1}$	[1]Mole Fraction Ethene,x_1
0	273.15	0.104	93900	123.6	0.00809
		0.241	124000	163.2	0.00613
		0.378	205000	269.7	0.00371
		0.557	333000	438.2	0.00228
5	278.15	0.104	101500	133.6	0.00749
		0.241	134000	176.3	0.00567
		0.378	224000	294.7	0.00339
		0.557	367000	482.9	0.00207
10	283.15	0.104	111000	146.1	0.00685
		0.241	147000	193.4	0.00517
		0.378	240000	315.8	0.00317
		0.557	393000	517.1	0.00193
15	293.15	0.104	121000	159.2	0.00628
		0.241	157200	206.8	0.00483
		0.378	262000	344.7	0.00290
		0.557	413000	543.4	0.00184

[1]Calculated by compiler; mole fraction ethene, x_1, is for a partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with a magnetic stirrer. Pressure measured with a Bourdon gauge. Samples of liquid analyzed by stripping out ethene. The solubilities were measured at several pressures below atmospheric and Henry's constant was determined. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. N-Methylpyrrolidinone source and purity not given.

   Properties used by authors:
   Normal boiling point = 479.15 K
   Density at 20°C = 1.0220 g/cm^3
   Refractive index n_D^{20} = 1.4700
3. Treatment not specified.

ESTIMATED ERROR:

$\delta K/K = \pm 0.02$

REFERENCES:

1. Shenderei, E.R.; Zelvenskii, Ya.D.; Ivanovskii, F.P. *Gaz. Prom.* 1958, *12*, 36.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Pyrrolidinone, 1-methyl-, (N-methylpyrrolidinone); C_5H_9NO; [872-50-4]
3. Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Wu, Z.; Zeck, S.; Langhorst, R.;

Knapp, H.

Proc. Int. Conf. Coal Gas and Air,

Beijing, China , 1985, *1* , 209-229.

VARIABLES: T/K = 298.15
P/kPa = 100 (1bar)
Conc. water/x'_3 = 0.08-0.96 mole fraction

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

For T/K = 298.15 K:

[3]Solvent Mole Fraction /x'_3	Gas Mole Fraction /[1]y_1	Mole Fraction Solubility, 10^4x_1 Given	[2]p_1=101.325 kPa	Henry's Constant K/bar	[2]H/atm(mole fraction)$^{-1}$	Ostwald Coefficient, L/cm^{3}gas (cm^3 solvent)$^{-1}$
0.960	0.970	1.231	1.29	7879	7777	0.147
0.918	0.972	1.609	1.68	6053	5962	0.168
0.849	0.975	2.587	2.69	3781	3720	0.222
0.747	0.979	4.784	4.95	2060	2020	0.326
0.582	0.985	12.02	12.36	811.9	808.8	0.607
0.544	0.987	15.04	15.44	657.2	647.7	0.708
0.421	0.991	25.21	25.8	398.3	388.0	0.986
0.371	0.992	33.01	33.7	331.7	296.6	1.113
0.277	0.994	40.63	41.4	248.2	241.4	1.336
0.194	0.996	49.53	50.4	202.7	198.5	1.502
0.083	0.998	62.97	63.9	159.6	156.4	1.721

[1] Values personally received from the first author for the gas and liquid phase compositions for a total pressure of 1 bar.

[2] Solubility for a partial pressure of 101.325 kPa calculated by compiler.

[3] The relationship between x_1 and x'_1 is as follows:

$$x_1 + x_2 + x_3 = 1 \; ; \quad x'_2 + x'_3 = 1 \; ; \quad x'_2 = x_2/(1-x_1) \; ; \quad x'_3 = x_3/(1-x_1)$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Ethylene gas was stored in a glass burette equipped with an accurate manometer for measuring pressure and situated in a constant temperature air bath. A known quantity of completely degassed solvent was charged into an equilibrium cell immersed in a liquid bath. The volume of gas absorbed was measured after the gas was admitted into the cell. The solubility was determined from the quantities of gas and solvent used. The apparatus and procedure are described in detail in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.9 vol. percent.
2. Solvent was provided by Merck with a minimum purity of 99.0% (GC). After treatment with molecular sieve drying agent the purity was analyzed to be 99.9%.
3. Water was bidistilled and had a conductivity of 2 micromhos/cm.

ESTIMATED ERROR:

δP/kPa = ± 0.05
δT/K = ± 0.01
$\delta L/L$ = ± 0.01

REFERENCES:

1. Zeck, S.

Doctoral Dissertation , Tech. Univ.

Berlin, FRG, 1985.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alkanes, neohexane and squalane	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 September, 1992

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubility in Alkanes, Neohexane and Squalane for Pressures up to 101.3 kPa

Data for solubilities of ethene have been reported by ten groups of researchers (1-10) for some of the alkane solvents from pentane to docosane as well as in the branch-chained solvents, 2,2 dimethylbutane (neohexane) and squalane, for pressures to 101.3 kPa and temperatures ranging from 213.2 K to 473.2 K. One group (10) measured ethene solubilities in a two-component solvent solution. Four groups of researchers, Jadot (1), Lenoir et al. (7), Ng et al. (8) and Simon and Lukacs (9), utilized gas chromatographic techniques which involve equilibrium at low gas partial pressures so that the values obtained are not always dependable when extrapolated to a partial pressure of 101.3 kPa. The data of McDaniel, obtained some 81 years ago, have often been questioned because of the technique used which tends to yield low values of solubility.

There are too few reliable data to define a relationship between the solubility at 298.15 K and the number of carbons in the alkane solvents (C_N). It is noted that the alkanes of carbon number greater than C_{16} are solids at this temperature. The paucity of solubility data for this class of solvents is particularly apparent; the data consist mainly of single measurements or those supplied by just one research group for any one solvent. Solubility data are available from two or more independent sources only for the solvents hexane and heptane.

Solubilities for the individual solvents are now discussed. Equations for interpolating consistent data and the applicable temperature ranges are included where possible.

Pentane; C_5H_{12}; [109-66-0]
Hexane; C_6H_{14}; [110-54-3]
2,2-Dimethylbutane (neohexane); C_6H_{14}; [75-83-2]

Jadot (1) reported the solubility of ethene in pentane and in hexane at 298.15 K in the form of Henry's constants. The single value for the solubility in pentane is classified as tentative. Sahgal et al. (2) measured the solubility of ethene in hexane at 298.15 K. Waters et al. (3) provided data for the ethene in hexane at four temperatures in the range of 263.15 K to 293.15 K, and at pressures between 26.7 kPa and 85.8 kPa. Tilquin et al. (4) provided a single value at 288.15 K, while McDaniel (5) furnished solubility values at four temperatures, from 295.15 K to 318.15 K. All five sets of data were plotted in the form of log x versus 1/T. The data of McDaniel (5) and the single value of Jadot (1) are about 30% lower than other comparable data, and are consequently rejected. The value of Waters et al. at 293.15 K is about 10% higher than the other data; hence, it too is rejected. Although the graph of these data is not shown, the equation of the line that best fit the data is:

$$\log x_1 = -3.349 + 498.07/(T/\mathrm{K}) \quad \text{for } 298 > T/\mathrm{K} > 263 \qquad (1)$$

Equation 1 has a coefficient of correlation of 0.9954 and the maximum deviation of the data points from the line is 3.3%, while the average deviation is 1.3%. The remaining data and Equation 1 are classified as tentative.

Tilquin et al. (4) reported a single value for the solubility of ethene in neohexane at 288.15 K. Their result is classified as tentative.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Alkanes, neohexane and squalane

EVALUATOR:

Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, ON
Canada K1N 6N5

September, 1992

CRITICAL EVALUATION:

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

Ethene solubilities in heptane were reported by four groups of researchers (1,2,5,6). Three values each were provided by Sahgal et al. (2) at temperatures from 273.15 K to 323.15 K, and by Leites and Ivanovskii (6) for temperatures from 213.15 K to 253.15 K. Four solubilities were reported by McDaniel (5) at temperatures from 295.55 K to 312.15 K, while Jadot (1) reported a single value at 298.15 K. All four sets of data were plotted in the form of log x versus 1/T, and all points were colinear except for the single value of Jadot (1) which deviated by about 16% (see Fig. 1). Omitting this point, the equation of the line which best fit the data is:

$$\log x_1 = -3.512 + 542.46/(T/\text{K}) \quad \text{for } 323 > T/\text{K} > 213 \qquad (2)$$

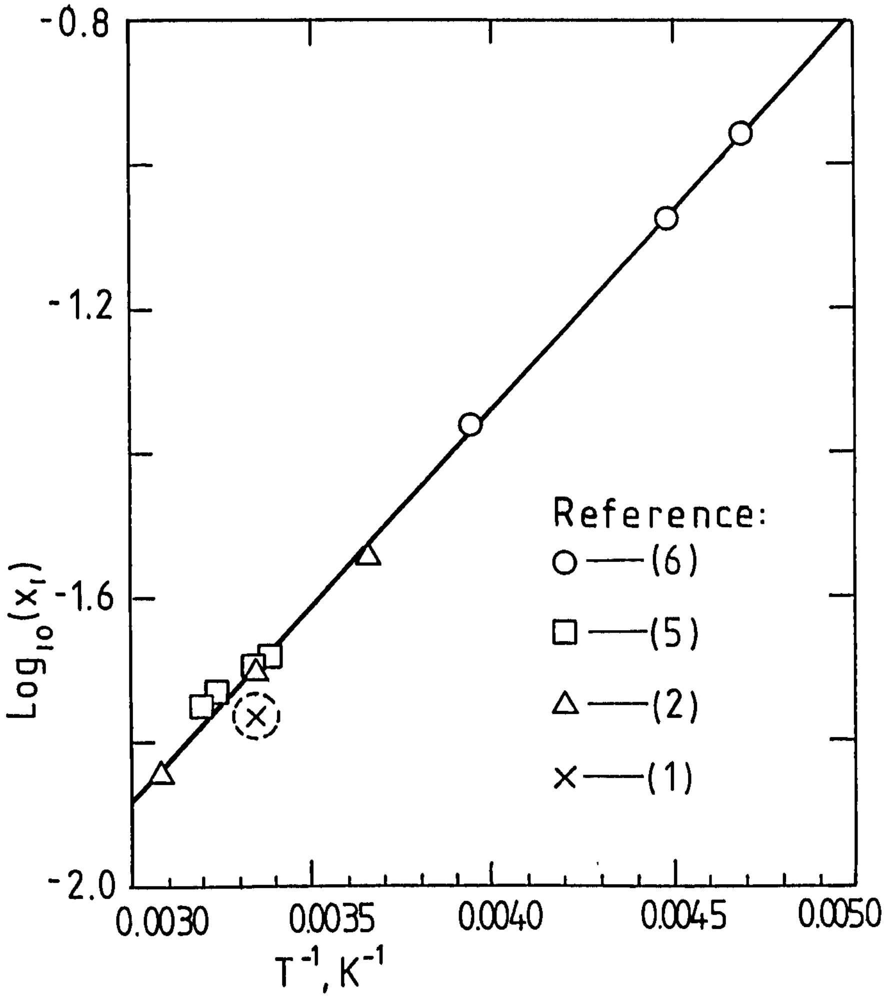

Figure 1 Mole fraction solubility of ethene in n-heptane at 298.15 K and 101.3 kPa gas partial pressure.

COMPONENTS: 1. Ethene; C_2H_4; [74-85-1] 2. Alkanes, neohexane and squalane	EVALUATOR: Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 September, 1992

CRITICAL EVALUATION:

Equation 2 has a correlation coefficient of 0.9988, and the average deviation of the data points from the regression line is 2.7%, while the maximum deviation is 6.0%. Equation 2 may be used to estimate ethene solubilities in heptane at temperatures between 213.15 K and 323.15 K and is classified as tentative along with the data on which it is based.

Octane; C_8H_{18}; [111-65-9]
Nonane; C_9H_{20}; [111-84-2]
Decane; C_1OH_{22}; [124-18-5]

Ethene solubilities in octane, nonane and decane were reported by Jadot (1). All were single values at 298.15 K. The solubilities showed a definite increase with an increase in the chain length of the alkane. These values are classified as tentative.

Dodecane; $C_{12}H_{26}$; [112-40-3]
Hexadecane; $C_{16}H_{34}$; [544-76-3]
Heptadecane; $C_{17}H_{36}$; [629-78-7]

Sahgal et al. (2) measured ethene solubilities in dodecane at 101.3 kPa pressure and at four temperatures ranging from 263.95 K to 339.15 K. The equation representing these data with deviations of less than 2.5% is:

$$\log x_1 = -3.6096 + 582.79/(T/K) \quad \text{for } 339 > T/K > 263 \qquad (3)$$

The data for dodecane are classified as tentative. Lenoir et al. (7) furnished single values for the solubility of ethene in hexadecane as well as heptadecane at 298.15 K, and 323.15 K, respectively. Both values are classified as tentative.

Octadecane; $C_{18}H_{38}$; [593-45-3]
Eicosane; $C_{20}H_{42}$; [112-95-8]
Docosane; $C_{22}H_{46}$; [629-97-0]
Tetracosane, 2,6,10,15,19,23-hexamethyl (squalane); $C_{30}H_{62}$; [110-01-3]

Ethene solubilities in octadecane, eicosane and docosane were measured by Ng et al. (8) at 101.3 kPa pressure and at temperatures from 308.2 K to 473.2 K. The three equations which best represent the data are:

For octadecane: $$\log x_1 = -3.2173 + 489.06/(T/K) \quad \text{for } 423 > T/K > 308 \qquad (4)$$

For eicosane: $$\log x_1 = -3.1861 + 479.10/(T/K) \quad \text{for } 413 > T/K > 323 \qquad (5)$$

For docosane: $$\log x_1 = -3.1820 + 484.71/(T/K) \quad \text{for } 483 > T/K > 333 \qquad (6)$$

All three sets of data are classified as tentative.

Ethene solubilities in squalane were reported by Simon and Lukacs (9) for temperatures between 293.15 K and 333.15 K. It is noted that this C_{30} hydrocarbon is a liquid at ambient conditions because of its branched structure. The solubilities were significantly higher than those measured by Ng et al. (8) for the C_{18} - C_{22} alkanes. The data of Simon and Lukacs (9) are classified as tentative.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alkanes, neohexane and squalane	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 September, 1992

CRITICAL EVALUATION:

Hexane and dodecane solvent solutions:
C_6H_{14}; [110-54-3]; $C_{12}H_{26}$; [112-40-3]

Sahgal and Hayduk (10) reported ethene solubilities in mixtures of hexane and dodecane at 298.15 K. The solubility of ethene was essentially insensitive to the amount of dodecane in the mixture until the mole fraction of dodecane exceeded 0.72. Thereafter, a small increase in solubility was observed. These data are classified as tentative.

References

1. Jadot, R. *J. Chim. Phys.* 1972, *69*, 1036.
2. Sahgal, A.; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354.
3. Waters, J.A.; Mortimer, G.A.; Clements, H.E. *J. Chem. Eng. Data* 1970, *15*, 174.
4. Tilquin, B.; Decanniere, L.; Fontaine, R.; Claes, P. *Ann. Soc. Sc. Bruxelles (Belgium)* 1967, *81*, 191.
5. McDaniel, A.S. *J. Phys. Chem.* 1911, *15*, 587.
6. Leites, I.L. and Ivanovskii, F.P. *Khim. Prom.* 1962, *9*, 653.
7. Lenoir, J.-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data* 1971 *16*, 340.
8. Ng, S.; Harris, H.G.; Prausnitz, J.M. *J. Chem. Eng. Data* 1969, *14*, 482.
9. Simon, F.; Lukacs, J. *Magy. Asvanyolaj-Foldaz. Intez. Kozl. (Hungary)* 1977, *18*, 57.
10. Sahgal, A.; Hayduk, W. *J. Chem. Eng. Data* 1979, *24*, 222.

COMPONENTS:

1. Ethene; C_2H_4 ; [74-85-1]
2. Pentane; C_5H_{12}; [109-66-0]
   or
   Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Jadot, R.

J. Chim. Phys. 1972, *69*, 1036-40.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.3$

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's Law Constant, H/atm	Mole fraction$^+$ at partial pressure of 101.3 kPa, $x_{C_2H_4}$	#ΔH^∞ /cal mol^{-1} (/J mol^{-1})
		Pentane; C_5H_{12}; [109-66-0]	
298.15	65.45	0.01528	-
		Hexane; C_6H_{14}; [110-54-3]	
298.15	62.82	0.01592	256 (1071)

+ Calculated by compiler assuming $x_{C_2H_4} = 1/H$.

Excess partial molar enthalpy of solution at infinite dilution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The conventional gas chromatographic technique was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since no allowance was made for surface adsorption.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$; $\delta H = \pm 2\%$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES:

T/K = 298.15

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1	Ostwald Coefficient L/(cm^3gas /cm^3 solvent)
25.0	298.15	0.0207	3.91

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. Hexane was from Fisher Chemicals, 99.0 mole % minimum purity.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 2%

$\delta T/K$ = ± 0.05

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Hexane; C_6H_{14}; [110-54-3]	Waters, J.A.; Mortimer, G.A.; Clements, H.E. *J. Chem. Eng. Data,* 1970, *15* , 174-176.
VARIABLES: T/K = 263-293 P/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	P/mm mercury	[2]Bunsen Coefficient α/cm^3 gas (NTP)/ cm^{3}solvent	[3]Solubility Mole/litre s	[3]Solubility [1]Average Mole Fraction, x_1
-10	263.15	200.4	6.53	0.291	0.0347
		346.9	6.35	0.284	
		465.9	6.33	0.283	
0	273.15	507.0	5.42	0.242	0.0297
		571.4	5.34	0.239	
10	283.15	543.3	4.77	0.213	0.0266
		611.9	4.70	0.210	
20	293.15	570.2	4.35	0.149	0.0244
		643.7	4.27	0.190	

[1] Calculated by compiler.

[2] Although not specified in paper, compiler confirms that α as given is the Bunsen coefficient.

[3] Solubility, s and x_1, are calculated for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

The method involved measuring the pressure change in a gas reservoir of known volume. Two glass bulbs were connected by tubing fitted with a pressure transducer, gas supply and vacuum lines. The solvent (100 cm^3) was degassed in one of the bulbs equipped with a stirrer using liquid nitrogen. Gas was charged to a higher pressure in the second bulb and quantitatively charged into the first bulb at the appropriate temperature. The final pressure in the equilibrium flask was measured.

SOURCE AND PURITY OF MATERIALS:

1. Ethene, Monsanto polymerization grade, purity 99.85 %.
2. Hexane was from Phillips Petroleum, purity 99.0%.

ESTIMATED ERROR:

δT/K = ± 0.01

$\delta s/s$ = ± 2%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene or ethylene; C_2H_4; [74-85-1] (2) Hexane; C_6H_{14}; [110-54-3]	McDaniel, A. S. *J. Phys. Chem.* 1911, *15*, 587-610.

VARIABLES:	PREPARED BY:
T/K = 295.15 - 318.15 p_1/kPa = 101.3 (1 atm)	H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Mol Fraction	Bunsen Coefficient[a]	Ostwald Coefficient[b]
t/°C	T/K	10^2x_1	α	L/cm³ cm⁻³
22.0	295.15	1.62	2.8141	3.0382
25.0	298.15	1.58	2.7389	2.9896[c]
35.0	308.15	1.47	2.5050	2.8265
45.0	318.15	1.32	2.2190	2.5863

[a] Bunsen coefficient, $\alpha/\text{cm}^3(\text{STP})\ \text{cm}^{-3}\ \text{atm}^{-1}$.

[b] Listed as absorption coefficient in the original paper. Interpreted to be equivalent to Ostwald coefficient by compiler.

[c] Ostwald coefficient (absorption coefficient) estimated as 298.15 K value by author.

[d] Mole fraction and Bunsen coefficient values calculated by compiler assuming ideal gas behavior.

EVALUATOR'S COMMENT: McDaniel's data should be used with caution. His values are often 20 percent or more too small when compared with more reliable data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is all glass. It consists of a gas buret connected to a contacting vessel. The solvent is degassed by boiling under reduced pressure. Gas pressure or volume is adjusted using mercury displacement. Equilibration is achieved at atm pressure by hand shaking, and incrementally adding gas to the contacting chamber. Solubility measured by obtaining total uptake of gas by known volume of the solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Prepared by reaction of 1,2-dibromoethane with zinc-copper.

(2) Hexane. No details given.

ESTIMATED ERROR:

$\delta L/L \geq -0.20$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Hexane; C_6H_{14}; [110-54-3]	Tilquin, B.; Decannière, L.; Fontaine, R.; Claes, P. *Ann. Soc. Sc. Bruxelles (Belgium)* 1967, *81*, 191-199.
VARIABLES: T/K: 288.15 P/kPa: 4.11-8.13	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

t/C	T/K	Ostwald coefficient,[a] L	Mole fraction,[b] x_1	Henry's constant[b] H/atm
15.0	288.15	4.445	0.0238	42.0

[a] Original data at low pressure reported as distribution coefficient; but if Henry's law and ideal gas law apply, distribution coefficient is equivalent to Ostwald coefficient as shown here.

[b] Calculated by compiler for a gas partial pressure of 101.325 kPa assuming that Henry's law and ideal gas law apply.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

All glass apparatus used at very low gas partial pressures, containing a replaceable degassed solvent ampule equipped with a breakable point which could be broken by means of a magnetically activated plunger. Quantity of gas fed into system determined by measuring the pressure change in a known volume. Quantity of liquid measured by weight. Pressure change observed after solvent released. Experimental details described by Rzad and Claes, ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Source not given; minimum purity specified as 99.0 mole per cent.
2. Fluka pure grade; minimum purity specified as 99.0 mole per cent.

ESTIMATED ERROR:

$\delta T/K = 0.05$; $\delta x_1/x_1 = 0.01$

(estimated by compiler).

REFERENCES:

1. Rzad, S.; Claes, P.
Bull. Soc. Chim. Belges
1964, *73*, 689.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2,2'-Dimethylbutane (Neo-hexane); C_6H_{14}; [75-83-2]

ORIGINAL MEASUREMENTS:

Tilquin, B.; Decannière, L.; Fontaine, R.; Claes, P.
Ann. Soc. Sc. Bruxelles (Belgium)
1967, *81*, 191-199.

VARIABLES:

T/K: 288.15
P/kPa: 2.05-2.11

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

t/C	T/K	Ostwald coefficient,[a] L	Mole fraction,[b] x_1	Henry's constant[b] H/atm
15.0	288.15	14.56	0.07506	13.32

[a] Original data at low pressure reported as distribution coefficient; but if Henry's law and ideal gas law apply, distribution coefficient is equivalent to Ostwald coefficient as shown here.

[b] Calculated by compiler for a gas partial pressure of 101.325 kPa assuming that Henry's law and ideal gas law apply.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

All glass apparatus used at very low gas partial pressures, containing a replaceable degassed solvent ampule equipped with a breakable point which could be broken by means of a magnetically activated plunger. Quantity of gas fed into system determined by measuring the pressure change in a known volume. Quantity of liquid measured by weight. Pressure change observed after solvent released. Experimental details described by Rzad and Claes, ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Source not given; minimum purity specified as 99.0 mole per cent.
2. Fluka pure grade; minimum purity specified as 99.0 mole per cent.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = 0.05$; $\delta x_1/x_1 = 0.01$

(estimated by compiler).

REFERENCES:

1. Rzad, S.; Claes, P.
Bull. Soc. Chim. Belges
1964, *73*, 689.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES:

T/K = 273-323
P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1	Ostwald Coefficient L/(cm^3 gas /cm^3 solvent)
0	273.15	0.0284	4.56
25	298.15	0.0198	3.35
50	323.15	0.0143	2.51

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. Heptane was chromatography grade from Matheson Coleman and Bell, 99.0 mole % minimum purity.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Heptane; C_7H_{16}; [142-82-5]	Leites, I.L.; Ivanovskii, F.P. *Khim. Prom.* 1962, *9*, 653-657.
VARIABLES: T/K = 213.15 - 253.15 p_1/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]$\log_{10} H'$, H'/mm Hg	[2]Henry's Constant, H/atm (mole fraction)$^{-1}$	[2]Mole Fraction Ethene, x_1
-60	213.15	3.841	9.12	0.1096
-50	223.15	3.965	12.14	0.0824
-20	253.15	4.243	23.02	0.0434

These results were part of a study for the behavior of solubilities in two-component solvent solutions.

[1] Only graphical results were available in this paper; values of log of Henry's constant (H') were read from enlarged graphs by the compiler.

[2] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler based on the graphical results.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A metal cryostat was cooled with dry-ice and acetone and controlled to a temperature to ± 0.05 K. The equilibrium cell was mounted in the cryostat. The solvent was purified by fractional distillation and analyzed by chromatography. Details were not given.	1. Ethene purity was stated to be 99.9%. 2. Heptane was distilled and analyzed by chromatography. Actual purity not given.
	ESTIMATED ERROR: δT/K = ± 0.05 $\delta x_1/x_1$ = ± 0.01 (Authors)
	REFERENCES:

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

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

ORIGINAL MEASUREMENTS:

McDaniel, A. S.

J. Phys. Chem. 1911, *15*, 587-610.

VARIABLES:

T/K = 295.55 - 312.15

p_1/kPa = 101.3 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Mol Fraction	Bunsen Coefficient[a]	Ostwald Coefficient[b]
t/°C	T/K	10^2x_1	α	L/cm³ cm⁻³
22.4	295.55	2.06	3.2071	3.4640
25.0	298.15	2.01	3.1205	3.4061[c]
35.0	308.15	1.85	2.8245	3.1860
39.0	312.15	1.79	2.7215	3.1100

[a] Bunsen coefficient, α/cm³(STP) cm⁻³ atm⁻¹.

[b] Listed as absorption coefficient in the original paper. Interpreted to be equivalent to Ostwald coefficient by compiler.

[c] Ostwald coefficient (absorption coefficient) estimated as 298.15 K value by author.

[d] Mole fraction and Bunsen coefficient values calculated by compiler assuming ideal gas behavior.

EVALUATOR'S COMMENT: McDaniel's data should be used with caution. His values are often 20 percent or more too small when compared with more reliable data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is all glass. It consists of a gas buret connected to a contacting vessel. The solvent is degassed by boiling under reduced pressure. Gas pressure or volume is adjusted using mercury displacement. Equilibration is achieved at atm pressure by hand shaking, and incrementally adding gas to the contacting chamber. Solubility measured by obtaining total uptake of gas by known volume of the solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Prepared by reaction of 1,2-dibromoethane with zinc-copper.

(2) Heptane. No details given.

ESTIMATED ERROR:

$\delta L/L \geq -0.20$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-] 2. Heptane; C_7H_{16}; [142-82-5] or Octane; C_8H_{18}; [111-65-9]	Jadot, R. *J. Chim. Phys.* 1972, *69*, 1036-40.
VARIABLES: T/K = 298.15 P/kPa = 101.3	PREPARED BY: C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's Law Constant, H/atm	Mole fraction$^+$ at partial pressure of 101.3 kPa, $x_{C_2H_4}$	#ΔH^∞ /cal mol^{-1} (/J mol^{-1})
		Heptane; C_7H_{16}; [142-82-5]	
298.15	57.88	0.01728	316 (1322)
		Octane; C_8H_{18}; [111-65-9]	
298.15	54.26	0.01843	420 (1757)

\+ Calculated by compiler assuming $x_{C_2H_4} = 1/H$.

\# Excess partial molar enthalpy of solution at infinite dilution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The conventional gas chromatographic technique was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since no allowance was made for surface adsorption.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

δT/K = ±0.05; δH = ±2%

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Nonane; C_9H_{20}; [111-84-2]
   or
   Decane; $C_{10}H_{22}$; [124-18-5]

ORIGINAL MEASUREMENTS:

Jadot, R.

J. Chim. Phys. 1972, *69*, 1036-40.

VARIABLES:

T/K = 298.15
P/kPa = 101.3

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's Law Constant, H/atm	Mole fraction$^+$ at partial pressure of 101.3 kPa, $x_{C_2H_4}$	#ΔH^∞ /cal mol^{-1} (/J mol^{-1})
	Nonane; C_9H_{20}; [111-84-2]		
298.15	50.97	0.01962	490 (2050)
	Decane; $C_{10}H_{22}$; [124-18-5]		
298.15	47.36	0.02111	540 (2259)

\+ Calculated by compiler assuming $x_{C_2H_4} = 1/H$.

\# Excess partial molar enthalpy of solution at infinite dilution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The conventional gas chromatographic technique was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since no allowance was made for surface adsorption.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

δT/K = ±0.05; δH = ±2%

REFERENCES:

COMPONENTS: 1. Ethene; C_2H_4; [74-85-1] 2. Dodecane; $C_{12}H_{26}$; [112-40-3]	ORIGINAL MEASUREMENTS: Sahgal, A.; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354-357.
VARIABLES: T/K = 264-339 P/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1	Ostwald Coefficient L/(cm^{3}gas /cm^3 solvent)
-9.2	263.95	0.0402	4.08
25	298.15	0.0216	2.35
48	321.15	0.0159	1.81
66	339.15	0.0131	1.55

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. Dodecane was research grade from Phillips Petroleum of 99.0 mole % minimum purity.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/\mathrm{K} = \pm 0.05$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene (Ethylene); C_2H_4; [74-85-1] 2. Hexadecane; $C_{16}H_{34}$; [544-76-3] or Heptadecane; $C_{17}H_{36}$; [629-78-7]	Lenoir, J-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data* 1971, *16*, 340-2.
VARIABLES: T/K = 298.15, 323.15 P/kPa = 101.3	PREPARED BY: C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant $H_{C_2H_4}$/atm	Mole fraction at 1 atm* $x_{C_2H_4}$
	Hexadecane	
298.15	42.8	0.0234
	Heptadecane	
323.15	52.0	0.0192

* Calculated by compiler assuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e. $x_{C_2H_4}$ (1 atm) = $1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

δT/K = ±0.1; δH/atm = ±6%
(estimated by compiler).

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Octadecane; $C_{18}H_{38}$; [593-45-3],
   Eicosane; $C_{20}H_{42}$; [112-95-8], or
   Docosane; $C_{22}H_{46}$; [629-97-0]

ORIGINAL MEASUREMENTS:

Ng. S.; Harris, H.G.;
Prausnitz, J.M.

J. Chem. Eng. Data

1969, *14*, 482-3.

VARIABLES:

T/K = 308.2 - 473.2

P/kPa = 101.3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant, H /atm	[1]Mole fraction ethene, x_1
	Octadecane; $C_{18}H_{38}$; [593-45-3]	
308.2	42.5	0.0235
323.2	50.6	0.0198
343.2	61.8	0.0162
363.2	74.4	0.0134
373.2	81.8	0.0122
423.2	114	0.00877
	Eicosane; $C_{20}H_{42}$; [112-95-8]	
323.2	50.5	0.0198
343.2	61.9	0.0162
373.2	79.8	0.0125
393.2	92.6	0.0108
413.2	106.4	0.00940
	Docosane; $C_{22}H_{46}$; [629-97-0]	
333.2	53.6	0.0187
383.2	82.6	0.0121
408.2	99.6	0.0100
433.2	112.7	0.00887
453.2	128	0.00781
473.2	147	0.00680

[1] Calculated by compiler for a partial pressure of 101.3 kPa assuming a mole fraction equal to $1/H$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas chromatographic method. Solvent supported on Chromosorb P in 6m column. Gas injected as sample, helium used as carrier gas. Henry's law constant calculated from knowledge of retention time and flow rate.

SOURCE AND PURITY OF MATERIALS:

1. Matheson sample, purity greater than 99 mole per cent.
2. Matheson, Coleman and Bell sample, m.p.t.:

Octadecane	27-28.5 °C
Eicosane	35-36.5 °C
Docosane	43-45 °C

ESTIMATED ERROR:

δT/K = ±0.1; δH/atm = ±5%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Tetracosane, 2,6,10,15,19,23-hexamethyl (squalane); $C_{30}H_{62}$; [110-01-3]	Simon, F.; Lukacs, J. *Magy. Asvanyolaj-Foldaz. Intez. Kozl. (Hungary)* 1977, *18*, 57-66.
VARIABLES: T/K = 293.15 - 333.15 p_1/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Bunsen Coefficient K_B/cm^3 gas at NTP cm^{-3} solvent	[2]Ostwald Coefficient L /cm^3 gas cm^{-3} solvent	[2]Mole Fraction Ethene, x_1
20	293.15	1.66	1.78	0.0373
40	313.15	1.25	1.43	0.0289
50	323.15	1.09	1.30	0.0257
60	333.15	0.970	1.18	0.0230

[1] The solubility results were in the form of two equations, the first describing the temperature effect at 101.3 kPa pressure and the second the effect of pressure, to 405.2 kPa, at 313.15 K:

$$\log K_B = 568.0378\ (T/K)^{-1} - 1.7185 \qquad \text{correlation coeff.} = 0.9985$$

$$K_B = 0.0101\ p/\text{atm} + 1.2241 \qquad \text{correlation coeff.} = 0.3171\ \text{(low)}$$

[2] The Ostwald coefficient and mole fraction solubility at 101.3 kPa were calculated by the compiler. The solvent densities were extrapolated.

Also available in the paper were ethene Bunsen coefficients in four transformer oils, the properties of which were not specified.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas solubility was determined using gas chromatography and employing helium as a carrier gas. Based on the retention times and column characteristics, the Bunsen coefficient was calculated.

SOURCE AND PURITY OF MATERIALS:

Sources and purities of gas and solvent not specified.

ESTIMATED ERROR:

δT/K = ± 0.1
δp_1 /kPa = 2.0
δK_B = ± 6-8% (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Hexane; C_6H_{14}; [110-54-3]
3. Dodecane; $C_{12}H_{26}$; [112-40-3]

ORIGINAL MEASUREMENTS:

Sahgal, A.; Hayduk, W.

J. Chem. Eng. Data 1979, *24*, 222-227.

VARIABLES:

T/K = 298.15
P/kPa = 101.325
x_3/Mole Fraction = 0-1.0

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Concentration of Solvent		Ethene Solubility	
t/C	T/K	z_3, Volume Fraction[1]	x_3, Mole Fraction[2]	Mole Fraction Ethene, x_1	Ostwald Coefficient L/(cm^{3}gas/cm^3 solvent)
		(Hexane)			
25	298.15	0	0	0.0207	3.91
		0.241	0.155	0.0207	3.51
		0.380	0.261	0.0206	3.27
		0.422	0.296	0.0205	3.17
		0.502	0.367	0.0206	3.06
		0.578	0.442	0.0205	2.92
		0.821	0.722	0.0207	2.564
		0.922	0.871	0.0214	2.470
		1.0	1.000	0.0216	2.352
		(Dodecane)			

[1] Volume fraction is based on volumes of two liquid components before mixing.

[2] Mole fraction is shown on a gas-free basis.

Values for pure solvents were previously given (in reference 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus utilized a continuous flow of deaerated solvent injected into a glass absorption spiral tube by means of a calibrated syringe pump. The mixed solvent was prepared volumetrically then deaerated and a sample analyzed by a density measurement. A mercury lift device was used for continuously adjusting the residual volume at constant pressure in a gas storage burette. Solvent injection and gas consumption rates were used to calculate solubilities. This paper also includes solution densities and refractive indices as well as ethene molecular diffusivities in the solutions.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson with minimum purity of 99.5 mole %. Molar volume used at 298.15 K and 101.325 kPa was 24,326 cm^3/mole.

2. Hexane was from Fisher; purity 99.0 mole %.

3. Dodecane was research grade from Phillips Petroleum, 99.0 mole % purity.

ESTIMATED ERROR:

$T/K = \pm 0.05$ $\delta P/P = \pm 0.01$

$\delta z_3 = \pm 0.001$ $\delta x_1/x_1 = \pm 0.02$

REFERENCES:

1. Sahgal, A.; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Propene and Alkanes from C_3 to C_{36}; for pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 June, 1993

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubility in Propene and in Ten Alkanes from Propane (C_3) to Hexatriacontane (C_{36}), for pressures exceeding 0.2 MPa

There are surprisingly few data for solubilities of ethene in alkane solvents at higher pressures and for some of these data it is not possible to accurately determine the gas partial pressures.

Ethene solubilities in individual solvents are now discussed:

Propane; C_3H_8; [74-98-6]
Propene; C_3H_6; [115-07-1]

Elshayal and Lu (1) reported ethene solubilities in propane for total pressures from 0.14 MPa to 3.92 MPa and for temperatures ranging from 199.8 K to 273.2 K. To check for consistency, the data were plotted as log x versus log p. Data for each isotherm were essentially linear over the whole range of partial pressures.

Although propene is not an alkane, the data for this solvent are included here because it is the only alkene for which data are available. The data of Rozhnov and Dorochinskaya (2) for 303.15 K and 323.15 K are reported only as Henry's constants.

Both of the above data are classified as tentative.

2-Methylpropane (isobutane); C_4H_{10}; [75-28-5]

The most extensive solubilities of ethene in 2-methylpropane solvent are those of Naumova and Tyvina (3) which span a temperature range from 293.15 K to 393.15 K and a pressure range from 0.30 MPa to 6.08 MPa. For constant temperatures all the data are essentially linear on a log x versus log p graph. There is a minimum solubility at a temperature of approximately 360 K. This is consistent with data for other gases of low solubility. The results of Kozorozov and Lisin (4) are consistent with those of Naumova and Tyvina at 333.15 K.

Both of the above data are classified as tentative.

The two solubilities of Benedict et al. (5) for 310.93 K and 455.26 K appear to be significantly lower than those from the other two sources for corresponding temperatures and pressures and are rejected.

Hexane; C_6H_{14}; [110-54-3]
Heptane; C_7H_{16}; [142-82-5]

Konobeev and Lyapin (6) reported solubilities for ethene in both n-hexane and n-heptane at temperatures from 293.15 K to 333.15 K and total pressures from 0.29 MPa to 3.2 MPa. However, the corresponding ethene partial pressures or gas phase compositions were not given. As expected, the solubilities in hexane and heptane are very similar in magnitude for the same temperatures and pressures. These data are classified as tentative.

Paratella (7) reported ethene solubilities in n-heptane for high temperatures, from 373.15 K to 473 K, and high total pressures, from 4.05 MPa to 10.13 MPa. Whereas these data appear self-consistent, no other comparable results are available. The data of Paratella are classified as tentative.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Propene and Alkanes from C_3 to C_{36}; for pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 June, 1993

CRITICAL EVALUATION:

Ethene solubilities in n-heptane were reported by Shenderei and Ivanovskii (8) for relatively low temperatures from 228.15 K to 248.15 K and for total pressures from 0.55 MPa to 1.66 MPa. Henry's constants were also given which permitted extrapolation of these data to solubilities corresponding to a pressure of 101.32 kPa. A comparison of the extrapolated Shenderei and Ivanovskii data with that obtained at low pressure (101.32 kPa) is very favorable, probably because both data were products of the same laboratory. These data are classified as tentative.

Octane; C_8H_{18}; [111-65-9]
Nonane; C_9H_{20}; [111-84-2]
Dodecane; $C_{12}H_{26}$; [112-40-3]

Data reported by Shenderei and Ivanovski (8) for ethene solubilities in n-octane are for the three temperatures 248.15 K, 238.15 K and 228.15 K and for pressures ranging from 0.25 MPa to 1.48 MPa. These low temperature data are entirely self-consistent.

Solubilities for ethene in n-nonane as reported by Konobeev and Lyapin (6) are for the temperatures 293.15 K, 313.15 K and 333.15 K and for total pressures ranging from 0.29 to 3.2 MPa. These data are entirely self-consistent.

The data for ethene solubilities in n-dodecane reported by Ribeiro et al. (10) are for relatively large temperature and pressure ranges, from 283.15 K to 348.15 K and from 0.51 MPa to 9.1 MPa. These data are also entirely self-consistent and are approximately consistent (within 8%) with the low pressure solubilities in n-dodecane.

The above data for n-octane, n-nonane and n-dodecane are classified as tentative.

Eicosane; $C_{20}H_{42}$; [112-95-8]
Octacosane; $C_{28}H_{58}$; [630-02-4]
Hexatriacontane; $C_{36}H_{74}$; [630-06-8]

Only the work of Chou and Chao (11) is available for the three wax-like paraffinic solvents at the relatively high temperatures from 373 K to 573 K and total pressures from 0.51 MPa to 9.12 MPa. These data are consistent with those of lower molecular weight alkane solvents and are classified as tentative.

References

1. Elshayal, I.M.; Lu, B.C.-Y. *Can. J. Chem. Eng.* 1975, *53*, 83-87.

2. Rozhnov, M.S.; Dorochinskaya, G.S. *Teploviz. Stoistva. Veshchestv.* 1969, 140-146.

3. Naumova, A.S.; Tyvina, T.N. *Zh. Prikl. Khim.* 1981, 2757-2758 (English Translation 2440-2441).

4. Kozorzov, Yu, E.; Lisin, V.E. *Khim. Prom.* 1978, *6*, 475.

5. Benedict, M.; Solomon, E.; Rubin, L.C. *Ind. Eng. Chem.* 1945, *37*, 55-59.

6. Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-116.

7. Paratella, A. *Riv. Combus.* 1963, *17*, 334-341.

COMPONENTS:
1. Ethene; C_2H_4; [74-85-1]

2. Propene and Alkanes from C_3 to C_{36}; for pressures greater than 0.2 MPa (2 atm)

EVALUATOR:
Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, ON
Canada K1N 6N5

June, 1993

CRITICAL EVALUATION:

8. Shenderi, E.R.; Ivanovskii, F.P. *Khim. Prom.* 1963, *91*, 18-37.

9. Kay, W.B. *Ind. Eng. Chem.* 1948, *40*, 1459-1464.

10. Ribeiro, W.J.; Susu, A.A.; Kohn, J.P. *J. Chem. Eng. Data* 1972, *17*, 79-80.

11. Chou, J.S.; Chao, K.C. *J. Chem. Eng. Data* 1989, *34*, 68-70.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Propene, C_3H_6; [115-07-1]

ORIGINAL MEASUREMENTS:

Rozhnov, M.S.; Dorochinskaya, G.S.

Teploviz. Svoistva. Veshchestv.
1969, 140-146.

VARIABLES:

T/K = 303.15, 323.15

P/MPa = to 4.05

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Henry's Constant, H/ atm (mol fraction)$^{-1}$	[2] Mole Fraction Ethene, x_1	[3] Vapor-liquid Equilibrium Constant, α
30	303.15	62.36	0.01604	2.55
50	323.15	83.33	0.01200	2.67

[1] Actual data were shown in the form of a graph only; Henry's constants were listed in the paper.

[2] The mole fraction solubility was calculated by the compiler for an ethene partial pressure of 101.3 kPa. Henry's law was shown by the authors to apply to 4.05 MPa (40 atm) total pressure.

[3] The authors showed that the vapor-liquid equilibrium compositions were described by the following equation:

$$x_1 + y_1 = \alpha \log \ (P/P_2^\circ)$$

For: α = Vapor-liquid equilibrium constant

x_1, y_1 = Ethene mole fraction in liquid and gas phases, respectively

P = Total pressure

P_2° = Propene vapor pressure

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The gas-liquid equilibrium compositions for the binary system were analyzed by chromatography. A membrane pressure gauge was used for measuring pressure. The equilibrium vessel of 110 cm^3 in volume, was placed in a constant temperature bath. A magnetic mixer was used.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. Propene purity measured by chromatography to be 99.95% pure.

ESTIMATED ERROR:

δT/K = ± 0.1 (authors)

$\delta x_1/x_1$ = ± 2% (compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Propane; C_3H_8; [74-98-6]	Elshayal, I.M.; Lu, B.C-Y. *Can. J. Chem. Eng.*1975, *53*, 83-87.
VARIABLES: T/K = 200-273 P/MPa = 0.14-3.92, (1.4-39 atm)	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

T/K	Total Pressure P/atm	Total Pressure P^1/MPa	Partial Pressure p_1^1/MPa	Mole Fraction Ethene liquid x_1	Mole Fraction Ethene vapor y_1
199.83	1.41	0.1429	0.1270	0.2505	0.8890
	1.64	0.1662	0.1512	0.3025	0.9098
	1.84	0.1864	0.1721	0.3469	0.9233
	2.56	0.2594	0.2482	0.522	0.9567
	3.66	0.3708	0.3653	0.9159	0.9224
	4.13	0.4185	0.3860	0.9159	0.9224
227.9	2.99	0.3030	0.2255	0.1856	0.7444
	4.00	0.4053	0.3334	0.2755	0.8226
	5.43	0.5502	0.4874	0.4065	0.8858
	7.07	0.7164	0.6651	0.5577	0.9284
	9.15	0.9271	0.8934	0.7485	0.9636
	11.34	1.149	1.139	0.9355	0.9909
255.38	3.77	0.3820	0.1222	0.054	0.3198
	8.08	0.8187	0.5851	0.254	0.7147
	11.27	1.141	0.9328	0.4	0.8169
	11.82	1.198	0.9933	0.425	0.8294
	12.67	1.284	1.087	0.463	0.8466
	12.82	1.299	1.103	0.4702	0.8495
	17.09	1.732	1.580	0.6565	0.9127
	19.37	1.963	1.840	0.7505	0.9377
	24.78	2.511	2.477	0.949	0.9865

[1] Calculated by compiler.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium cell was a chamber drilled into a copper rod. The cell was equipped with viewing windows, with gauges for pressure measurement and temperature measurement using two thermocouples for the liquid and gas phases. The low temperatures were achieved by immersing the copper extension of the cell in liquid nitrogen provided with a pressure controller and utilizing an intermediate electric heater. The cell itself was surrounded by a steel vacuum jacket for insulation. An electromagnetic plunger-type stirrer was used. In most of the experiments only the liquid phase was analyzed and that by GC.

SOURCE AND PURITY OF MATERIALS:

1. Ethene from Matheson of purity 99.9 mole %.
2. Propane from Matheson of purity 99.9 mole %.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 1\%$ $\delta T/\mathrm{K} = 0.02$

$\delta P/P = \pm 0.5\%$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Propane; C_3H_8; [74-98-6]

ORIGINAL MEASUREMENTS:

Elshayal, I.M.; Lu, B.C-Y.

Can. J. Chem. Eng. 1975, *53*, 83-87.

VARIABLES:

T/K = 200-273

P/MPa = 0.14-3.92, (1.4-39 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

T/K	Total Pressure P/atm	Total Pressure P^1/MPa	Partial Pressure p_1^1/MPa	Mole Fraction Ethene liquid, x_1	Mole Fraction Ethene vapor, y_1
273.06	7.72	0.7822	0.3208	0.0996	0.4101
	10.53	1.067	0.6208	0.1905	0.5818
	11.79	1.195	0.7561	0.2308	0.6329
	15.24	1.544	1.130	0.3402	0.7316
	17.66	1.789	1.394	0.4157	0.7793
	20.13	2.040	1.667	0.4915	0.8175
	22.00	2.229	1.875	0.5466	0.8410
	24.53	2.486	2.161	0.6216	0.8693
	25.96	2.630	2.323	0.6617	0.8832
	29.13	2.952	2.689	0.7478	0.9111
	32.15	3.258	3.046	0.8238	0.9350
	35.41	3.588	3.442	0.8980	0.9593
	38.69	3.920	3.856	0.9635	0.9836

[1] Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium cell was a chamber drilled into a copper rod. The cell was equipped with viewing windows, with gauges for pressure measurement and temperature measurement using two thermocouples for the liquid and gas phases. The low temperatures were achieved by immersing the copper extension of the cell in liquid nitrogen provided with a pressure controller and utilizing an intermediate electric heater. The cell itself was surrounded by a steel vacuum jacket for insulation. An electromagnetic plunger-type stirrer was used. In most of the experiments only the liquid phase was analyzed and that by GC.

SOURCE AND PURITY OF MATERIALS:

1. Ethene from Matheson of purity 99.9 mole %.

2. Propane from Matheson of purity 99.9 mole %.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 1\%$ $\delta T/K = 0.02$

$\delta P/P = \pm 0.5\%$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. 2-Methylpropane (isobutane); C_4H_{10}; [75-28-5]

ORIGINAL MEASUREMENTS:

Naumova, A.A.; Tyvina, T.N.

Zh. Prikl. Khim. 1981, *54*, 2757-8.

or *J. Appl. Chem. USSR* 1981, *54*, 2440-1.

VARIABLES:

T/K = 293.15-393.15

P/MPa = 0.30-6.08, (3-60 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Total Pressure $P/10^3$ hPa	Total Pressure [1]P/MPa	[1] Ethene Partial Pressure p_1/MPa	Ethene Mole Fraction Liquid, x_1	Ethene Mole Fraction Gas, y_1
20	293.15	2.98	0.298	0	0	0
		10.1	1.01	0.713	0.198	0.706
		20.3	2.03	1.746	0.427	0.860
		30.4	3.04	2.815	0.605	0.926
		40.5	4.05	3.831	0.765	0.946
		50.6	5.06	4.807	0.895	0.950
40	313.15	5.22	0.522	0	0	0
		10.1	1.01	0.505	0.100	0.500
		20.3	2.03	1.462	0.285	0.720
		30.4	3.04	2.420	0.445	0.796
		40.5	4.05	3.382	0.587	0.835
		50.6	5.06	4.296	0.718	0.849
		60.8	6.08	5.168	0.845	0.850
60	333.15	8.63	0.863	0	0	0
		10.1	1.01	0.131	0.025	0.130
		20.3	2.03	1.096	0.187	0.540
		30.4	3.04	1.961	0.334	0.645
		40.5	4.05	2.835	0.460	0.700
		50.6	5.06	3.653	0.576	0.722
		60.8	6.08	4.408	0.685	0.725

[1] Calculated by compiler.

...continued

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A static type of solubility equipment was used.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.

2. 2-Methylpropane source and purity not given.

ESTIMATED ERROR:

δT/K = ± 0.5

$\delta x_1/x_1$ = ± 0.02 (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Methylpropane (isobutane); C_4H_{10}; [75-28-5]

ORIGINAL MEASUREMENTS:

Naumova, A.A.; Tyvina, T.N.

Zh. Prikl. Khim. 1981, *54*, 2757-8.

or *J. Appl. Chem. USSR* 1981, *54*, 2440-1.

VARIABLES:

T/K = 293.15-393.15

P/MPa = 0.30-6.08, (3-60 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

		Total Pressure		[1] Ethene Partial Pressure	Ethene Mole Fraction	
t/C	T/K	$P/10^3$ hPa	[1]P/MPa	p_1/MPa	Liquid, x_1	Gas, y_1
80	353.15	13.43	1.343	0	0	0
		20.3	2.03	0.641	0.096	0.316
		30.4	3.04	1.450	0.225	0.477
		40.5	4.05	2.195	0.349	0.542
		50.6	5.06	2.914	0.458	0.576
		60.8	6.08	3.567	0.565	0.585
100	373.15	19.93	1.993	0	0	0
		20.3	2.03	0.016	0.005	0.008
		30.4	3.04	0.775	0.130	0.255
		40.5	4.05	1.462	0.241	0.361
		50.6	5.06	2.964	0.350	0.408
120	393.15	28.38	2.838	0	0	0
		30.4	3.04	0.109	0.024	0.036
		40.5	4.05	0.648	0.140	0.160

[1] Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A static type of solubility equipment was used.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. 2-Methylpropane source and purity not given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.5$

$\delta x_1/x_1 = \pm 0.02$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. 2-Methylpropane (isobutane); C_4H_{10}; [75-28-5]

ORIGINAL MEASUREMENTS:

Benedict, M.; Solomon, E.;

Rubin, L.C.

Ind. Eng. Chem. 1945, *37*, 55-59.

VARIABLES: T/K = 310.93, 344.26

P/MPa = 3.447 (34.02 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Total Pressure		[1] Ethene Partial Pressure	Ethene Mole Fraction	
t/C	T/K	P/atm	[1] P/MPa	p_1/MPa	Liquid, x_1	Gas, y_1
37.78	310.93	34.02	3.447	2.897	0.497	0.8405
71.11	344.26	34.02	3.447	2.151	0.296	0.624

[1] Calculated by compiler; the partial pressure is based on the gas phase composition.

This paper contains a listing of three-component phase equilibria for methane, ethene and 2-methylpropane at several temperatures and pressures. These have been compiled and may be found in the *Methane* volume. The data here are all that are available for the two-component system.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A steel cell is used for the solubility measurements. The solvent floats on mercury. The mercury is in contact with a free-piston and weights for pressure measurement. Equilibration is aided by rocking the cell and contents. As the gas is slowly sampled, mercury flows into the cell to keep the pressure constant. When only liquid remains, the pressure is increased and a liquid sample is obtained. The gas phase densities and olefin content are determined for the samples at low pressure.

SOURCE AND PURITY OF MATERIALS:

1. Ethene, anesthesia grade, was obtained from Ohio Chemical. It was purified by flash distillation and estimated to have 0.5 mole % ethane.

2. 2-Methylpropane of the CP grade was from Phillips Petroleum with a purity of 99.2%.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.02$

$\delta P/P = \pm 0.001$

$\delta x_1/x_1 = \pm 0.02$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Propane, 2-methyl (isobutane); C_4H_{10}; [75-28-5]

ORIGINAL MEASUREMENTS:

Kozorezov, Yu.I.; Lisin, V.E.

Khim. Prom. 1978, *6*, 475.

VARIABLES: T/K = 293-333

P/MPa = 0.097-0.782

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Gas Partial Pressure		Solubility	
t /C	T/K[1]	p_1/atm	p_1/MPa[1]	s/cm^3 (NTP)$(g)^{-1}$	x_1,mole fraction
20	293.15	0.96	0.097	13.17	0.033
		1.93	0.196	28.85	0.070
		2.89	0.293	40.86	0.096
		4.82	0.488	75.27	0.162
		7.72	0.782	122.40	0.241
30	303.15	0.96	0.097	11.52	0.029
		1.93	0.196	23.30	0.057
		2.89	0.293	34.98	0.083
		4.82	0.488	62.43	0.139
		7.72	0.782	102.60	0.210
40	313.15	0.96	0.097	9.22	0.023
		1.93	0.196	19.84	0.049
		2.89	0.293	32.20	0.077
		4.82	0.488	54.51	0.124
60	333.15	0.96	0.097	7.43	0.019
		1.93	0.196	14.00	0.035
		2.89	0.293	22.20	0.054
		3.86	0.391	36.12	0.089

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[1] Calculated by compiler.

Although Henry's law constants were calculated by authors, they are not listed here because data obey Henry's law only very approximately.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 650 cm^3 vessel kept at constant temperature was charged with 400-450 cm^3 of liquid isobutane. The vessel was provided with a mixer for equilibration. The isobutane was saturated at constant pressure with gas. A sample of the saturated solution was withdrawn for chromatographic analysis. Method for determining gas partial pressure was not given in paper.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 99.6%.
2. Isobutane purity 99.3%.

ESTIMATED ERROR:

$\delta s/s = \pm 3\%$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967,*43*, 114-6.

VARIABLES:

$T/K = 293.15 - 333.15$

$P/MPa = 0.28 - 3.2$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5Pa$	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.090	0.060
	8.106	0.156
	15.60	0.291
	32.12	0.576
313.15	2.827	0.040
	8.248	0.123
	17.43	0.266
	32.42	0.471
333.15	2.847	0.031
	8.278	0.100
	17.53	0.221
	32.53	0.396

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.
2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$; $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967, *43*, 114-6.

VARIABLES:

T/K = 293.15 - 333.15

P/MPa = 0.29 - 3.2

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5$Pa	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.090	0.056
	8.106	0.153
	15.50	0.285
	17.43	0.318
	31.92	0.573
313.15	2.878	0.040
	8.177	0.129
	17.53	0.267
	32.32	0.464
333.15	2.888	0.025
	8.238	0.092
	17.63	0.207
	32.42	0.364

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

δT/K = ±0.1; δP = ±0.5%; $\delta x_{C_2H_4}$ = ±0.002

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

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

Khim. Prom. 1963, *91*, 18-37.

VARIABLES:

T/K = 228.15 - 248.15

P/MPa = 0.552 - 1.663

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	P/Atm	[1]P/MPa	Mole fraction ethene, x_1	Solubility cm^3 (STP)/g
-25	248.15	5.45	0.552	0.2376	69.06
		5.49	0.556	0.2561	76.26
		8.65	0.876	0.3789	135.16
		8.90	0.902	0.4091	153.44
		10.19	1.033	0.4686	195.37
		13.64	1.382	0.6169	356.80
		14.73	1.493	0.6834	478.25
		15.76	1.597	0.7196	568.00
		16.41	1.663	0.7657	723.96
-35	238.15	5.44	0.551	0.3085	98.84
		5.54	0.561	0.3170	102.85
		7.76	0.786	0.4572	186.62
		8.56	0.867	0.4909	213.97
		12.88	1.305	0.7747	766.11
		12.92	1.309	0.7649	721.04

[1] Calculated by compiler.

Henry's constant determined for pressures below atmospheric. Graphs given for low pressure range showing that Henry's law is obeyed.

T/K	228.15	238.15	248.15
H/Atm (mole fraction)$^{-1}$	13.5	17.2	20.9

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus utilized an absorption tube with a magnetic stirrer. The temperature controlled bath had two compartments, one containing methanol solution, the other containing solid dry ice in acetone. The walls of the vessels served as the heat transfer medium. Capillary tubing connected the absorber to pressure devices, gas and solvent vessels and a vacuum system. A known amount of solvent was charged into the absorber and the quantity of gas was determined by pressure difference in the gas supply vessel.

SOURCE AND PURITY OF MATERIALS:

1. Purified and analyzed by GC. Actual purity not given.
2. Not given.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta x_1/x_1$ = ± 2% (compiler)

REFERENCES:

1. Shenderei, E.R.; Zelvenski, Ya.D.; Ivanovskii, F.P.

   Khim. Prom. 1960, *5*, 370.

COMPONENTS:

1. Ethene; C_2H_4 ; [74-85-1]
2. Heptane; C_7H_{16} ; [142-82-5]

ORIGINAL MEASUREMENTS:

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

Khim. Prom. 1963, *91* , 18-37.

VARIABLES:

T/K = 228.15 - 248.15

P/MPa = 0.552 - 1.663

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ....continued

t/C	[1] T/K	P/Atm	[1] P/MPa	Mole fraction ethene, x_1	Solubility cm^3(STP)/g
-35	238.15	14.06	1.425	0.8550	1305.30
		14.22	1.441	0.8539	1294.80
		14.84	1.504	0.8945	1877.70
-45	228.15	4.90	0.496	0.3636	126.58
		5.21	0.528	0.3765	133.80
		5.18	0.525	0.3742	132.50
		7.55	0.765	0.5742	298.76
		7.84	0.794	0.5929	322.74
		7.87	0.797	0.5962	324.24
		10.19	1.033	0.8161	981.15
		10.29	1.043	0.8218	1022.30
		10.55	1.069	0.8413	1176.70
		10.96	1.111	0.8908	1806.70
		11.17	1.132	0.9012	2024.69

[1] Calculated by compiler.

Henry's constant determined for pressures below atmospheric. Graphs given for low pressure range showing that Henry's law is obeyed.

T/K	228.15	238.15	248.15
H/Atm(mole fraction)$^{-1}$	13.5	17.2	20.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus utilized an absorption tube with a magnetic stirrer. The temperature controlled bath had two compartments, one containing methanol solution, the other containing solid dry ice in acetone. The walls of the vessels served as the heat transfer medium. Capillary tubing connected the absorber to pressure devices, gas and solvent vessels and a vacuum system. A known amount of solvent was charged into the absorber and the quantity of gas was determined by pressure difference in the gas supply vessel.

SOURCE AND PURITY OF MATERIALS:

1. Purified and analyzed by GC. Actual purity not given.
2. Not given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$

$\delta x_1/x_1 = \pm 2\%$ (compiler)

REFERENCES:

1. Shenderei, E.R.; Zelvenski, Ya.D.; Ivanovskii, F.P.

   Khim. Prom., 1960, *5*, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Paratella, A.

Riv. Combust. 1963, *17*, 334-341.

VARIABLES:

T/K = 373.15 - 473.15

P/MPa = 4.05 - 10.13

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

				Equilibrium Constants:			
Temperature		Total Pressure		Ethene	Heptane	[2]Ethene Mole Fraction	
t/C	[1]T/K	P/atm	[1]P/MPa	$K_1 = y_1/x_1$	$K_2 = y_2/x_2$	Vapor, y_1	Liquid, x_1
100	373.15	40	4.05	2.95	0.144	0.900	0.306
		60	6.08	2.04	0.148	0.919	0.450
		80	8.11	1.51	0.237	0.905	0.599
		100	10.13	1.08	0.724	0.837	0.775
150	423.15	40	4.05	3.16	0.298	0.775	0.245
		60	6.08	2.21	0.283	0.822	0.371
		80	8.11	1.63	0.354	0.925	0.506
		100	10.13	1.14	0.716	0.764	0.670
200	473.15	40	4.05	2.67	0.596	0.520	0.195
		60	6.08	1.93	0.595	0.586	0.304
		80	8.11	1.39	0.702	0.602	0.433

[1] Calculated by Compiler.

[2] Liquid and vapor compositions were calculated by the Compiler to satisfy the Equilibrium Constants; these were not given in the paper although they were shown in a graph.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A high pressure apparatus employing a glass capillary tube immersed in mercury was used. Agitation was by means of a magnetically-operated agitation system. A cathetometer was used to determine the quantity of solvent charged and a microburette was used to measure the volumes of gas dissolved.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was prepared by reaction of Zn with dibromoethane in an alcohol solution. The purity was determined at 99.5%.
2. Heptane was from Phillips Petroleum of the highest purity grade (unspecified).

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.1$

$\delta \Pi/\mathrm{atm} = \pm 0.5$

$\delta x_1 = \pm 0.02$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Kay, W.B.

Ind. Eng. Chem. 1948, *40*, 1459-1464.

VARIABLES:

T/K = 211.5 - 522.0

P/MPa = 0.677 - 19.15

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Fraction Ethene in Liquid		Temperature		[1]Equilibrium Constant for Ethene	Total Pressure	
w, mass	x_1, mol	t/°F	[1]T/K	K = y_1/x_1	P/psia	[1]p/MPa
0.0208	0.0704	183.0	357.04	12.94	100	0.689
		260.2	399.93	11.38	150	1.034
		317.1	431.54	9.87	200	1.379
		360.7	455.76	8.66	250	1.724
		396.0	475.37	7.70	300	2.068
		426.7	492.43	6.89	350	2.413
		454.6	507.93	6.15	400	2.758
		480.0	522.04	5.50	450	3.103
0.0596	0.1846	36.0	275.37	5.41	100	0.689
		86.8	303.59	5.38	150	1.034
		131.5	328.43	5.34	200	1.379
		173.4	351.71	5.28	250	1.724
		214.2	374.37	5.18	300	2.068
		253.0	395.93	5.05	350	2.413
		289.6	416.26	4.90	400	2.758
		325.1	435.98	4.71	450	3.103
		359.1	454.87	4.50	500	3.447
		392.0	473.15	4.27	550	3.792
		424.9	491.43	4.01	600	4.137
		468.0	515.37	3.58	650	4.482

[1]Calculated by compiler. Raoult's law was used to calculate the vapor composition and K, both being approximations.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Heptane was charged into the high pressure cell, degassed, and its quantity determined by volume. A measured volume of ethene gas was added from a storage bomb at constant temperature to give a known liquid composition by a material balance. The liquid composition was considered to remain constant for the changes in temperature and pressure involved in each series of experiments because of the small gas volume used. Densities and critical properties of the solutions were also given at high pressure. Details of experimental method given in reference 1. Vapor-liquid equilibria for eight ethene compositions are reported. The results for four of the compositions, in which the mole fractions are less than 0.5, may be considered solubility equilibria and are listed here.

SOURCE AND PURITY OF MATERIALS:

1. Commercial high purity ethene was fractionated then degassed by repeated freezing, evacuation and melting. Actual purity not indicated.
2. Heptane purity not specified.

ESTIMATED ERROR:

δT/K = $\pm$ 0.02
$\delta P/P$ = $\pm$ 0.005
$\delta x_1/x_1$ = $\pm$ 0.03 (Compiler)

REFERENCES:

1. Kay, W.B.
Ind. Eng. Chem. 1938, *30*, 459.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Kay, W.B.

Ind. Eng. Chem. 1948, *40*, 1459-1464.

VARIABLES:

T/K = 211.5 - 522.0

P/MPa = 0.677 - 19.15

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

Fraction Ethene in Liquid w,mass	Fraction Ethene in Liquid x_1,mol	Temperature t/°F	Temperature [1]T/K	[1]Equilibrium Constant for Ethene K = y_1/x_1	Total Pressure P/psia	Total Pressure [1]p/MPa
0.1007	0.2857	-5	252.59	3.50	100	0.689
		32	273.15	3.50	150	1.034
		64	290.93	3.49	200	1.379
		93.9	307.54	3.49	250	1.724
		122.2	323.26	3.48	300	2.068
		149.8	338.59	3.46	350	2.413
		176.7	353.54	3.45	400	2.758
		203.2	368.26	3.42	450	3.103
		230.1	383.21	3.40	500	3.447
		257.2	398.26	3.36	550	3.792
		284.6	413.48	3.32	600	4.137
		312.5	428.98	3.26	650	4.482
		341	444.82	3.19	700	4.826
		372	462.04	3.11	750	5.171
		411.3	483.87	2.97	800	5.516
0.2005	0.4725	80.5	300.09	2.114	400	2.758
		96.2	308.82	2.113	450	3.103
		111.4	317.26	2.112	500	3.447
		126.2	325.48	2.110	550	3.792
		141	333.71	2.109	600	4.137

[1] Calculated by compiler. Raoult's law was used to calculate the vapor composition and K, both being approximations.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Heptane was charged into the high pressure cell, degassed, and its quantity determined by volume. A measured volume of ethene gas was added from a storage bomb at constant temperature to give a known liquid composition by a material balance. The liquid composition was considered to remain constant for the changes in temperature and pressure involved in each series of experiments because of the small gas volume used. Densities and critical properties of the solutions were also given at high pressure. Details of experimental method given in reference 1. Vapor-liquid equilibria for eight ethene compositions are reported. The results for four of the compositions, in which the mole fractions are less than 0.5, may be considered solubility equilibria and are listed here.

SOURCE AND PURITY OF MATERIALS:

1. Commercial high purity ethene was fractionated then degassed by repeated freezing, evacuation and melting. Actual purity not indicated.
2. Heptane purity not specified.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.02$

$\delta P/P = \pm 0.005$

$\delta x_1/x_1 = \pm 0.03$ (Compiler)

REFERENCES:

1. Kay, W.B.

   Ind. Eng. Chem. 1938, *30*, 459.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Kay, W.B.

Ind. Eng. Chem. 1948, *40*, 1459-1464.

VARIABLES:

T/K = 211.5 - 522.0

p/MPa = 0.677 - 19.15

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

Fraction Ethene in Liquid w,mass	Fraction Ethene in Liquid x_1,mol	Temperature t/°F	Temperature ^1T/K	^{1}Equilibrium Constant for Ethene K = y_1/x_1	Total Pressure P/psia	Total Pressure ^1p/MPa
0.2005	0.4725	155.8	341.93	2.107	650	4.482
		170.5	350.09	2.104	700	4.826
		186.0	358.71	2.101	750	5.171
		201.3	367.21	2.098	800	5.516
		217.0	375.93	2.094	850	5.861
		233.5	385.09	2.089	900	6.205
		250.7	394.65	2.083	950	6.550
		269.0	404.82	2.076	1000	6.895
		288.2	415.48	2.067	1050	7.239
		310.0	427.59	2.031	1100	7.584
		343.0	445.93	2.031	1150	7.929

[1] Calculated by compiler. Raoult's law was used to calculate the vapor composition and K, both being approximations.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Heptane was charged into the high pressure cell, degassed, and its quantity determined by volume. A measured volume of ethene gas was added from a storage bomb at constant temperature to give a known liquid composition by a material balance. The liquid composition was considered to remain constant for the changes in temperature and pressure involved in each series of experiments because of the small gas volume used. Densities and critical properties of the solutions were also given at high pressure. Details of experimental method given in reference 1.
Vapor-liquid equilibria for eight ethene compositions are reported. The results for four of the compositions, in which the mole fractions are less than 0.5, may be considered solubility equilibria and are listed here.

SOURCE AND PURITY OF MATERIALS:

1. Commercial high purity ethene was fractionated then degassed by repeated freezing, evacuation and melting. Actual purity not indicated.

2. Heptane purity not specified.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.02$

$\delta P/P = \pm 0.005$

$\delta x_1/x_1 = \pm 0.03$ (Compiler)

REFERENCES:

1. Kay, W.B.

Ind. Eng. Chem. 1938, *30*, 459.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

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

Khim. Prom. 1963, *91*, 18-37.

VARIABLES:

T/K = 228.15 - 248.15

P/MPa = 0.285 - 1.48

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1] T/K	P/atm	[1] P/MPa	Mole fraction ethene, x_1	Solubility cm^3(STP)/g
-25	248.15	5.29	0.536	0.2370	60.38
		12.82	1.299	0.5937	284.02
		14.63	1.482	0.6811	415.10
-35	238.15	2.18	0.285	0.1458	33.19
		2.96	0.300	0.1568	36.14
		4.64	0.470	0.2578	67.53
		4.80	0.486	0.2656	70.29
		4.87	0.493	0.2803	75.71
		6.32	0.640	0.3692	113.75
		9.24	0.936	0.5261	215.18
		10.70	1.084	0.6210	318.43
		11.74	1.190	0.6773	407.94
		12.62	1.279	0.7483	577.85
		13.39	1.357	0.7820	697.83
		13.44	1.362	0.8083	819.73
		14.11	1.430	0.8337	974.60

[1] Calculated by compiler.

Henry's constant determined for pressures below atmospheric. Graphs given for low pressure range showing that Henry's law is obeyed.

T/K	228.15	238.15	248.15
H/Atm(mole fraction)$^{-1}$	14.2	17.0	20.2

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus utilized an absorption tube with a magnetic stirrer. The temperature controlled bath had two compartments, one containing methanol solution, the other containing solid dry ice in acetone. The walls of the vessels served as the heat transfer medium. Capillary tubing connected the absorber to pressure devices, gas and solvent vessels and a vacuum system. A known amount of solvent was charged into the absorber and the quantity of gas was determined by pressure difference in the gas supply vessel.

SOURCE AND PURITY OF MATERIALS:

1. Purified and analyzed by GC. Actual purity not given.

2. Not given.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta x_1/x_1$ = ± 2% (compiler)

REFERENCES:

1. Shenderei, E.R.; Zelvenski, Ya.D.; Ivanovskii, F.P.

   Khim. Prom., 1960, *5*, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

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

Khim. Prom. 1963, *91*, 18-37.

VARIABLES:

T/K = 228.15 - 248.15

P/MPa = 0.253 - 1.048

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ....continued

t/C	^1T/K	P/atm	^1P/MPa	Mole fraction ethene, x_1	Solubility cm^3 (STP)/g
-45	228.15	2.50	0.253	0.1715	40.23
		2.85	0.289	0.1950	47.09
		3.58	0.363	0.2583	67.68
		4.52	0.458	0.3169	90.17
		5.55	0.562	0.4032	132.38
		7.46	0.756	0.5457	233.47
		7.97	0.808	0.5924	282.48
		9.40	0.952	0.6991	474.88
		10.34	1.048	0.8164	864.13

[1] Calculated by compiler.

Henry's constant determined for pressures below atmospheric. Graphs given for low pressure range showing that Henry's law is obeyed.

T/K	228.15	238.15	248.15
H/Atm(mole fraction)$^{-1}$	14.2	17.0	20.2

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus utilized an absorption tube with a magnetic stirrer. The temperature controlled bath had two compartments, one containing methanol solution, the other containing solid dry ice in acetone. The walls of the vessels served as the heat transfer medium. Capillary tubing connected the absorber to pressure devices, gas and solvent vessels and a vacuum system. A known amount of solvent was charged into the absorber and the quantity of gas was determined by pressure difference in the gas supply vessel.

SOURCE AND PURITY OF MATERIALS:

1. Purified and analyzed by GC. Actual purity not given.
2. Not given.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta x_1/x_1$ = ± 2% (compiler)

REFERENCES:

1. Shenderei, E.R.; Zelvenski, Ya.D.; Ivanovskii, F.P.

   Khim. Prom., 1960, *5*, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Nonane; C_9H_{20}; [111-84-2]

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967, *43*, 114-6.

VARIABLES:

T/K = 293.15 - 333.15

P/MPa = 0.29 - 3.19

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5$Pa	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.050	0.063
	8.106	0.154
	15.50	0.282
	31.51	0.562
313.15	2.867	0.043
	8.238	0.124
	17.33	0.242
	31.82	0.453
333.15	2.888	0.036
	8.248	0.104
	17.43	0.217
	31.92	0.380

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

δT/K=±0.1; δP=±0.5%; $\delta x_{C_2H_4}$ =±0.002

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Dodecane; $C_{12}H_{26}$; [112-40-3]

ORIGINAL MEASUREMENTS:

Ribeiro, V.J.; Susu, A.A.;
Kohn, J.P.

J. Chem. Eng. Data 1972, *17*, 79-80.

VARIABLES:

T/K = 283-348

P/MPa = 0.51-9.12

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	Total Pressure P/atm	[1]P/MPa	Ethene in liquid Mole Fraction, x_1	Liquid Solution Molar Volume V_L/cm^3 (mole)$^{-1}$ [1]
10	283.15	5.00	0.507	0.135	200.8
		10.00	1.013	0.245	182.8
		15.00	1.520	0.350	165.4
		20.00	2.026	0.445	149.8
		25.00	2.533	0.530	135.7
		30.00	3.040	0.610	122.7
		35.00	3.546	0.690	110.3
		40.00	4.053	0.770	98.8
		45.00	4.560	0.850	87.5
25	298.15	5.00	0.507	0.100	212.3
		10.00	1.013	0.190	198.0
		15.00	1.520	0.270	185.3
		20.00	2.026	0.350	172.7
		25.00	2.533	0.425	160.7
		30.00	3.040	0.500	148.6
		35.00	3.546	0.570	137.2
		40.00	4.053	0.635	126.7
		45.00	4.560	0.690	117.5
		50.00	5.066	0.742	109.2
		55.00	5.573	0.795	101.0
		60.00	6.080	0.860	91.4
		65.00	6.586	0.950	82.0

[1] Calculated by compiler.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 10-cm^3 borosilicate glass equilibrium cell containing a known mass of degassed solvent was mounted in a constant temperature bath. Gas was quantitatively ($\pm$ 0.006 cm^3) charged from a reservoir, kept at constant pressure, by mercury displacement. Pressure gauges mounted on the cell and the reservoir were accurate to 0.07 atm. Liquid volumes inside the cell could be read using calibration marks on the cell wall. Agitation was by using a magnetically activated stainless steel ball. The solubility was determined from the volume of gas consumed. Saturated solution volumes were read from the observed volumes in the cell. Additional details in reference 1. The dodecane vapor pressure was considered negligible even at 75°C when it corresponded to 4.2 mm mercury.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson; minimum purity 99.5%. Gas critical temperature and pressure measured as 9.34°C at 50.09 atm.
2. Dodecane was from Humphrey-Wilkinson; 99.0% minimum purity.
   Freezing point: -9.57°C.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm\ 0.01$ $\quad T/K = \pm\ 0.02$

$\delta P/P = \pm\ 0.01$

REFERENCES:

1. Lee, K.H.; Kohn, J.P.
   J. Chem. Eng. Data 1969, *14*, 292.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Dodecane; $C_{12}H_{26}$; [112-40-3]

ORIGINAL MEASUREMENTS:

Ribeiro, V.J.; Susu, A.A.;

Kohn, J.P.

J. Chem. Eng. Data 1972, *17*, 79-80.

VARIABLES: T/K = 283-348

P/MPa = 0.51-9.12

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/C	^1T/K	Total Pressure P/atm	Total Pressure ^1P/MPa	Ethene in liquid Mole Fraction, x_1	Liquid Solution Molar Volume V_L/cm^3 (mole)$^{-1}$
50	323.15	5.00	0.507	0.075	222.6
		10.00	1.013	0.140	212.3
		15.00	1.520	0.206	201.8
		20.00	2.026	0.270	191.7
		25.00	2.533	0.330	182.0
		30.00	3.040	0.385	173.2
		35.00	3.546	0.435	165.2
		40.00	4.053	0.485	157.2
		45.00	4.560	0.530	150.0
		50.00	5.066	0.575	142.8
		55.00	5.573	0.612	136.8
		60.00	6.080	0.650	130.5
		65.00	6.586	0.685	125.0
		70.00	7.093	0.720	119.5
		75.00	7.600	0.753	113.9
		80.00	8.106	0.785	109.3
		85.00	8.613	0.817	104.3
		90.00	9.119	0.850	99.0

Calculated by compiler.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 10-cm^3 borosilicate glass equilibrium cell containing a known mass of degassed solvent was mounted in a constant temperature bath. Gas was quantitatively (±0.006 cm^3) charged from a reservoir, kept at constant pressure, by mercury displacement. Pressure gauges mounted on the cell and the reservoir were accurate to 0.07 atm. Liquid volumes inside the cell could be read using calibration marks on the cell wall. Agitation was by using a magnetically activated stainless steel ball. The solubility was determined from the volume of gas consumed. Saturated solution volumes were read from the observed volumes in the cell. Additional details in reference 1. The dodecane vapor pressure was considered negligible even at 75 °C when it corresponded to 4.2 mm mercury.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson; minimum purity 99.5%. Gas critical temperature and pressure measured as 9.34 °C at 50.09 atm.
2. Dodecane was from Humphrey-Wilkinson; 99.0% minimum purity. Freezing point: -9.57 °C.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.01$ $T/K = \pm 0.02$

$\delta P/P = \pm 0.01$

REFERENCES:

1. Lee, K.H.; Kohn, J.P. *J. Chem. Eng. Data* 1969, *14*, 292.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Dodecane; $C_{12}H_{26}$; [112-40-3]

ORIGINAL MEASUREMENTS:

Ribeiro, V.J.; Susu, A.A.;

Kohn, J.P.

J. Chem. Eng. Data 1972, *17*, 79-80.

VARIABLES:

T/K = 283-348

P/MPa = 0.51-9.12

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

t/C	[1] T/K	Total Pressure P/atm	[1] P/MPa	Ethene in liquid Mole Fraction, x_1	Liquid Solution Molar Volume V_L/cm^3 (mole)$^{-1}$
75	348.15	5.00	0.507	0.065	230.7
		10.00	1.013	0.120	221.7
		15.00	1.520	0.170	213.7
		20.00	2.026	0.220	205.3
		25.00	2.533	0.265	198.0
		30.00	3.040	0.310	190.8
		35.00	3.546	0.353	183.7
		40.00	4.053	0.395	177.0
		45.00	4.560	0.435	170.5
		50.00	5.066	0.475	164.0
		55.00	5.573	0.510	158.2
		60.00	6.080	0.542	152.8
		65.00	6.586	0.575	147.2
		70.00	7.093	0.602	142.5
		75.00	7.600	0.632	137.2
		80.00	8.106	0.660	132.7
		85.00	8.613	0.685	128.2
		90.00	9.119	0.712	123.5

[1] Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 10-cm^3 borosilicate glass equilibrium cell containing a known mass of degassed solvent was mounted in a constant temperature bath. Gas was quantitatively (± 0.006 cm^3) charged from a reservoir, kept at constant pressure, by mercury displacement. Pressure gauges mounted on the cell and the reservoir were accurate to 0.07 atm. Liquid volumes inside the cell could be read using calibration marks on the cell wall. Agitation was by using a magnetically activated stainless steel ball. The solubility was determined from the volume of gas consumed. Saturated solution volumes were read from the observed volumes in the cell. Additional details in reference 1. The dodecane vapor pressure was considered negligible even at 75 °C when it corresponded to 4.2 mm mercury.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson; minimum purity 99.5%. Gas critical temperature and pressure measured as 9.34°C at 50.09 atm.

2. Dodecane was from Humphrey-Wilkinson; 99.0% minimum purity.
Freezing point: -9.57°C.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.01$ T/K = ± 0.02

$\delta P/P = \pm 0.01$

REFERENCES:

1. Lee, K.H.; Kohn, J.P.

J. Chem. Eng. Data 1969, *14*, 292.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Eicosane (n-Eicosane); $C_{20}H_{42}$; [112-95-8]

ORIGINAL MEASUREMENTS:

Chou, J.S.; Chao, K. C.

J. Chem. Eng. Data 1989, *34*, 68-70.

VARIABLES:

T/K = 373.25 - 573.15
P/MPa = 1.01 - 5.06

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	[1]T/K	Pressure P/atm	 [1]P/MPa	Mole Fraction, Ethene, x_1
100.1	373.25	1.0	0.1013	0.0123 [2]
		10.10	1.023	0.123
		20.06	2.033	0.228
		29.94	3.034	0.320
		40.04	4.057	0.395
		49.95	5.061	0.456
200.0	473.15	1.0	0.1013	0.0081 [2]
		10.18	1.031	0.0820
		20.03	2.030	0.155
		29.91	3.031	0.221
		39.96	4.049	0.281
		49.91	5.057	0.335
300.0	573.15	1.0	0.1013	0.0065 [2]
		10.12	1.025	0.0659
		20.06	2.033	0.132
		29.95	3.035	0.190
		39.98	4.051	0.245
		49.93	5.059	0.296

[1] Calculated by Compiler.
[2] Estimated by Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/ PROCEDURE

Ethene is bubbled through a presaturator and then through the equilibrium cell, both being filled with the molten solvent. The cell is thermostated in a nitrogen bath. After saturation, a (molten) liquid sample is withdrawn into an evacuated trap connected to a gas handling system. The solvent solidifies, and the volume of the gas released is measured in a burette over water at a known temperature and pressure. The mass of the solid solvent is determined. Further details are in Ref. 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson Gas Products at a specified purity of 99.5%.
2. Eicosane was from Sigma Chemicals at a specified purity of 99.0%.

ESTIMATED ERROR:

δT/K = 0.1
δP/atm = 0.05
$\delta x/x$ = 0.02 (Compiler)

REFERENCES:

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

   Fluid Phase Equil. 1987, *36*, 141.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Octacosane; $C_{28}H_{58}$; [630-02-4]

ORIGINAL MEASUREMENTS:

Chou, J.S.; Chao, K. C.

J. Chem. Eng. Data 1989, *34*, 68-70.

VARIABLES:

T/K = 373.05 - 573.05
P/MPa = 1.01 - 5.06

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	[1]T/K	Pressure P/atm	Pressure [1]P/MPa	Mole Fraction, Ethene, x_1
99.9	373.05	1.0	0.1013	0.0146[2]
		10.04	1.017	0.147
		20.06	2.033	0.255
		30.02	3.042	0.344
		39.98	4.051	0.422
		49.94	5.060	0.488
199.9	473.05	1.0	0.1013	0.0098[2]
		10.03	1.016	0.0979
		20.00	2.026	0.181
		29.97	3.037	0.251
		39.99	4.052	0.311
		49.89	5.055	0.369
299.9	573.05	1.0	0.1013	0.0080[2]
		9.99	1.012	0.0804
		20.07	2.034	0.151
		30.01	3.041	0.214
		40.00	4.053	0.273
		49.98	5.064	0.321

[1] Calculated by Compiler.
[2] Estimated by Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Ethene is bubbled through a presaturator and then through the equilibrium cell, both being filled with the molten solvent. The cell is thermostated in a nitrogen bath. After saturation, a (molten) liquid sample is withdrawn into an evacuated trap connected to a gas handling system. The solvent solidifies, and the volume of the gas released is measured in a burette over water at a known temperature and pressure. The mass of the solid solvent is determined. Further details are in Ref. 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson Gas Products at a specified purity of 99.5%.
2. Octacosane was from the Aldrich Chemical Company at a specified purity of 99.0%.

ESTIMATED ERROR:

δT/K = 0.1
δP/atm = 0.05
$\delta x/x$ = 0.02 (Compiler)

REFERENCES:

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

Fluid Phase Equil. 1987, *36*, 141.

COMPONENTS:

1. **Ethene; C_2H_4; [74-85-1]**
2. **Hexatriacontane; $C_{36}H_{74}$; [630-06-8]**

ORIGINAL MEASUREMENTS:

Chou, J.S.; Chao, K. C.

J. Chem. Eng. Data 1989, *34*, 68-70.

VARIABLES:

T/K = 373.25 - 573.25
P/MPa = 1.02 - 5.06

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	[1] T/K	Pressure P/atm	Pressure [1] P/MPa	Mole Fraction, Ethene, x_1
100.1	373.25	1.0	0.1013	0.0170[2]
		10.13	1.026	0.172
		19.99	2.026	0.292
		29.97	3.037	0.393
		39.97	4.050	0.467
		49.93	5.059	0.527
199.9	473.05	1.0	0.1013	0.0112[2]
		10.09	1.022	0.113
		20.06	2.033	0.205
		29.95	2.964	0.280
		40.01	4.054	0.352
		49.97	5.063	0.403
299.9	573.05	1.0	0.1013	0.0093[2]
		10.10	1.023	0.0937
		20.07	2.034	0.177
		29.99	3.039	0.242
		39.97	4.050	0.306
		50.01	5.067	0.361

[1] Calculated by Compiler.
[2] Estimated by Compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Ethene is bubbled through a presaturator and then through the equilibrium cell, both being filled with the molten solvent. The cell is thermostated in a nitrogen bath. After saturation, a (molten) liquid sample is withdrawn into an evacuated trap connected to a gas handling system. The solvent solidifies, and the volume of the gas released is measured in a burette over water at a known temperature and pressure. The mass of the solid solvent is determined. Further details are in Ref. 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson Gas Products at a specified purity of 99.5%.
2. Hexatriacontane was from the Aldrich Chemical Company at a specified purity of 99.0%.

ESTIMATED ERROR:

δT/K = 0.1
δP/atm = 0.05
$\delta x / x$ = 0.02 (Compiler)

REFERENCES:

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

   Fluid Phase Equil. 1987, *36*, 141.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic, cyclic and alicyclic compounds for pressures less than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 October, 1993

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Aromatic, Cyclic and Alicyclic Compounds for Pressures less than 0.2 MPa

The solubilities of ethene in aromatic, cyclic and alicyclic compounds for a pressure of essentially 101.3 kPa were reported by some ten groups of researchers (1-10). Three groups of researchers reported their results in the form of graphs or correlations only (4,7,8) and from these solubility values were determined or calculated for comparison with other data.

For the solvents composed of carbon-ring structures, some general observations can be made concerning their solvating ability for ethene. It is observed that the ethene solubility is increased when the number of methyl side groups on a carbon ring compound is increased. The solubility is also increased when the degree of saturation of an unsaturated carbon-ring compound is increased. Finally, solvents having a ring structure all appear to have similar temperature coefficients of solubility for ethene. These observations are based on the fact that at the same temperatures the solubility in decahydronaphthalene is higher than in tetrahydronaphthalene, in methylbenzene it is higher than in benzene, and in turn in dimethyl benzene it is higher still than in methylbenzene. Finally, the solubilities in methylcyclohexane, when extrapolated, appear higher than those in cyclohexane solvent for the same temperatures.

Solubilities in individual solvents are now discussed in more detail below.

Benzene; C_6H_6; [71-43-2]

Horiuti (1) reported solubility data for ethene in benzene at low pressures for temperatures ranging from 278.15 K to 323.15 K. In spite of the date of the publication (1931/1932), Horiuti's data are known to be of high accuracy. Narasimhan and Nageshwar (2), and Jadot (3) reported ethene solubilities at 293.15 K, and at 298.15 K, respectively. Krauss and Gestrich (4) reported their results as a correlation utilizing an enthalpy of solution which permitted the calculation of solubilities in the temperature range from 293.15 to 313.15 K. The early results of McDaniel (5), while of historical interest, have been usually found to be significantly lower than those of more recent researchers as in this case, and are rejected. When compared with the other data, the result of Jadot is also rejected because it is approximately 9% lower than comparable data. The single value of Narasimhan and Nageshwar (2) is 4% higher than those of the remaining two research groups and is also rejected.

The remaining data are well represented by the following equation applicable for a temperature range from 278.15 K to 323.15 K and having a correlation coefficient of 0.9995:

$$\ln x_1 = -8.0954 + 1103.8/(T/K) \qquad (1)$$

Equation (1) has a maximum deviation from the experimental data of 0.9%. This equation and the data on which it is based are classified as tentative. It is noted that while both constants of Equation (1) are different than those listed in the compilation of the Horiuti data (1), the calculated values are virtually identical, differing by a maximum of only one figure in the fourth significant place.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic, cyclic and alicyclic compounds for pressures less than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 October, 1993

CRITICAL EVALUATION:

The mole fraction solubilities for ethene in benzene at 101.3 kPa pressure as calculated by means of Equation (1) are tabulated below:

T/K	$10^2\ x_1$	T/K	$10^2\ x_1$
278.15	1.606	303.15	1.158
283.15	1.518	308.15	1.093
288.15	1.398	313.15	1.036
293.15	1.327	318.15	0.9828
298.15	1.229	323.15	0.9327

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

Solubilities of ethene in methylbenzene at low pressure of four groups of researchers(4,6,7,8) are available over a wide temperature range, from 213.15 K (-60°C) to 313.15 K (40°C). The data of Waters et al. (6) were obtained using three different methods; hence, it is unlikely that systematic errors occurred. The data of Krauss and Gestrich (4) as well as of Hannaert et al. (7) were presented only as correlations. Values of the latter two groups were calculated for the temperature ranges for which the measurements were made. Leites and Ivanoskii (8) reported solubilities at low temperatures. A consistency test indicated that there is a good correlation for the temperature range from 243.15 K to 313.15 K, provided that the low temperature data of Leites and Ivanovskii are omitted. The equation obtained for the temperature range from 243.15 K to 313.15 K, having a correlation coefficient of 0.9980, an average deviation of 1.2% and a maximum deviation of 3.2% is:

$$\ln x_1 = -8.1440 + 1161.47/(T/\mathrm{K}) \qquad (2)$$

The data on which it is based and Equation (2) are classified as tentative. The value of Leites and Ivanovskii (8) is about 6% higher than the correlation of Hannaert et al. at 243.15 K. The low temperature data are also significantly higher, by about 10%, than Equation (2). It is, however, impossible to ascertain whether the data are too high or there is a curvature in the solubility-temperature relation. Until additional solubilities become available, the data of Leites and Ivanovskii are classified as tentative.

The mole fraction solubilities for ethene in methylbenzene at 101.3 kPa pressure were calculated by means of Equation (2) and are tabulated below:

T/K	$10^2\ x_1$	T/K	$10^2\ x_1$
243.15	3.449	293.15	1.527
253.15	2.856	398.15	1.429
263.15	2.399	303.15	1.340
273.15	2.041	313.15	1.186
283.15	1.756		

Dimethylbenzenes (xylenes); C_8H_{10}; [108-38-3]

Two research groups reported ethene solubilities in dimethylbenzene. Krauss and Gestrich (4) and Hannaert et al. (7), both reported their results as correlations only, but for different temperature ranges. Four values of solubility were calculated from each correlation and together were found to be very consistent. The correlating line representing data from both sources is:

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic, cyclic and alicyclic compounds for pressures less than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 October, 1993

CRITICAL EVALUATION:

$$\ln x_1 = -8.19193 + 1186.94/(T/K) \qquad (3)$$

Equation (3) covers temperatures from 243.15 K to 313.15 K, has a correlation coefficient of r = 0.9992 and maximum, and average deviations from the equation of 2.4%, and 1.1%, respectively. Attention is drawn to the fact that the solvent used by Hannaert et al. (7) contained only 90% dimethylbenzene of an unspecified isomer, with the remaining components being methylbenzene and ethylbenzene. Similarly, the solvent purity and isomer type used by Krauss and Gestrich (4) likewise were not specified. Hence, it is not possible to determine in which isomer the solubilities were obtained. However, because there is a relatively small difference in ethene solubilities in methylbenzene and in dimethylbenzene, it appears likely that the solubilities in all three dimethylbenzene isomers are similar. Equation (3) and the data on which it is based are classified as tentative.

Cyclohexane; C_6H_{12}; [110-82-7] and methylcyclohexane; C_7H_{14}; [108-87-2]

Only the results of Krauss and Gestrich (4), expressed as a correlation, are available for the solubilities of ethene in cyclohexane. The temperature range is from 293.15 K to 313.15 K. Only the results of Leites and Ivanovskii at low temperature (8) are available for solubilities in methylcyclohexane. These data are both classified as tentative.

Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2] and decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

Only the results of Krauss and Gestrich (4) for the temperature range from 293.15 to 313.15 K are available for the solubility of ethene in tetrahydronaphthalene. Again, only the results of Lenoir et al. (9) are available at two temperatures for the solubility in decahydronaphthalene. These data are both classified as tentative.

(R)-1-Methyl-4-(1-methylethenyl)cyclohexene, (Limonene); $C_{10}H_{16}$; [5989-27-5]

The result of McDaniel (5) is the only solubility of ethene available in limonene. As with most of McDaniel's results, a caution is expressed because his results have been found to be more than 20% too low. Hence, this result is considered to be of qualitative value only, and is rejected.

1,1'-Methylenebis(methylbenzene) or ditolylmethane; $C_{15}H_{16}$; [1335-47-3]

Glazunova et al. (10) reported ethene solubilities in 1,1'-methylenebis(methylbenzene) at temperatures to 413.15 K. These solubilities appear consistent and no other source of data is available for this solvent. These data are classified as tentative.

Two component solvent solutions composed of n-heptane; C_7H_{16}; [142-82-5] and methylbenzene; C_7H_8; [108-88-3], as well as of methylcyclohexane; C_7H_{14}; [108-87-2] and methylbenzene.

The solubilities of ethene in the mixed solvent solutions were reported for both solvent solutions for the low temperatures of 223.15 K and 213.15 K by Leites and Ivanovskii (8). These results were shown only graphically as Henry's constants and were recalculated as mole fraction solute. There is a maximum mole fraction solubility of ethene in

COMPONENTS: 1. Ethene; C_2H_4; [74-85-1] 2. Aromatic, cyclic and alicyclic compounds for pressures less than 0.2 MPa (2 atm)	EVALUATOR: Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 October, 1993

CRITICAL EVALUATION:

methylcyclohexane-methylbenzene solutions at about 25% methylbenzene, whereas, the solubility in n-heptane-methylbenzene solutions increases with increasing heptane concentrations. These results appear consistent and are classified as tentative.

References

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5. McDaniel, A.S. *J. Phys. Chem.* 1911, *15*, 587-610.

6. Waters, J.A.; Mortimer, G.A.; Clements, H.E. *J. Chem. Eng. Data* 1970, *15*, 174-176.

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9. Lenoir, J.-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data* 1971, *16*, 340-342.

10. Glazunova, T.V.; Ryabov, M.I.; Lipshtein, R.A. *Sov. At. Energ.* 1987, *62*, 449-451.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, *17*, 125 - 256.

VARIABLES:

T/K: 278.15 - 323.15

p_1/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick

H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^2x_1	Bunsen Coefficient α/cm^3(STP)cm^{-3}atm^{-1}	Ostwald Coefficient L/cm^{3}cm^{-3}
278.15	1.606	4.191	4.268
283.15	1.518	3.875	4.017
288.15	1.398	3.598	3.796
293.15	1.327	3.346	3.591
298.15	1.229	3.118	3.403
303.15	1.158	2.920	3.241
308.15	1.093	2.736	3.087
313.15	1.036	2.578	2.955
318.15	0.9828	2.428	2.828
323.15	0.9327	2.289	2.708

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

Smoothed Data: For use between 278.15 and 323.15 K.

$$\ln x_1 = -8.0797 + 10.9921/(T/100\text{K})$$

The standard error about the regression line is 8.15 x 10^{-5}.

T/K	Mol Fraction 10^2x_1	T/K	Mol Fraction 10^2x_1
278.15	1.612	298.15	1.236
283.15	1.503	303.15	1.163
288.15	1.405	313.15	1.036
293.15	1.317	323.15	0.930

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) Ethene. Prepared by dropping ethanol into orthophosphoric acid. The gas was cooled, passed through several wash solutions, dried, and fractionated from liquid air several times.

(2) Benzene. Merck. Extra pure and free of sulfur. Refluxed with sodium amalgam, distilled. Boiling point (760 mmHg) 80.18°C.

ESTIMATED ERROR:

$\delta T/\text{K} = 0.05$

$\delta x_1/x_1 = 0.01$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Nageshwar, G.W.

Chem. Petro-Chem. J. (India)

1979, *10*, 13-15.

VARIABLES: $T/K = 293.15$

$P/kPa = 101.325$ kPa

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1, for: $^1P = 101.325$	$^2P_1 = 101.325$	^{2}Ostwald Coefficient L/cm^3 gas$(\mathrm{cm}^3$ solvent$)^{-1}$
20	293.15	0.01235	0.01369	3.737

[1] Although not specifically stated in the paper, it is assumed that the mole fraction solubility is for a total pressure of 101.325 kPa.

[2] Calculated by compiler; a gas molar volume of 23910 cm^3/mole was used at 293.15 K and 101.325 kPa for the calculation of L, and Henry's law was assumed to apply for the calculation of x_1.

It was confirmed by personal communication that the solubilities were measured at atmospheric pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. Benzene was distilled twice in a laboratory packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A.

Anal. Chem. 1948, *20*, 624.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Krauss, V.W.; Gestrich, W.

Khemie - Technik 1977, *6*, 513-516.

VARIABLES:

T/K = 293.15 - 313.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	[1]Mole Fraction Ethene, x_1	[1]Ostwald Coefficient L/cm^3 gas (cm^3 solvent)$^{-1}$	[1]Bunsen Coefficient α/cm^3 (STP)cm^{-3}atm^{-1}
20	293.15	0.0132	3.60	3.36
25	298.15	0.0124	3.41	3.12
30	303.15	0.0116	3.23	2.91
40	313.15	0.0103	2.92	2.54

[1] There were no direct results, only a correlation. The results were calculated by the compiler for a gas partial pressure of 101.325 kPa using equations given in the paper for the applicable temperature range as follows:

$H = H_0 \exp(-\Delta H_L/fRT)$; $C = HP$

C = Solubility, mol/l; P = Pressure, bar

H = Henry's constant, mol/l.bar

H_0 = A constant, 0.00195, mol/l.bar

$-\Delta H_L$ = Enthalpy of solution, 10544, W s/mol

R = Gas constant, l.bar/mol.K

fR = Conversion factor, 8.324, W s.l.bar (mol^2.K)$^{-1}$ (determined by compiler from graphs of H versus T^{-1})

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel whose volume was 160 ml, containing a thermometer and stirring bar, was mounted in a constant temperature bath. A volume of about 100 ml of solvent was degassed then pressurized with ethene to a pressure not exceeding 2 bar in the absorption vessel. After equilibrium was achieved, the gas was slowly released into an evacuated gas expansion system connected to a mercury manometer. Any solvent vapor present in the gas was condensed in a low temperature coil. By material balance, considering the volumes of gas in the system, it was possible to calculate solubilities as Henry's constants.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Jadot, R.

J. Chim. Phys. 1972, *69*, 1036-40.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.3$

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's Law Constant, H/atm	Mole fraction$^+$ at partial pressure of 101.3 kPa, $x_{C_2H_4}$	#ΔH^∞ /cal mol^{-1} (/J mol^{-1})
298.15	89.46	0.01118	625 (2615)

\+ Calculated by compiler assuming $x_{C_2H_4} = 1/H$.

\# Excess partial molar enthalpy of solution at infinite dilution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The conventional gas chromatographic technique was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since no allowance was made for surface adsorption.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$; $\delta H = \pm 2\%$

REFERENCES:

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McDaniel, A. S.

J. Phys. Chem. 1911, *15*, 587-610.

VARIABLES:

T/K = 295.15 - 323.15

p_1/kPa = 101.3 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Mol Fraction	Bunsen Coefficient[a]	Ostwald Coefficient[b]
t/°C	T/K	10^2x_1	α	L/cm³ cm⁻³
22.0	295.15	1.10	2.7865	3.0100
25.0	298.15	1.06	2.6826	2.9281[c]
35.0	308.15	0.94	2.3530	2.6545
50.0	323.15	0.86	2.1000	2.4820

[a] Bunsen coefficient, α/cm^3(STP) cm^{-3} atm^{-1}.

[b] Listed as absorption coefficient in the original paper. Interpreted to be equivalent to Ostwald coefficient by compiler.

[c] Ostwald coefficient (absorption coefficient) estimated as 298.15 K value by author.

[d] Mole fraction and Bunsen coefficient values calculated by compiler assuming ideal gas behavior.

EVALUATOR'S COMMENT: McDaniel's data should be used with caution. His values are often 20 percent or more too small when compared with more reliable data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is all glass. It consists of a gas buret connected to a contacting vessel. The solvent is degassed by boiling under reduced pressure. Gas pressure or volume is adjusted using mercury displacement. Equilibration is achieved at atm pressure by hand shaking, and incrementally adding gas to the contacting chamber. Solubility measured by obtaining total uptake of gas by known volume of the solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Prepared by reaction of 1,2-dibromoethane with zinc-copper.

(2) Benzene.

ESTIMATED ERROR:

$\delta L/L \geq -0.20$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Methylbenzene (toluene); C_7H_8; [108-88-3]	Leites, I.L.; Ivanovskii, F.P. *Khim. Prom.* 1962, *9*, 653-657.
VARIABLES: T/K = 213.15 - 243.15 p_1/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] $\log_{10}H'$, H' /mm Hg	[2]Henry's Constant, H/atm (mole fraction)$^{-1}$	[2] Mole Fraction Ethene, x_1
-60	213.15	3.998	13.10	0.0764
-50	223.15	4.119	17.31	0.0578
-30	243.15	4.304	26.50	0.0377

These results were part of a study for the behavior of solubilities in two-component solvent solutions.

[1] Only graphical results were available in this paper; values of log of Henry's constant (H') were read from enlarged graphs by the compiler.

[2] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler based on the graphical results.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and controlled to a temperature to ± 0.05 K. The equilibrium cell was mounted in the cryostat. The solvent was purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Methylbenzene was distilled and analyzed by chromatography. Actual purity not given.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors).

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methylbenzene (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.

VARIABLES:

T/K = 250-295
P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	P/mm mercury	[2]Bunsen Coefficient α/cm^3 gas NTP (cm^3 solvent)$^{-1}$	[3]Solubility Mole/litre s	[3]Solubility [1]Average Mole Fraction, x_1
-23	250.15	760.0	6.894	0.311^B	0.0306
-20	253.15	760.0	6.320	0.283^B	0.0280
-10	263.15	222.6	5.310	0.237^A	0.0236
		359.9	5.240	0.234^A	
		475.6	5.270	0.235^A	
0	273.15	243.3	4.450	0.199^A	0.0201
		393.6	4.380	0.196^A	
		520.1	4.400	0.196^A	
		594.5	4.410	0.196^A	
		765.0	4.412	0.197^B	
		765.0	4.444	0.199^C	
10	283.15	260.9	3.850	0.172^A	0.0176
		422.6	3.770	0.168^A	
20	293.15	275.4	3.420	0.153^A	0.0159
		445.6	3.360	0.150^A	
22	295.15	760.0	3.189	0.142^B	0.0149

[1] Calculated by compiler.
[2] Although not specified in paper, compiler confirms that α as given is the Bunsen coefficient.
[3] Solubility, s and x_1, are calculated for a gas partial pressure of 101.325 kPa.
A,B,C, Refers to methods used as described below.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two of three methods used involved measuring the pressure change in a gas reservoir of known volume. The third involved weighing.
Method A: Two glass bulbs were connected by tubing fitted with a pressure transducer, gas supply and vacuum lines. The solvent (100 cm^3) was degassed in one bulb equipped with a stirrer using liquid nitrogen. Gas at a higher pressure in the second bulb was quantitatively charged into the first bulb at the appropriate temperature. The final pressure in the equilibration flask was measured.
Method B: For larger quantities of gas a stainless steel supply bomb connected to a pressure gauge was filled to about 12 atm. Equilibration was in a glass flask equipped with a mercrury manometer.
Method C: The increase in mass of the solution was measured.

SOURCE AND PURITY OF MATERIALS:

1. Ethene, Monsanto polymerization grade, minimum purity 99.85%.
2. Methyl benzene, Fisher spectrophotometric grade; purity not specified.

ESTIMATED ERROR:

δT/K = ± 0.01 (A); ± 0.02 (B)

$\delta s/s$ = 0.02

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Methylbenzene (toluene);

C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Krauss, V.W.; Gestrich, W.

Khemie - Technik 1977, *6*, 513-516.

VARIABLES:

$T/K = 293.15 - 313.15$

$p_1/kPa = 101.32$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	$^1T/K$	^{1}Mole Fraction Ethene, x_1	^{1}Ostwald Coefficient L/cm^3 gas$(cm^3$ solvent$)^{-1}$	^{1}Bunsen Coefficient α/cm^3 (STP)cm^{-3} atm^{-1}
20	293.15	0.0154	3.51	3.27
25	298.15	0.0144	3.32	3.04
30	303.15	0.0134	3.14	2.83
40	313.15	0.0119	2.83	2.47

[1] There were no direct results, only a correlation. The results were calculated by the compiler for a gas partial pressure of 101.325 kPa using equations given in the paper for the applicable temperature range as follows:

$$H = H_\circ \exp(-\Delta H_L/fRT); \quad C = HP$$

C = Solubility, mol/l; P = Pressure, bar

H = Henry's constant, mol/l.bar

$H_\circ$ = A constant, 0.00175, mol/l.bar

$-\Delta H_L$ = Enthalpy of solution, 10742, W s/mol

R = Gas constant, l.bar/mol.K

f R = Conversion factor, 8.324, W.s.l.bar $(mol^2.K)^{-1}$ (determined by compiler from graphs of H versus T^{-1})

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel whose volume was 160 ml, containing a thermometer and stirring bar, was mounted in a constant temperature bath. A volume of about 100 ml of solvent was degassed then pressurized with ethene to a pressure not exceeding 2 bar in the absorption vessel. After equilibrium was achieved, the gas was slowly released into an evacuated gas expansion system connected to a mercury manometer. Any solvent vapor present in the gas was condensed in a low temperature coil. By material balance, considering the volumes of gas in the system, it was possible to calculate solubilities as Henry's constants.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methylbenzene(toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 243.15 - 293.15

p_1/kPa = 101.3

PREPARED BY:

W. Hayduk
H.L. Clever

EXPERIMENTAL VALUES:

t/C	T/K	[1]Mole fraction Ethene, x_1
-30	243.15	0.0356
-10	263.15	0.0241
10	283.15	0.0172
20	293.15	0.0148

[1]Mole fraction solubility calculated by compilers for a gas partial pressure of 101.3 kPa using the equation developed by the authors with $\nu = 1$, for the applicable temperature range:

$$\log (K\pi\nu) = 3.68 - (\Delta H /\text{cal mol}^{-1})/(2.3R(T/\text{K}))$$

The authors' definitions are:

ΔH = 2,480 cal mol^{-1}, Enthalpy of dissolution

$$K = y_1 / x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π / atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = $(f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the least accurate.

The apparatus is of glass and consists of a burette in which the gas is confined over mercury, two bulbs for the solvent, one above the other, a mercury manometer and a constant temperature bath. A measured volume of solvent is degassed in the top bulb at ambient temperature and charged to the absorption bulb in the bath. Gas is charged to the desired pressure. The quantity of gas added at constant pressure is measured. Agitation is manual.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. For narcosis, 99.9 per cent.
2. Methylbenzene. Qualite UCB. Density, ρ^{20}/g cm^{-3} = 0.8689.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 10 to 15% (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Dimethylbenzene, (xylene), actual type not specified; C_8H_{10}; taken to be m-xylene [108-38-3]

ORIGINAL MEASUREMENTS:

Krauss, V.W.; Gestrich, W.

Khemie - Technik 1977, *6*, 513-516.

VARIABLES:

T/K = 293.15 - 313.15

p_1 /kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	[1]Mole Fraction Ethene, x_1	[1]Ostwald Coefficient L/cm^{3}gas(cm^3 solvent)$^{-1}$	[1]Bunsen Coefficient α/cm^3(STP)cm^{-3} atm^{-1}
20	293.15	0.0161	3.19	2.98
25	298.15	0.0150	3.00	2.75
30	303.15	0.0140	2.83	2.55
40	313.15	0.0123	2.53	2.21

[1] There were no direct results, only a correlation. The results were calculated by the compiler for a gas partial pressure of 101.325 kPa using equations given in the paper for the applicable temperature range as follows:

$$H = H_0 \exp(-\Delta H_L/fRT); \quad C = HP$$

C = Solubility, mol/l; P = Pressure, bar

H = Henry's constant, mol/l.bar

H_0 = A constant, 0.00126, mol/l.bar

$-\Delta H_L$ = Enthalpy of solution, 11309, W s/mol

R = Gas constant, l.bar/mol.K

f R = Conversion factor, 8.324, W s.l.bar.(mol^2.K)$^{-1}$ (determined by compiler from graphs of H versus T^{-1})

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel whose volume was 160 ml, containing a thermometer and stirring bar, was mounted in a constant temperature bath.
A volume of about 100 ml of solvent was degassed then pressurized with ethene to a pressure not exceeding 2 bar in the absorption vessel. After equilibrium was achieved, the gas was slowly released into an evacuated gas expansion system connected to a mercury manometer. Any solvent vapor present in the gas was condensed in a low temperature coil. By material balance, considering the volumes of gas in the system, it was possible to calculate solubilities as Henry's constants.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Dimethylbenzenes (xylenes); C_8H_{10}; [108-38-3]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 243.15 - 293.15

p_1/kPa = 101.3

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Mole Fraction Ethene, x_1
-30	243.15	0.0368
-10	263.15	0.0251
10	283.15	0.0180
20	293.15	0.0155

[1]Mole fraction solubility calculated by compiler for a gas partial pressure of 101.3 kPa using the equation developed by the authors with $\nu = 1$, for the applicable temperature range:

$$\log(K\pi\nu) = 3.63 - (\Delta H/\text{cal mol}^{-1})/(2.3R(T/\text{K}))$$

The authors' definitions are:

ΔH = 2,440 cal mol^{-1}, Enthalpy of dissolution

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π / atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = $(f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the least accurate.

The apparatus is of glass and consists of a burette in which the gas is confined over mercury, two bulbs for the solvent, one above the other, a mercury manometer and a constant temperature bath. A measured volume of solvent is degassed in the top bulb at ambient temperature and charged to the absorption bulb in the bath. Gas is charged to the desired pressure. The quantity of gas added at constant pressure is measured. Agitation is manual.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%.
2. Dimethylbenzenes. Merck and Co. Mixture of 90% dimethylbenzenes, 5% methylbenzene, and 5% ethylbenzene.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm$ 10 to 15% (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Krauss, V.W.; Gestrich, W.

Khemie - Technik 1977, *6*, 513-516.

VARIABLES:

T/K = 293.15 - 313.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1] T/K	[1] Mole Fraction Ethene, x	[1] Ostwald Coefficient L/cm^3 gas(cm^3 solvent)$^{-1}$	[1] Bunsen Coefficient α /cm^3 (STP)cm^{-3} atm^{-1}
20	293.15	0.0161	3.63	3.38
25	298.15	0.0150	3.40	3.12
30	303.15	0.0139	3.20	2.88
40	313.15	0.0122	2.85	2.48

[1] There were no direct results, only a correlation. The results were calculated by the compiler for a gas partial pressure of 101.325 kPa using equations given in the paper for the applicable temperature range as follows:

$$H = H_0 \exp(- \Delta H_L/fRT); \quad C = H\,P$$

C = Solubility, mol/l; P = Pressure, bar

H = Henry's constant, mol/l.bar

H_0 = A constant, 0.00123, mol/l.bar

$-\Delta H_L$ = Enthalpy of solution, 11679, W s/mol

R = Gas constant, l.bar/mol.K

f R = Conversion factor, 8.324, W.s.l.bar (mol^2.K)$^{-1}$ (determined by compiler from graphs of H versus T^{-1})

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel whose volume was 160 ml, containing a thermometer and stirring bar, was mounted in a constant temperature bath. A volume of about 100 ml of solvent was degassed then pressurized with ethene to a pressure not exceeding 2 bar in the absorption vessel. After equilibrium was achieved, the gas was slowly released into an evacuated gas expansion system connected to a mercury manometer. Any solvent vapor present in the gas was condensed in a low temperature coil. By material balance, considering the volumes of gas in the system, it was possible to calculate solubilities as Henry's constants.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methylcyclohexane; C_7H_{14}; [108-87-2]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

T/K = 213.15, 223.15

p_1/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] $\log_{10}(H'/\text{mmHg})$	[2] Henry's Constant, H/atm (mole fraction)$^{-1}$	[2] Mole Fraction Ethene, x_1
-60	213.15	3.909	10.67	0.0937
-50	223.15	4.037	14.33	0.0698

These results were part of a study for the behavior of solubilities in two-component solvent solutions.

[1] Only graphical results were available in this paper; values of log of Henry's constant (H') were read from enlarged graphs by the compiler.

[2] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler based on the graphical results.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and controlled to a temperature to ± 0.05 K. The equilibrium cell was mounted in the cryostat. The solvent was purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Methylcyclohexane was distilled and analyzed by chromatography. Actual purity not given.

ESTIMATED ERROR:

$\delta T/\text{K} = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene (Ethylene); C_2H_4; [74-85-1] 2. Decahydronaphthalene, (Decalin) $C_{10}H_{18}$; [91-17-8]	Lenoir, J-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data* 1971, *16*, 340-2.
VARIABLES: T/K = 298.15, 323.15 P/kPa = 101.3 (1 atm)	PREPARED BY: C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant $H_{C_2H_4}$/atm	Mole fraction at 1 atm* $x_{C_2H_4}$
298.15	72.2	0.0139
323.15	84.9	0.0118

* Calculated by compiler asssuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e. $x_{C_2H_4}$ (1 atm) = $1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

δT/K = ± 0.1; δH/atm = $\pm 6\%$ (estimated by compiler).

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Naphthalene, 1,2,3,4-tetrahydro-, (tetralin); $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Krauss, V.W.; Gestrich, W.

Khemie - Technik 1977, *6*, 513-516.

VARIABLES:

$T/\text{K} = 293.15 - 313.15$

$p_1/\text{kPa} = 101.32$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	[1]Mole Fraction Ethene, x_1	[1]Ostwald Coefficient $L/\text{cm}^3\text{gas}(\text{cm}^3\text{solvent})^{-1}$	[1]Bunsen Coefficient $\alpha/\text{cm}^3(\text{STP})\text{cm}^{-3}\text{atm}^{-1}$
20	293.15	0.0127	2.25	2.09
25	298.15	0.0119	2.15	1.97
30	303.15	0.0113	2.05	1.85
40	313.15	0.0101	1.88	1.64

[1] There were no direct results, only a correlation. The results were calculated by the compiler for a gas partial pressure of 101.325 kPa using equations given in the paper for the applicable temperature range as follows:

$H = H_0 \exp(- \Delta H_L /\text{fRT})$; $C = H P$

C = Solubility, mol/l; P = Pressure, bar

H = Henry's constant, mol/l.bar

H_0 = A constant, 0.00212, mol/l.bar

$-\Delta H_L$ = Enthalpy of solution, 9190, W s/mol

R = Gas constant, l.bar/mol.K

f R = Conversion factor, 8.324, W.s.l.bar $(\text{mol}^2.\text{K})^{-1}$ (determined by compiler from graphs of H versus T^{-1})

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The absorption vessel whose volume was 160 ml, containing a thermometer and stirring bar, was mounted in a constant temperature bath. A volume of about 100 ml of solvent was degassed then pressurized with ethene to a pressure not exceeding 2 bar in the absorption vessel. After equilibrium was achieved, the gas was slowly released into an evacuated gas expansion system connected to a mercury manometer. Any solvent vapor present in the gas was condensed in a low temperature coil. By material balance, considering the volumes of gas in the system, it was possible to calculate solubilities as Henry's constants.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) (R)-1-Methyl-4-(1-methylethenyl) cyclohexene or Limonene; $C_{10}H_{16}$; [5989-27-5] see also [499-97-8]

ORIGINAL MEASUREMENTS:

McDaniel, A. S.

J. Phys. Chem. 1911, *15*, 587-610.

VARIABLES:

T/K = 295.15

p_1/kPa = 101.3 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature		Ostwald Coefficient
t/°C	T/K	L/cm^3 cm^{-3}
22.0	295.15	2.753 → 3.05 in 12 h. Equilibrium not established

EVALUATOR'S COMMENT: McDaniel's data should be used with caution. His values are often 20 percent or more too small when compared with more reliable data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is all glass. It consists of a gas buret connected to a contacting vessel. The solvent is degassed by boiling under reduced pressure. Gas pressure or volume is adjusted using mercury displacement. Equilibration is achieved at atm pressure by hand shaking, and incrementally adding gas to the contacting chamber. Solubility measured by obtaining total uptake of gas by known volume of the solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Prepared by reaction of 1,2-dibromoethane with zinc-copper.

(2) Limonene.

ESTIMATED ERROR:

$\delta L/L \geq -0.20$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane; C_7H_{16}; [142-82-5]
3. Methylbenzene (toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

T/K = 213.15, 223.15
p_1/kPa = 101.325
x_3 = 0 - 1.0

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Solvent Composition, x_3, Mole Fraction Toluene	[2]$\log_{10}(H'/\text{mmHg})$	[3]Henry's Constant H/atm (mole fraction)$^{-1}$	[3]Mole Fraction Ethene, x_1
-60	213.15	0 (heptane)	3.841	9.12	0.110
		0.25	3.848	9.27	0.108
		0.50	3.863	9.60	0.104
		0.75	3.900	10.45	0.0957
		1.0 (toluene)	3.998	13.10	0.0764
-50	223.15	0 (heptane)	3.965	12.14	0.0824
		0.25	3.978	12.51	0.0800
		0.50	3.996	13.04	0.0767
		0.75	4.030	14.10	0.0709
		1.0 (toluene)	4.119	17.31	0.0578

[1] Compositions of two-component solvent solutions are given on a solute-free basis.

[2] Only graphical results were available; values of log Henry's constant (H') were read from an enlarged graph by the compiler.

[3] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and the temperature was controlled to ± 0.05 K. The equilibration cell was mounted in the cryostat. The solvents were purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Heptane was distilled and analyzed by chromatography. Purity not specified.
3. Methylbenzene was distilled and analyzed by chromatography. Purity not specified.

ESTIMATED ERROR:

$\delta T/\text{K} = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methylcyclohexane; C_7H_{14}; [108-87-2]
3. Methylbenzene (toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

T/K = 213.15, 223.15
p_1/kPa = 101.325
x_3 = 0 - 1.0

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Solvent Composition, x_3, Mole Fraction Toluene	[2]$\log_{10}(H'/\text{mmHg})$	[3]Henry's Constant H/atm (mole fraction)$^{-1}$	[3]Mole Fraction Ethene, x_1
-60	213.15	0 (m.c.hexane)	3.909	10.67	0.0937
		0.25	3.900	10.45	0.0957
		0.50	3.900	10.45	0.0957
		0.75	3.915	10.82	0.0924
		1.0 (toluene)	3.998	13.10	0.0763
-50	223.15	0 (m.c.hexane)	4.037	14.33	0.0698
		0.25	4.020	13.78	0.726
		0.50	4.028	14.03	0.0713
		0.75	4.056	14.97	0.0668
		1.0 (toluene)	4.119	17.31	0.0578

[1] Compositions of two-component solvent solutions are given on a solute-free basis.

[2] Only graphical results were available; values of log Henry's constant (H') were read from an enlarged graph by the compiler.

[3] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and the temperature was controlled to ± 0.05 K. The equilibration cell was mounted in the cryostat. The solvents were purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Methylcyclohexane was distilled and analyzed by chromatography. Purity not specified.
3. Methylbenzene was distilled and analyzed by chromatography. Purity not specified.

ESTIMATED ERROR:

δT/K = ± 0.05

$\delta x_1/x_1$ = ± 0.01 (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1,1'-Methylenebis(methylbenzene), (ditolyl methane); $C_{15}H_{16}$; [1335-47-3]

ORIGINAL MEASUREMENTS:

Glazunova, T.V.; Ryabov, M.I.; Lipshtein, R.A.
Sov. At. Energ., 1987, *62*, 449-451.

VARIABLES:

T/K = 291-413
P_1/kPa = 101.3

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

t/°C	T/K	Bunsen coefficient	Mole fraction at partial pressure of 1 atm.[a]
18	291	1.7149	0.01512
50	323	1.2607	0.01116
140	413	0.7444	0.00662

[a] Calculated by compiler assuming the ideal gas law and the molar volume of component 2 is 200.7 $cm^3\ mol^{-1}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE

Single pass flow system in which sample of solvent was saturated with gas at or near atmospheric pressure. Sample of solvent withdrawn and analysed using gas chromatography fitted with thermal conductivity detector.

SOURCE AND PURITY OF MATERIALS:

1. Purity at least 99.8 per cent by volume.
2. Technical grade to TU 3810298-76 standard.

ESTIMATED ERROR:

$\delta T/K = \pm\ 0.5$; $\delta x/x = \pm 0.10$

REFERENCES:

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic and Alicyclic compounds T/K = 196 - 423 P/MPa up to 19.3	C.L. Young School of Chemistry University of Melbourne Parkville, Victoria Australia, 3052 December 1993

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Cyclohexane and Various Aromatic Hydrocarbons for Pressures greater than 0.2 MPa (2 atm)

Ten groups of researchers (1-10) have measured solubilities for ethene in cyclohexane and in various aromatic hydrocarbons at elevated pressures. Solubilities were measured by two or more groups for benzene, toluene and xylenes but in general there are relatively few data available so that extensive evaluations are not possible. One group (3) has studied two-component solvent systems.

Few sets of data included both the liquid and gas phase compositions. In this evaluation we have, where possible, checked if the available data give a linear relationship for log x versus log P, which is indicative but not conclusive of consistent data. Furthermore, where possible we have compared extrapolated values at a partial pressure of 0.1013 MPa with values determined at or near 0.1013 MPa pressure. Correlating equations have been included where possible.

Cyclohexane; C_6H_{12}; [110-82-7]

This system has been investigated (1) at six temperatures from 303 K to 423 K at pressures between 1.7 MPa and 9.0 MPa. Linear plots were obtained at all temperatures when log x was plotted against log P. There are no gross inconsistencies in the data. Considerable uncertainty is involved in the long extrapolation of the data to 101.3 kPa. but the values obtained appear about 10% greater than the values obtained from the work of Krauss and Gestrich (11) (Please see low pressure Critical Evaluation). The values of Zhuze et al. (1) are therefore classified as tentative.

Benzene; C_6H_6; [71-43-2]

Ethene solubilities in benzene have been reported by five groups of research workers (2,4,8-10) for total pressures from 0.28 MPa to 19.3 MPa and for temperatures ranging from 293 to 423 K. The results of Paratella and Sagramora (8) are rejected. Their solubilities are considerably lower than those of any other group and extrapolate to 101.3 kPa to give values considerably smaller than the tentative low pressure values. The data of Hiraoka (10) are difficult to evaluate; the lower temperature solubilities are broadly consistent with Henry's law constants determined from low pressure measurements but there are no low pressure results at the higher temperatures for comparison. The data of Ellis et al. (9) at 348.15 K are broadly consistent with the data of Kozorezov et al. (4) at the same temperature. The data of Kozorezov et al. (4) appear to have a reasonable temperature dependency and together with the limited data of Ellis et al. are classified as tentative. The data of Konobeev and Lyapin (2) are consistent with the data of Kozorezov et al. (4) and are also classified as tentative.

Methylbenzene; C_7H_8; [108-88-3]

This system has been studied by four groups of workers (2, 5-7) for temperatures ranging from 228 K to 473 K and total pressures from 0.1 to 6 MPa. It is difficult to evaluate the data because of the different temperature and pressure ranges involved. Frank (7) measured the solubilities of ethene in toluene at four temperatures between 273 and 323 K up to pressures of 0.4 MPa. The values of the solubilities extrapolated to 0.1013 MPa are several percent lower than the values measured at or near 0.1013 MPa. The Henry's law constants obtained from the graphs given by Tyvina et al. (5) can be used to calculate the mole fraction solubility of ethane in toluene at a partial pressure of 0.1013 MPa. The values are in fair agreement with the values measured at or near 0.1013

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic and Alicyclic compounds T/K = 196 - 423 P/MPa up to 19.3	C.L. Young School of Chemistry University of Melbourne Parkville, Victoria Australia, 3052 December 1993

CRITICAL EVALUATION:

MPa considering the problem of obtaining the solubility from the graphs. The results of Knonbeev and Lyapin (2) are consistent with the values of Tyvina et al. (5). The data of Shenderei et al. (6) are the only low temperature data available at elevated pressures. The values extrapolated to 0.1013 MPa and 238.15 and 248.15 K are consistent with the low pressure data of Leites and Ivanovskii (12). Please see low pressure Critical Evaluation. None of the sets of data can be recommended but the data of Shenderei et al. (6), Tyvina et al. (5) and Konobeev and Lyapin (2) are classified as tentative for the temperature and pressure range covered by the respective data. Please see Table 1.

Table 1. Comparison of Extrapolated High Pressure Solubilities with Low Pressure Results for the System Ethene - Methylbenzene

T/K	Av. extrapolated solubility[a]		Solubility measured at low pressure[a]	% deviation
	Ref. 5	Ref. 7		
273.15		0.0204	0.0207	-1.4
293.15	0.0139		0.0152	-8.5
		0.0146		-3.9
308.15		0.0114	0.0124	-8.1
313.15	0.0108		0.0116	-6.9

[a] at a partial pressure of 0.1013 MPa

1,2-Dimethylbenzene; C_8H_{10}; [106-42-3]
1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]
1,4-Dimethylbenzene; C_8H_{10}; [95-47-6]

Ethene solubilities in a mixture of xylenes were reported by Konobeev and Lyapin (2) at pressures from 0.28 MPa to 3.21 MPa and temperatures from 293 K to 333 K. Nakamura et al. (3) reported ethene solubilities in each xylene isomer at six temperatures ranging from 213 K to 303 K and total pressures up to 1.28 MPa. Although the authors did not provide ethene partial pressures, they gave average Henry's constants for each operating temperature. Assuming a direct inverse relationship between Henry's law constant and the mole fraction solubility at an ethene partial pressure of 101.3 kPa, the latter was calculated and plotted against $1/T$. A linear relationship was obtained in all cases and this shows some degree of consistency of the data. The equation of the line of best fit was determined for each of the isomers. The equations of the lines and the corresponding correlation coefficients are:

1,2-dimethylbenzene

$$\log x = -3.74 + 569.3/(T/\mathrm{K}) \quad \text{coeff.} = 0.9991 \qquad (1)$$

1,3-dimethylbenzene

$$\log x = -3.85 + 591.2/(T/\mathrm{K}) \quad \text{coeff.} = 0.9998 \qquad (2)$$

1,4-dimethylbenzene

$$\log x = -3.90 + 599.7/(T/\mathrm{K}) \qquad (3)$$

It is not meaningful to give a correlation coefficient for the 1,4-dimethylbenzene solubilities since half of the values were obtained by extrapolation of data for the binary solvent (1,4-dimethylbenzene + ethylbenzene) results.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic and Alicyclic compounds T/K = 196 - 423 P/MPa up to 19.3	C.L. Young School of Chemistry University of Melbourne Parkville, Victoria Australia, 3052 December 1993

CRITICAL EVALUATION:

In Table 2 the extrapolated high pressure solubility data of Nakamura et al. (3) have been compared with the low pressure measurements of Krauss and Gestrich (11) for 1,3-dimethylbenzene. The average deviation between the two sets of data was 3.9%. At 293.15 K the data of Konobeev and Lyapin (2) for the dimethylbenzene mixture are consistent with those of Nakamura et al. (3) at the same temperature. Both are classified as tentative.

Table 2. Comparison of Extrapolated High Pressure Solubilities with Low Pressure for the System Ethene - 1,3-Dimethylbenzene

T/K	Av. extrapolated solubility[a]	Solubility measured at low pressure[a]	% deviation
293.15	0.0151	0.0159	-5.0
273.15	0.0205	0.0214	-4.0
252.65	0.0313	0.0304	+2.7

[a] at a partial pressure of 0.1013 MPa

Ethylbenzene; C_8H_{10}; [100-41-4]

Nakamura et al. (3) reported solubility data for ethene in ethylbenzene at temperatures ranging from 196 K to 293 K and Kororezov et al. (4) measured ethene solubilities at similar pressures but for temperatures in the range 323 K to 423 K. Both workers gave Henry's constants and using these constants values of solubilities at a partial pressure of 101.3 kPa were calculated. The data of the two groups of workers gave colinear points on a plot of log x versus $1/T$ and are thus considered to be consistent with each other. The equation of the best fit line is:

$$\log x = -3.628 + 534.5/(T/\mathrm{K}) \quad (4)$$

Since this equation has a correlation coefficient of 0.9983 it provides a suitable estimate of the solubility of ethene in ethylbenzene over the temperature range 196 K to 423 K.

The data of Nakamura et al. (3) and Kororezov et al. (4) are both classified as tentative.

Diethylbenzene; $C_{10}H_{14}$; [25340-17-4]

Ethene solubilities in diethylbenzene were reported by Kozorezov et al. (4) for total pressures from 0.25 MPa to 1.52 MPa at temperatures ranging from 323 to 423 K. The authors gave Henry's constants and the mole fraction solubilities at partial pressures of 101.3 kPa were calculated (assuming a direct inverse relationship) and were plotted against 1/T.

A linear plot was obtained; therefore, the data of Kozorezov et al. (4) are classified as tentative.

Benzene,1,4-dimethyl-,(p-xylene); C_8H_{10}; [106-42-3]
and Ethylbenzene, C_8H_{10}; [100-41-4] solvent mixtures
Benzene,1,3-dimethyl-,(m-xylene); C_8H_{10}; [108-38-3] and Ethylbenzene; C_8H_{10}; [100-41-4] solvent mixtures

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Aromatic and Alicyclic compounds T/K = 196 - 423 P/MPa up to 19.3	C.L. Young School of Chemistry University of Melbourne Parkville, Victoria Australia, 3052 December 1993

CRITICAL EVALUATION:

Benzene,1,2-dimethyl-,(o-xylene); C_8H_{10}; [95-47-6] and Ethylbenzene; C_8H_{10}; [100-41-4] solvent mixtures

Nakamura et al. [3] measured the solubilities of ethene in two component solvent mixtures containing ethylbenzene and each of the three xylene isomers at temperatures in the range of 213.15 K to 273.15 K. The working pressures were in the range of 192.5 kPa to 983 kPa. Based on the evaluation of the data in the pure solvents by these authors, these data also are classified as tentative.

References

1. Zhuze, T.P.; Zhurba, A.S.; Esakov, E.A. *Bull. Acad. Sci. USSR, Inst. Geol. Min. Fuels*, 1960, *2*, 2150-2152.
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8. Paratella, A., Sagramora, G. *Ric. Sci. (Italy)*, 1959, *29*, 2605-2613.
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11. Krauss, V.W.; Gestrich, W. *Khemie - Technik*, 1977, *6*, 513-516.
12. Leites, I.L.; Ivanovskii, F.P. *Khim. Prom.*, 1962, *9*, 653-657.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Zhuze, T.P.; Zhurba, A.S.;

Esakov, E.A.

Bull. Acad. Sci. USSR, Inst. Geol. Min. Fuels. 1960, *2*, 2150-2152.

VARIABLES:

T/K = 300-423

P/MPa = 2 - 10, (20-100 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Pressure	Partial Pressure[1]		Mole Fraction Ethylene[2]	
t/°C	T/K	P/Atm	p_1/Atm	p_1/MPa	liquid, x_1	vapor, y_1
30	303.15	20	19.8	2.01	0.245	0.990
		40	39.8	4.03	0.520	0.995
		60	59.4	6.02	0.830	0.990
50	323.15	20	19.5	1.98	0.200	0.975
		40	39.2	3.97	0.405	0.980
		60	58.8	5.96	0.510	0.980
		80	76.4	7.74	0.845	0.955
75	348.15	20	19.0	1.93	0.160	0.950
		40	38.6	3.91	0.315	0.965
		60	58.5	5.93	0.460	0.975
		80	76.8	7.78	0.635	0.960
		100	88.0	8.92	0.860	0.880

[1] Calculated by compiler.

[2] Only graphical data available in reference; data read from enlarged graph by compiler.

Liquid solution molar volumes are also shown as a graph.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method is similar to that described by Sage and Lacey. Accurately known masses of solvent and gas were charged into an evacuated equilibrium vessel. The temperature was controlled to ± 0.05 K. The volume occupied by the system in the equilibrium vessel was varied by forcing a definite amount of mercury into it from a graduated mercury supply vessel equipped with a movable electric indicator. Equilibrium was attained using an electromagnetic stirrer. The pressure was measured using pressure guages. A sample of the gas phase was passed to a trap cooled to 213 K with acetone and dry ice. From a reading of a gas burette connected to the trap, the volume of ethylene was determined. From the increase in weight of the trap (0.5-1.5g) the solvent content of the gas phase was obtained.

SOURCE AND PURITY OF MATERIALS:

1. Ethene contains 2.9% ethane.
2. Cyclohexane properties given as:

   Density at 20°C = 0.7801 g/cm^3

   n_D^{20} = 1.4271

   Normal boiling point = 80.9 °C.

ESTIMATED ERROR:

Original data: $\delta x_1/x_1$ = ± 2%

Tabulated values: $\delta x_1/x_1$ = ± 4%

REFERENCES:

Sage, B.H.; Lacey, W.N.

Trans. Am. Inst. Mining Met. Eng., 1940, *136*, 138.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Zhuze, T.P.; Zhurba, A.S.;

Esakov, E.A.

Bull. Acad. Sci. USSR, Inst. Geol.

Min. Fuels. 1960, *2*, 2150-2152.

VARIABLES:

T/K = 300-423

P/MPa = 2 - 10, (20-100 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

		Pressure	Partial Pressure[1]		Mole Fraction Ethylene[2]	
t/°C	T/K	P/Atm	p_1/Atm	p_1/MPa	liquid, x_1	vapor, y_1
100	373.15	20	17.9	1.81	0.125	0.895
		40	37.2	3.77	0.260	0.930
		60	56.1	5.68	0.380	0.935
		80	75.2	7.62	0.525	0.940
		100	91.0	9.22	0.670	0.910
125	398.15	20	16.7	1.69	0.105	0.835
		40	35.0	3.55	0.220	0.875
		60	53.7	5.44	0.335	0.895
		80	72.0	7.30	0.450	0.900
		100	88.5	8.97	0.580	0.885
150	423.15	20	--	--	0.085	--
		40	--	--	0.185	--
		60	--	--	0.290	--
		80	--	--	0.390	--
		100	--	--	0.520	--

[1] Calculated by compiler.

[2] Only graphical data available in reference; data read from enlarged graph by compiler.

Liquid solution molar volumes are also shown as a graph.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method is similar to that described by Sage and Lacey. Accurately known masses of solvent and gas were charged into an evacuated equilibrium vessel. The temperature was controlled to ±0.05 K. The volume occupied by the system in the equilibrium vessel was varied by forcing a definite amount of mercury into it from a graduated mercury supply vessel equipped with a movable electric indicator. Equilibrium was attained using an electromagnetic stirrer. The pressure was measured using pressure guages. A sample of the gas phase was passed to a trap cooled to 213 K with acetone and dry ice. From a reading of a gas burette connected to the trap, the volume of ethylene was determined. From the increase in weight of the trap (0.5-1.5g) the solvent content of the gas phase was obtained.

SOURCE AND PURITY OF MATERIALS:

1. Ethene contains 2.9% ethane.
2. Cyclohexane properties given as:

   Density at 20°C = 0.7801 g/cm^3

   n_D^{20} = 1.4271

   Normal boiling point = 80.9°C.

ESTIMATED ERROR:

Original data: $\delta x_1/x_1$ = ± 2%

Tabulated values: $\delta x_1/x_1$ = ± 4%

REFERENCES:

Sage, B.H.; Lacey, W.N.

Trans. Am. Inst. Mining Met. Eng.,

1940, *136*, 138.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Benzene; C_6H_6; [71-43-2]	Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-6.
VARIABLES: $T/K = 293.15 - 333.15$ $P/MPa = 0.286 - 3.23$	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5 Pa$	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.070	0.036
	8.106	0.096
	14.19	0.172
	17.43	0.224
	21.08	0.288
	31.82	0.502
313.15	2.857	0.024
	8.258	0.076
	17.63	0.174
	23.31	0.220
	32.12	0.380
333.15	2.878	0.018
	8.268	0.061
	17.43	0.136
	32.32	0.278

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$; $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Kozorezov, Yu.I.; Rusakov, A.P.; Pikalo, N.M.

Khim. Prom. <u>1969</u>, *5*, 343-5.

VARIABLES:

$T/K = 323.15 - 423.15$

$P/MPa = 0.25 - 1.54$

PREPARED BY:

C.L. Young
W. Hayduk

EXPERIMENTAL VALUES:

T/K	$^1P/10^5Pa$	P/atm	Mole fraction of ethene in liquid, $x_{C_2H_4}$	Solubility cm^3 (STP)/g
323.15	2.5	2.5	0.020	6.0
	5.1	5.0	0.040	11.9
	10.1	10.0	0.081	25.4
	15.2	15.0	0.122	39.9
373.15	2.5	2.5	0.004	1.3
	5.1	5.0	0.017	5.1
	10.1	10.0	0.043	13.0
	15.2	15.0	0.072	22.3
403.15	5.1	5.0	0.006	1.7
	10.1	10.0	0.030	8.6
	15.2	15.0	0.051	14.9
423.15	6.6	6.5	0.003	1.0
	10.1	10.0	0.010	5.1
	15.2	15.0	0.047	12.1

[1] Calculated by compilers.

Henry's constant given as atm/mole fraction as follows:

T/K	323.15	373.15	403.15	423.15
H, atm /mole fraction	115.2	181.0	204.0	229.0

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Single pass flow apparatus. Ethene allowed to flow through solvent for 3 to 5 hours. Liquid sample withdrawn and analysed by stripping out ethene and measuring amount volumetrically. Solvent in sample estimated gravimetrically.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.93 mole per cent.
2. Boiling point 80°C; melting point 54°C

   $d_4^{20} = 0.8796$; $n_D^{20} = 1.5010$.

ESTIMATED ERROR:

$\delta T/K = \pm 0.5$; $\delta P/10^5Pa = \pm 0.1$; $\delta x_{C_2H_4} = \pm 0.001$

(estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Benzene; C_6H_6; [71-43-2]	Hiraoka, H. *Rev. Phys. Chem. Japan*, 1958, *28*, 64-66.
VARIABLES:	**PREPARED BY:**
T/K = 298-423 P/MPa = 4.1 - 19.3, (40-189 atm)	W. Hayduk

EXPERIMENTAL VALUES:

T/K	Total Pressure kg/cm^2	Total Pressure MPa[1]	Partial Pressure[2] p_1/Atm	Partial Pressure[2] p_1/MPa	Mole Fraction Ethene liquid, x_1	Mole Fraction Ethene vapor,[2] y_1
298.15	42	4.12	40.6	4.11	0.559	0.999
323.15	42	4.12	40.4	4.10	0.421	0.995
	103	10.1	99.6	10.1	0.786	0.999
373.15	42	4.12	39.3	3.98	0.264	0.967
	70	6.86	66.7	6.76	0.445	0.985
	103	10.1	99.1	10.0	0.654	0.994
	197	19.3	189.8	19.2	0.526	0.995
423.15	42	4.12	35.7	3.62	0.186	0.879
	70	6.86	63.7	6.46	0.333	0.940
	103	10.1	96.6	9.78	0.483	0.969
	154	15.1	146.7	14.9	0.617	0.984
	197	19.3	187.8	19.0	0.527	0.985

[1] Calculated by compiler.

[2] Calculated by compiler assuming Raoult's Law.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium was acheived by bubbling gas at constant temperature and pressure through benzene solvent stored in a stainless steel vessel. Gas and liquid phases were sampled and analyzed. The gas phase was condensed with liquid air then slowly warmed to room temperature. The residual liquid after evaporation of ethylene was considered to be benzene. The liquid phase was sampled at constant pressure by slowly displacing the mercury in a sample bomb and adding gas at a rate required to keep the pressure constant. The liquid sample was analyzed. Further details of analysis and calculations were not given in this paper, although some earlier work was mentioned but the reference to it was not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by dehydration of ethanol and purified by distillation. Infra-red spectrum indicated no ether.

2. Benzene source and purity not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = 0.02$

REFERENCES:

114

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Paratella, A.; Sagramora, G.

Ric. Sci. (Italy), 1959, *29*,

2605-2613.

VARIABLES:

T/K = 298.15,348.15

P/MPa = 2.94-9.81, (29-97 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	^1T/K	Total Pressure P/kg cm^{-2}	^1P/MPa	^{1}Partial Pressure p_1/MPa	Mole Fraction, x_1	^{1}Henry's Constant H/atm (mole fraction)$^{-1}$
25.0	298.15	30	2.942	2.930	0.0212	1364
		60	5.884	5.872	0.0521	1112
75.0	348.15	30	2.942	2.856	0.00719	3920
		60	5.884	5.800	0.0251	2281
		100	9.807	9.738	0.2050	469

[1] Calculated by compiler.

It is noted by compiler that these results are in serious disagreement with all other results.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A dynamic method was used in which the solvent was saturated by bubbling the gas through the solvent. The body of the cell was constructed of metal. Saturation was achieved by passing the gas through the solvent. The consumption of gas was high (20-40 l/h). The solvent was initially fed into the cell, and solution subsequently withdrawn, by means of a valve and capillary tubing. Details of the pressure control and analytical systems were not available.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was spectroscopy grade at 99.7% purity.
2. Benzene source and purity not given.

ESTIMATED ERROR:

δT/K = ± 0.3

Probable error in solubility is high. (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Ellis, S.R.M.; Valteris, R.L.;
Harris, G.J.

Chem. Eng. Prog. Symp. Ser.,
1968, *64*, 16-21.

VARIABLES:

T/K = 348.15

P/MPa = 1.4-8.3 (14-82 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

P /atm	Partial pressure[1]		Mole fraction ethene	
	p_1/atm	p_1/MPa	in liquid, x_1	in vapor, y_1
15.0	13.9	1.41	0.099	0.925
21.1	20.1	2.04	0.144	0.954
29.9	28.5	2.88	0.205	0.952
38.1	36.7	3.72	0.259	0.964
57.1	55.3	5.60	0.398	0.968
73.5	70.5	7.14	0.554	0.959
81.6	78.0	7.90	0.599	0.956
87.1	81.8	8.29	0.665	0.939
90.0	82.1	8.32	0.710	0.912

[1] Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A static method with a 500 cm stainless steel vessel equipped with a plunger, perforated-cup stirrer was used. The perforated cup was attached to a soft iron rod which was raised up by means of an electromagnet, and dropped downward under its own weight. Ethylene was displaced from a reservoir by mercury using a volumetric piston pump to the desired pressure. After equilibration, samples of gas and liquid were withdrawn for analysis. During the sampling process, an equivalent volume of mercury was allowed to flow from the sample bomb back to the equilibration vessel. The liquid portion of the samples was condensed at atmospheric pressure using dry-ice and acetone whereas the gas portion was aspirated volumetrically over water. Analysis was by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.03$ T/K = ± 2

$\delta P/P = \pm 0.01$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methylbenzene (toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Frank, V.H.P.

Österr. Chemik.- Zeitung 1967, *68*, 360-361.

VARIABLES:

T/K = 273.15 - 323.15

p/MPa = 0.1013 - 0.4053

PREPARED BY:

W. Hayduk

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EXPERIMENTAL VALUES:

T/K	Partial Pressure Ethene p/atm	Partial Pressure Ethene [1]p_1/MPa	Percent by Weight Ethene, w_1	[1] Mole Fraction Ethene, x_1	[2] Values of k
273.15 (0°C)	1	0.1013	0.63	0.0204	0.55
	2	0.2026	1.3	0.0415	
	3	0.3040	1.9	0.0598	
	4	0.4053	2.7	0.0835	
293.15 (20°C)	1	0.1013	0.45	0.0146	0.40
	2	0.2026	0.90	0.0290	
	3	0.3040	1.4	0.0446	
	4	0.4053	1.9	0.0598	
308.15 (35°C)	1	0.1013	0.35	0.0114	0.30
	2	0.2026	0.70	0.0226	
	3	0.3040	1.1	0.0352	
	4	0.4053	1.5	0.0476	
323.15 (50°C)	1	0.1013	0.25	0.00816	0.20
	2	0.2026	0.50	0.0162	
	3	0.3040	0.75	0.0242	
	4	0.4053	1.1	0.0352	

[1] Calculated by compiler.

[2] Values of a type of Henry's constant (actually H^{-1}) were also given in the form of the following equation:

$$C = k.p$$

C = Equilibrium concentration, g ethene/100 ml of solvent
k = A type of Henry's constant
p = Gas partial pressure, atm

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The source of the data was stated to be reference 1. Only a graph is available in that reference. It was also stated that the Hoechst company (Germany) used these values of solubility.

There were no details of apparatus or procedure.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not given.

ESTIMATED ERROR:

$\delta w_1/w_1 = \pm 0.04$ (compiler)

REFERENCES:

1. Bier, G.; Lehmann, G. *"Copolymerization" Chap. IVB of High Polymers, G. Ham, Ed.* 1964, *Vol. XVIII Interscience, New York*, 169.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Methylbenzene (Toluene); C_7H_8; [108-88-3]	Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-6.
VARIABLES: T/K = 293.15 - 333.15 P/MPa = 0.284 - 3.16	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5$Pa	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.070	0.040
	8.197	0.109
	14.89	0.199
	31.11	0.430
313.15	2.837	0.029
	8.268	0.087
	31.41	0.347
333.15	2.837	0.022
	8.299	0.070
	17.73	0.151
	31.61	0.287

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

δT/K=±0.1; δP=±0.5%; $\delta x_{C_2H_4}$ =±0.002

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene, methyl-, (toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Zhur. Fiz. Khim. 1962, *36*, 801-808.

OR *Russian J. Phys. Chem.* 1962, *36*, 415-419.

VARIABLES:

T/K = 228.05 - 248.15

P/bar = 1 - 18.2

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

11f

x_1 S

T/K	P/atm	P/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	Solubility $^+$
248.15	1	1.0	0.0330	8.24
	3	3.0	0.1010	26.80
	5	5.1	0.1700	49.42
	10	10.1	0.3600	135.61
	12	12.2	0.4410	191.31
	15	15.2	0.5832	336.90
	18	18.2	0.7390	682.40
238.15	1	1.0	0.0408	10.29
	3	3.0	0.1280	35.40
	5	5.1	0.2135	67.22
	10	10.1	0.4881	229.71
	12	12.2	0.6200	294.60
	15	15.2	0.8263	1505.00
228.05	1	1.0	0.510	12.95
	3	3.0	0.1680	48.71
	5	5.1	0.2930	99.90
	10	10.1	0.7300	651.60

$+$ $cm^3 g^{-1}$ at p_1 = 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with magnetic stirrer. Pressure measured with Bourdon gauge. Samples of liquid analysed by stripping out ethene. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Prepared from ethanol by dehydration and purified by absorption in cuprous chloride under pressure.
2. Distilled.

ESTIMATED ERROR:

δT/K = ±0.1; δP/bar = ±0.3; $\delta x_{C_2H_4}$ = ±2%.

(estimated by compiler).

REFERENCES:

1. Shenderei, E.R.; Zel'venskii, Ya. D.; Ivanovskii, F.P.

   Khim. Prom. 1960, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methylbenzene (toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Tyvina, T.N.; Naumova, A.A.; Polyakov, S.A.

Zhur. Prikl. Khim. 1979, *52*, 949-952.
OR
J. Appl. Chem. USSR 1979, *52*, 910-913.

VARIABLES:

T /K = 293.15 - 473.15

P/MPa = 0.507 - 6.08

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		[1] Henry's Constants		
t/C	T/K	H'/atm (mol fraction)$^{-1}$	H/MPa (mol fraction)$^{-1}$	[1] Mole Fraction Ethene, x_1
20	293.15	72.2	7.32	0.0139
40	313.15	92.8	9.40	0.0108
60	333.15	112.7	11.42	0.00888
80	353.15	135.4	13.72	0.00739
100	373.15	156.1	15.82	0.00641
120	393.15	170.3	17.25	0.00587
140	413.15	184.7	18.71	0.00542
160	433.15	196.7	19.93	0.00508
180	453.15	200.7	20.33	0.00498
200	473.15	203.3	20.60	0.00493

No numerical data were given; only a graph showing total pressure as a function of mole fraction toluene was included.

[1] Values of Henry's constants and mole fraction ethene for a partial pressure of 101.3 kPa were calculated from total pressures and compositions read from an enlarged graph by the compiler. Raoult's law was assumed for the solvent vapor pressure. Henry's law was obeyed for ethene concentrations of at least up to 0.30 mole fraction.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was described in reference 1. The ethene absorber was a 1-litre pressure vessel submerged in a constant temperature bath. Ethene was bubbled through the solvent continuously at constant pressure for 3-5 hours. The ethene was passed through a reflux condenser to minimize the escape of solvent vapor. After saturation was complete, a sample of the solution was directed to an evacuated separator and allowed to flash to a low temperature and pressure. The quantity of solvent from the flashing step was weighed, while the quantity of ethene released was determined by measuring the increase in pressure, by manometer, in a gas accumulator of known volume and temperature.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was specified to be 99.9%.
2. Methylbenzene was of the CP grade.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 4\%$ (compiler)

REFERENCES:

1. Kozorezov, Yu. I.; Rusakov, A.P.; Pikalo, N.M.

   Khim. Prom. 1963, *5*, 343.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Xylene (mixture of the three isomers); C_8H_{10};

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967, *43*, 114-6.

VARIABLES:

$T/K = 293.15 - 333.15$

$P/MPa = 0.286 - 3.21$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5 Pa$	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.080	0.044
	8.106	0.117
	14.49	0.206
	20.67	0.316
	31.71	0.455
313.15	2.857	0.030
	8.238	0.091
	32.02	0.360
333.15	2.867	0.024
	8.248	0.074
	20.97	0.193
	32.12	0.300

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.
2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$; $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethylbenzene; C_8H_{10}; [100-41-4]

ORIGINAL MEASUREMENTS:

Kozorezov, Yu.I., Rusakov, A.P.; Pikalo, N.M.

Khim. Prom. 1969, *5*, 343-5.

VARIABLES:

T/K = 323.15 - 423.15

P/MPa = 0.25 - 1.52

PREPARED BY:

C.L. Young
W. Hayduk

EXPERIMENTAL VALUES:

T/K	[1]$P/10^5$Pa	P/atm	Mole fraction of ethene in liquid, $x_{C_2H_4}$	Solubility, cm^3 (STP)/g
323.15	2.5	2.5	0.024	5.2
	5.1	5.0	0.047	10.5
	10.1	10.0	0.099	23.1
	15.2	15.0	0.152	37.5
373.15	2.5	2.5	0.013	2.8
	5.1	5.0	0.029	6.4
	10.1	10.0	0.061	13.9
	15.2	15.0	0.097	22.6
403.15	5.1	5.0	0.022	4.8
	10.1	10.0	0.050	11.1
	15.2	15.0	0.078	17.9
423.15	6.6	6.5	0.024	5.3
	10.1	10.0	0.041	8.9
	15.2	15.0	0.068	15.5

[1] Calculated by compilers.

Henry's constant reported as atm./mole fraction as follows:

T/K	323.15	373.15	403.15	423.15
H, atm / mole fraction	101.6	158.6	183.7	205.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Single pass flow apparatus. Ethene allowed to flow through solvent for 3 to 5 hours. Liquid sample withdrawn and analysed by stripping out ethene and measuring amount volumetrically. Solvent in sample estimated gravimetrically.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.93 mole per cent.
2. Boiling point 135.8°C,

   d_4^{20} = 0.8673; n_D^{20} = 1.4960.

ESTIMATED ERROR:

δT/K = ±0.5; $\delta P/10^5$Pa = ±0.1;
$\delta x_{C_2H_4}$ = ±0.001.
(estimated by compiler).

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Diethylbenzene; $C_{10}H_{14}$; [25340-17-4]

ORIGINAL MEASUREMENTS:

Kozorezov, Yu.I.; Rusakov, A.P.; Pikalo, N.M.

Khim. Prom. 1969, *5*, 343-5.

VARIABLES:

T/K = 323.15 - 423.15

P/MPa = 0.25 - 1.52

PREPARED BY:

C.L. Young
W. Hayduk

EXPERIMENTAL VALUES:

T/K	$^1P/10^5$Pa	P/ atm	Mole fraction of ethene in liquid, $x_{C_2H_4}$	Solubility, cm^3 (STP)/g
323.15	2.5	2.5	0.026	4.6
	5.1	5.0	0.053	9.3
	10.1	10.0	0.106	20.1
	15.2	15.0	0.163	32.6
373.15	2.5	2.5	0.017	2.9
	5.1	5.0	0.035	6.0
	10.1	10.0	0.070	12.6
	15.2	15.0	0.106	20.0
403.15	5.1	5.0	0.028	4.8
	10.1	10.0	0.056	10.1
	15.2	15.0	0.089	16.2
423.15	6.6	6.5	0.034	5.7
	10.1	10.0	0.050	8.9
	15.2	15.0	0.079	14.6

[1] Calculated by compilers.

Henry's constants given as atm./mole fraction as follows:

T/K	323.15	373.15	403.15	423.15
H, atm / mole fraction	94.1	141.2	170.1	185.0

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Single pass flow apparatus. Ethene allowed to flow through solvent for 3 to 5 hours. Liquid sample withdrawn and analysed by stripping out ethene and measuring amount volumetrically. Solvent in sample estimated gravimetrically.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.93 mole per cent.
2. Boiling point range 179-182°C; d_4^{20} = 0.8643; n_D^{20} = 1.4962; (60.9% m-isomer and 35.5% o- and p-isomers by chromatographic analysis).

ESTIMATED ERROR:

δT/K = ±0.5; $\delta P/10^5$Pa = ±0.1;
$\delta x_{C_2H_4}$ = ±0.001

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Benzene,1,2-dimethyl-, (o-xylene); C_8H_{10}; [95-47-6]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;

Amemiya, T.

Kogyo Kagaku Zasshi , 1966, *69*, 42-47.

VARIABLES:

T/K = 213.15-293.15

P/kPa = 182.4-1276.7 (1.8-12.6 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	Total Pressure P/atm	[1]P/kPa	Mole Fraction Ethene, x_1	Average Henry's Constant H/atm (mole fraction)$^{-1}$
20.0	293.15	3.9	395.2	0.056	69.1
		6.8	689.0	0.097	
		9.7	982.9	0.140	
0.0	273.15	3.9	395.2	0.076	50.9
		6.8	689.0	0.134	
		9.7	982.9	0.190	
-21.6	251.55	3.9	395.2	0.119	33.2
		6.8	689.0	0.203	
		9.7	982.9	0.288	
		12.6	1276.7	0.379	
-30.0	243.15	4.8	486.4	0.173	27.5
		4.8	486.4	0.175	
		6.8	689.0	0.247	
		8.7	881.5	0.322	
		8.7	881.5	0.322	
		9.7	982.9	0.361	
		12.6	1276.7	0.482	

[1] Calculated by compiler. The solvent vapor pressure was neglected.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was chaken, gas evacuated and cell reachaged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%; the impurity consisted of 0.4% nitrogen.

2. The 1,2-dimethylbenzene purity was 99.9% as checked by GC after drying using solid sodium.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta P/P$ = ± 0.01

$\delta x_1/x_1$ = ± 0.02 (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Benzene,1,2-dimethyl-, (o-xylene); C_8H_{10}; [95-47-6]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.; Amemiya, T.

Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 213.15-293.15

P/kPa = 182.4-1276.7 (1.8-12.6 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

...continued

t /C	[1] T/K	Total Pressure P/atm	[1] P/kPa	[2] Mole Fraction Ethene, x_1	Average Henry's Constant H/atm (mole fraction)$^{-1}$
-40.0	233.15	1.8	182.4	0.091	21.0
		3.9	395.2	0.184	
		5.8	587.7	0.276	
		6.8	689.0	0.328	
-60.0	213.15	1.9	192.5	0.162	11.9
		3.9	395.2	0.319	

[1] Calculated by compiler.

[2] The solubilities in xylene at temperatures lower than the xylene freezing point were calculated from the data for ethylbenzene-xylene mixtures given elsewhere in this volume.

The solvent vapor pressure was neglected.

An equation for Henry's constant was given: $\log_{10} H = 3.90-601\ (T/K)^{-1}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%; the impurity consisted of 0.4% nitrogen.

2. The 1,2-dimethylbenzene purity was 99.9% as checked by GC after drying using solid sodium.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta P/P$ = ± 0.01

$\delta x_1/x_1$ = ± 0.02 (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Benzene,1,3-dimethyl-, (m-xylene); C_8H_{10}; [108-38-3]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;
Amemiya, T.

Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 213.15-293.15

P/kPa = 182.4-1276.7 (1.8-12.6 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	^1T/K	Total Pressure P/atm	^1P/kPa	Mole Fraction Ethene, x_1	Average Henry's Constant H/atm(mole fraction)$^{-1}$
20.0	293.15	3.9	395.2	0.058	66.3
		6.8	689.0	0.103	
		9.7	982.9	0.146	
0.0	273.15	3.9	395.2	0.080	48.7
		6.8	689.0	0.141	
		9.7	982.9	0.119	
-20.5	252.65	3.9	395.2	0.120	32.0
		6.8	689.0	0.207	
		9.7	982.9	0.302	
		12.6	1276.7	0.395	
-40.0	233.15	3.9	395.2	0.189	20.5
		6.8	689.0	0.332	
		9.7	982.9	0.510	
-50.0	223.15	1.8	182.4	0.120	15.5
		3.9	395.2	0.250	
		5.8	587.7	0.388	
-60.0	^{2}213.15	1.9	192.5	0.164	11.8
		3.9	395.2	0.331	
		4.8	486.4	0.441	

[1] Calculated by compiler.

[2] The solubilities at temperatures lower than the xylene freezing point were calculated from the data for ethylbenzene-xylene mixtures given elsewhere in this volume.

The solvent vapor pressure was neglected.

An equation for Henry's constant was given: $\log_{10} H = 3.84 - 591\ (T/K)^{-1}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%; the impurity consisted of 0.4% nitrogen.
2. The 1,3-dimethylbenzene purity was 99.9% as checked by GC after drying using solid sodium.

ESTIMATED ERROR:

$\delta T/K = \pm\ 0.1$

$\delta P/P = \pm\ 0.01$

$\delta x_1/x_1 = \pm\ 0.02$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene,1,4-dimethyl-, (p-xylene); C_8H_{10}; [106-42-3]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;
Amemiya, T.
Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 233.15-303.15

P/kPa = 192.5-982.9 (1.9-9.7 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	^1T/K	Total Pressure P/atm	^1P/kPa	Mole Fraction Ethene, x_1	Average Henry's Constant, H/atm(mole fraction)$^{-1}$
30.0	303.15	3.9	395.2	0.050	71.2
		3.9	395.2	0.051	
		6.8	689.0	0.091	
		6.8	689.0	0.091	
		9.7	982.9	0.132	
20.0	293.15	3.9	395.2	0.061	62.8
		6.8	689.0	0.106	
		9.7	982.9	0.154	
10.0	283.15	6.8	689.0	0.125	54.4
		9.7	982.9	0.177	
0.0	^{2}273.15	3.9	395.2	0.081	46.9
		6.8	689.0	0.145	
		9.7	982.9	0.206	
-21.2	^{2}251.95	3.9	395.2	0.130	30.7
		6.8	689.0	0.221	
		9.7	982.9	0.311	
-40.0	^{2}233.15	1.9	192.5	0.104	19.6
		3.9	395.2	0.197	
		6.8	689.0	0.360	

[1] Calculated by compiler.

[2] The solubilities at temperatures lower than the xylene freezing point were calculated from the data for ethylbenzene-xylene mixtures given elsewhere in this volume.

The solvent vapor pressure was neglected.

An equation for Henry's constant was given: $\log_{10} H = 3.71 - 561\ (T/K)^{-1}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%; the impurity consisted of 0.4% nitrogen.
2. The 1,4-dimethylbenzene purity was 99.9% as checked by GC after drying using solid sodium.

ESTIMATED ERROR:

$\delta T/K = \pm\ 0.1$
$\delta P/P = \pm\ 0.01$
$\delta x_1/x_1 = \pm\ 0.02$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethylbenzene; C_8H_{10}; [100-41-4]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;
Amemiya, T.

Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 195.15-293.15

P/kPa = 121.6-1277 (1.2-12.6 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	$^1T/K$	Total Pressure P/atm	$^1p/kPa$	Mole Fraction Ethene Ethene, x_1	Average Henry's Constant H/atm (mole fraction)$^{-1}$
20.0	293.15	3.9	395.2	0.057	65.8
		6.8	689.0	0.103	
		9.7	982.9	0.147	
0.0	273.15	3.9	395.2	0.080	48.4
		6.8	689.0	0.139	
		9.7	982.9	0.201	
-21.2	251.95	3.9	395.2	0.121	31.8
		6.8	689.0	0.210	
		9.7	982.9	0.306	
		12.6	1276.7	0.395	
-40.0	233.15	3.9	395.2	0.190	20.6
		6.8	689.0	0.329	
		9.7	982.9	0.516	
-60.0	213.15	1.9	192.5	0.160	12.1
		3.9	395.2	0.338	
		4.8	486.4	0.495	
-77.2	195.95	1.2	121.6	0.159	7.3
		1.9	192.5	0.279	
		1.9	192.5	0.284	
		2.9	293.8	0.476	
		2.9	293.8	0.464	

[1] Calculated by compiler. The solvent vapor pressure was neglected.

An equation for Henry's constant was given: $\log_{10}H = 3.77 - 571\,(T/K)^{-1}$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%; the impurity was nitrogen, 0.4%.
2. Ethyl benzene source and purity not given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$
$\delta P/P = \pm 0.01$
$\delta x_1/x_1 = \pm 0.02$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene,1,2-dimethyl-, (o-xylene); C_8H_{10}; [95-47-6]
3. Ethylbenzene; C_8H_{10}; [100-41-4]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;
Amemiya, T.

Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 213.15-233.15
P/kPa = 182.4-689.0 (1.8-6.8 atm)
Ethylbenzene mole fr., x'_3=0.311-0.593

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	Total Pressure P/atm	[1]P/kPa	Number of [2] Solvent	Moles, Ethene	[3] Mole Fraction Ethylbenzene in Solvent, x'_3	Mole Fraction Ethene, x_1
-40.0	233.15	1.8	182.4	o:0.5545 e:0.2504	0.0809	0.311	0.091
		3.9	395.2	o:0.4854 e:0.2192	0.1608	0.311	0.186
		5.8	587.7	o:0.5497 e:0.2482	0.3066	0.311	0.278
		6.8	689.0	o:0.5249 e:0.2370	0.3722	0.311	0.328
-60.0	213.15	1.9	192.5	o:0.3272 e:0.4768	0.1540	0.593	0.161
		3.9	395.2	o:0.3263 e:0.4755	0.3961	0.593	0.331

[1] Calculated by compiler.

[2] The symbols o, and e, refer to actual number of moles of o-xylene, and ethylbenzene, in gas-free solvent solution, respectively.

[3] The ethene-free solvent composition (x'_3) was calculated by the compiler.

The purpose of these low temperature measurements was to determine the hypothetical solubility in xylene below the xylene freezing point.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the vol ume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%.
2. 1,2-Dimethylbenzene purity was 99.9% as determined by GC.
3. Ethylbenzene source and purity not given.

ESTIMATED ERROR:

δT/K = ± 0.1
$\delta P/P$ = ± 0.01
$\delta x_1/x_1$ = ± 0.02 (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene,1,3-dimethyl-, (m-xylene); C_8H_{10}; [108-38-3]
3. Ethylbenzene; C_8H_{10}; [100-41-4]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;

Amemiya, T.

Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 213.15
P/kPa = 192.5-486.4 (1.9-4.8 atm)
Ethylbenzene mole fr., x_3' = 0.298

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	Total Pressure P/atm	[1]P/kPa	Number of Moles, [2]Solvent	Ethene	[3]Mole Fraction Ethylbenzene in Solvent, x_3'	Mole Fraction Ethene, x_1
-60.0	213.15	1.9	192.5	m:0.5630 e:0.2387	0.1561	0.2977	0.163
		3.9	395.2	m:0.5677 e:0.2408	0.4032	0.2978	0.333
		4.8	486.4	m:0.5677 e:0.2408	0.6210	0.2978	0.435

[1] Calculated by compiler.

[2] The symbols m, and e, refer to actual number of moles of m-xylene, and ethylbenzene, in gas-free solvent solution, respectively.

[3] The ethene-free solvent composition (x_3') was calculated by the compiler.

The purpose of these low temperature measurements was to determine the hypothetical solubility in xylene below the xylene freezing point.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%.
2. 1,3-Dimethylbenzene purity was 99.9%.
3. Ethylbenzene purity not given.

ESTIMATED ERROR:

δT/K = ± 0.1
$\delta P/P$ = ± 0.01
$\delta x_1/x_1$ = ± 0.02 (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene,1,4-dimethyl-, (p-xylene); C_8H_{10}; [106-42-3]
3. Ethylbenzene; C_8H_{10}; [100-41-4]

ORIGINAL MEASUREMENTS:

Nakamura, E.; Koguchi, K.;

Amemiya, T.

Kogyo Kagaku Zasshi, 1966, *69*, 42-47.

VARIABLES:

T/K = 233.15-273.15

P/kPa = 192.5-982.9 (1.9-9.7 atm)

Ethylbenzene mole fr.x'_3=0.304-0.729

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	Total Pressure P/atm	[2]P/kPa	Number of [2] Solvent	Moles, Ethene	[3]Mole Fraction Ethylbenzene in Solvent, x'_3	Mole Fraction Ethene, x_1
0.0	273.15	3.9	395.2	p:0.5525 e:0.2415	0.0699	0.3042	0.081
		6.8	689.0	p:0.5613 e:0.2453	0.1358	0.3041	0.144
		9.7	982.9	p:0.5567 e:0.2433	0.2053	0.3041	0.204
-21.2	251.95	3.9	395.2	p:0.3505 e:0.4459	0.1144	0.5599	0.126
		6.8	689.0	p:0.3536 e:0.4498	0.2214	0.5599	0.216
		9.7	982.9	p:0.3530 e:0.4490	0.3540	0.5599	0.306
-40.0	233.15	1.9	192.5	p:0.2172 e:0.5828	0.0834	0.7285	0.094
		3.9	395.2	p:0.2177 e:0.5843	0.1904	0.7285	0.192
		6.8	689.0	p:0.2197 e:0.5894	0.4125	0.7285	0.338

[1] Calculated by compiler.

[2] The symbols p, and e, refer to actual number of moles of p-xylene, and ethylbenzene, in gas-free solvent solution, respectively.

[3] The ethene-free solvent composition (x'_3) was calculated by the compiler. The purpose of these low temperature measurements was to determine the hypothetical solubility in xylene below the xylene freezing point.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For lower pressures a 200 cm^3 graduated glass cell was used. Solvent was charged to 100 cm^3; then the cell and contents were weighed. For degassing, ethene was pressured into the cell from a 170 cm^3 ss bomb; then the cell was shaken, gas evacuated and cell recharged with ethene several times. After degassing, the cell contents were equilibrated at constant temperature and pressure for 3-4 h. After the volume of solution was measured, the sealed cell was placed in a dessicator and later weighed at room temperature. For higher pressures two cells, one glass the other ss, of identical volume were used simultaneously. The same procedure was used except that the solution volume was measured in the glass cell and the final mass in the ss cell. The glass tended to fail at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.6%.
2. 1,4-Dimethylbenzene purity was 99.9% as determined by GC.
3. Ethylbenzene source and purity not given.

ESTIMATED ERROR:

δT/K = ± 0.1

$\delta P/P$ = ± 0.01

$\delta x_1/x_1$ = ± 0.02 (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Alcohols; pressures less than 0.2 MPa (2 atm)

EVALUATOR:

W. Hayduk
Chemical Engineering
University of Ottawa
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June, 1992

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubility in Alkanols and Other Alcohols for pressures Less than 0.2 MPa

The solubilities of ethene in normal alkanols for a pressure of essentially 101.3 kPa were reported by some seven groups of researchers (1-7). Only for two of these solvents, for methanol and butanol, were data provided over temperature range greater than 10 K. In addition, ethene solubilities are available for 2-propanol (7), cyclohexanol (8), dipropylene glycol (9), phenol (9) and benzyl alcohol (9). Finally, solubilities are available for a two-component solvent solution composed of 1-butanol and 1,2-ethanediol (ethylene glycol) (10) at 298.15 K.

It is useful to test whether the solubility of ethene at one temperature (298.15 K) follows a linear relation in the normal alcohols when plotted as log x_1 versus log C_n where x_1 is the mole fraction solubility and C_n is the number of carbon atoms in each of the alkanols. It was previously found that such a linear relation was obtained for the solubilities of ethane (11) and for propane, butane and 2-methylpropane as well (12). Only three research groups reported ethene solubilities in more than one alkanol solvent. Boyer and Bircher (2) provided solubility data for all the alkanols from methanol to 1-octanol at 298.15, Narasimhan et al. (4) for ethanol to 1-pentanol and Yano et al. (5) provided data for methanol to 1-propanol. These data especially, provide a means for testing the consistency of the data at 298.15 K among three groups.

Figure 1 shows all the available data for ethene solubilities at 298.15 K in the alkanols from methanol to 1-octanol as the mole fraction solubility, x_1, versus the solvent carbon number on log scales. It may be observed that the data appear consistent except for the solubilities in methanol. For this solvent only, the data of Boyer and Bircher (2) appear consistent while that of Narasimhan et al. (4) and Yano et al. (5) appear too high by more than 5% whereas the data of Ohgaki et al. (3) appear too low by more than 5%. It will be shown subsequently that the data of Boyer and Bircher in methanol are also consistent with the extrapolated data of Hannaert et al. (6) and Shenderei et al. (1). The resulting linear relation for the solubility of ethene in the alkanols for a gas partial pressure of 101.3 kPa and a temperature of 298.15 K, excluding the data outside the 5% range mentioned above, and expressed in two ways is:

$$\log x_1 = 0.5140 \log C_n - 2.3702 \qquad (1)$$

$$x_1 = 0.004264\, C_n^{0.5140}$$

The correlation coefficient for equation (1) is 0.9950 and the maximum deviation of the 15 data points from the calculated line is 5%. Based on equation (1) the solubilities were calculated and are shown in Table 1.

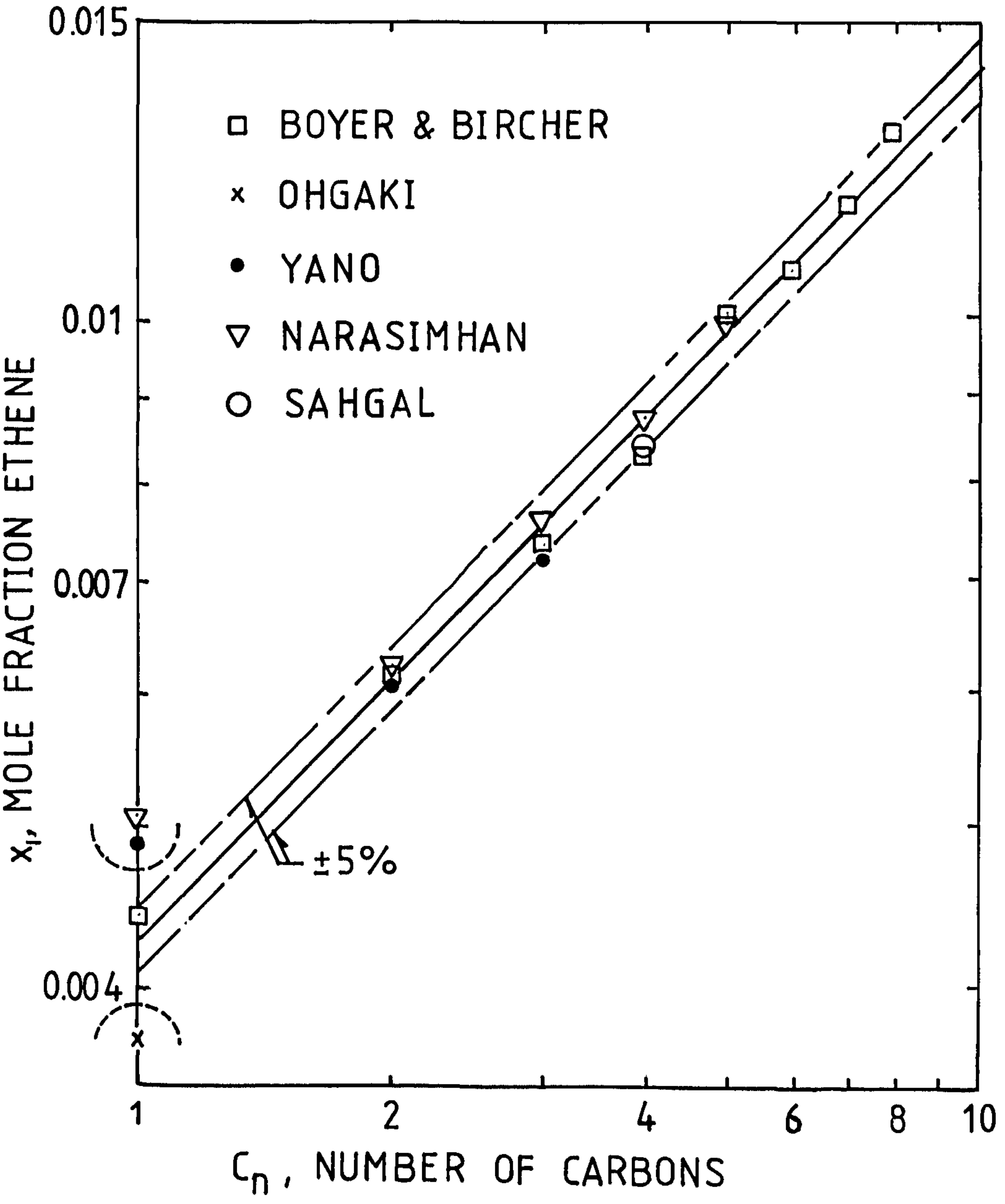
Table 1: Calculated solubility of ethene in the alkanols at 298.15 K and 101.3 kPa partial pressure

C_n	1 (methanol)	2 (ethanol)	3 (propanol)	4 (butanol)
x_1	0.00426	0.00609	0.00750	0.00869
C_n	5 (pentanol)	6 (hexanol)	7 (heptanol)	8 (octanol)
x_1	0.00975	0.0107	0.0116	0.0124

COMPONENTS: 1. Ethene; C_2H_4; [74-85-1] 2. Alkanols; methanol to 1-octanol for pressures less than 0.2 MPa (2 atm)	EVALUATOR: W. Hayduk Chemical Engineering University of Ottawa Ottawa, Ontario Canada K1N 6N5 June, 1992

CRITICAL EVALUATION:

Fig. 1 Solubility of ethene in alkanols from methanol to 1-octanol at 298.15 K and an ethene partial pressure of 101.3 kPa.



COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Alcohols; pressures less than 0.2 MPa (2 atm)

EVALUATOR:

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June, 1992

CRITICAL EVALUATION:

Solubilities in the individual solvents are discussed in more detail below.

Methanol; CH_4O; [67-56-1]

Solubilities of ethene in methanol were measured at temperatures from 298.15 K (25°C) to 217.15 K (-56°C) but, surprisingly, there are no data above 298.15 K. The low temperature values of Shenderei et al. (1) and Hannaert et al. (6) as well as that of Boyer and Bircher (2) at 298.15 K are highly consistent and can be represented by the following linear relationship in which T is in K and x_1 is the mole fraction solubility:

$$\log x_1 = 574.8/(T/\mathrm{K}) - 4.284 \qquad (2)$$

The correlation coefficient for the regression line is 0.9992. The values for the ethene solubility in methanol as expressed by equation (2) are classified as tentative for the temperature range from 217.15 K to 298.15 K and are shown in Table 2.

Table 2: Calculated values for mole fraction solubility of ethene in methanol

t, °C	T,K	x_1, Mole fraction ethene
25	298.15	0.00440
20	293.15	0.00475
10	283.15	0.00557
0	273.15	0.00661
-10	263.15	0.00795
-20	253.15	0.00970
-30	243.15	0.0120
-40	233.15	0.0152
-50	223.15	0.0196

Ethanol; C_2H_6O; [64-17-5]

The three values of Boyer and Bircher (2), Narasimhan et al. (4) and Yano et al. (5) for ethene solubility in ethanol at 298.15 K are within 2% of the average value which corresponds to a mole fraction at an ethene partial pressure of 101.3 kPa of $x_1 = 0.00614$. The solubility of Narisamhan et al. at 293.15 K is consistent with those at 298.15 K. These solubilities are classified as tentative.

Further, if it is assumed that the temperature coefficient of solubility is the same as for methanol, extrapolation to other temperatures may be made using the following equation:

$$\log x_1 = 574.8/(T/\mathrm{K}) - 4.140 \qquad (3)$$

The above equation is not recommended if accurate results are required and for extrapolation to temperatures far from the ambient.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Alcohols; pressures less than 0.2 MPa (2 atm)

EVALUATOR:

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June, 1992

CRITICAL EVALUATION:

1-Propanol; C_3H_8O; [71-23-8]

The three values of Boyer and Bircher (2), Narasimhan et al. (4) and Yano et al. (5) for ethene solubility in 1-propanol at 298.15 K are within 3% of the average value which corresponds to a mole fraction at an ethene partial pressure of 101.3 kPa of $x_1 = 0.00737$. The solubilities of Narisamhan et al., and Boyer and Bircher at 293.15 K, and 308.15 K, respectively, are consistent with those at 298.15 K. These solubilities are classified as tentative.

Further, if it is assumed that the temperature coefficient of solubility in 1-propanol is the same as that in 1-butanol (see below), extrapolation to other temperatures may be made using the following equation:

$$\log x_1 = 543.6/(T/\mathrm{K}) - 3.956 \qquad (4)$$

The temperature span for 1-propanol alone is insufficient to provide an accurate temperature coefficient of solubility. The above equation is not recommended if accurate data are required outside the temperature range within which experimental results are available.

1-Butanol; $C_4H_{10}O$; [71-36-3]

Three research groups have contributed to the solubility data for ethene in 1-butanol; these are Narasimhan et al. (4) Boyer and Bircher (2) and Sahgal et al. (7). The temperature span of the data, nearly 80 K, permits a reasonably good estimate of the temperature coefficient of solubility. A regression line including the 8 data points yields the following equation with a maximum deviation of 5% and a correlation coefficient of 0.9942:

$$\log x_1 = 543.6/(T/\mathrm{K}) - 3.890 \qquad (5)$$

The above equation is considered to be the best available relation for the solubility of ethene in 1-butanol and is classified as tentative for the temperature range for which data are available, that is from 263.95 K to 343.15 K. Solubilities calculated by means of equation (5) are listed in Table 3.

Table 3: Ethene solubilities in 1-butanol for a gas partial pressure of 101.3 kPa as calculated using equation (5).

t, °C	T, K	x_1, Mole fraction ethene
-10	263.15	0.0150
0	273.15	0.0126
10	283.15	0.0107
20	293.15	0.00921
25	298.15	0.00858
30	303.15	0.00800
40	313.15	0.00701
50	323.15	0.00620
60	333.15	0.00552
70	343.15	0.00495

1-Pentanol; $C_5H_{12}O$; [71-41-0]

The two values for ethene solubilities in 1-pentanol at 298.15 K (2,4) are within 2% of the average value which corresponds to a mole

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alcohols; pressures less than 0.2 MPa (2 atm)	W. Hayduk Chemical Engineering University of Ottawa Ottawa, Ontario Canada K1N 6N5 June, 1992

CRITICAL EVALUATION:

fraction of $x_1 = 0.0102$. The solubilities of Narisamhan et al. (4) and Boyer and Bircher (2), at 293.15 K and 308.15 K, respectively, are consistent with those at 298.15 K. These solubilities are classified as tentative.

Further, if it is assumed that the temperature coefficient of solubility in 1-pentanol is the same as that in 1-butanol, extrapolation to other temperatures may be made using the following equation:

$$\log x_1 = 543.6/(T/\mathrm{K}) - 3.185 \qquad (6)$$

While the above equation represents the limited solubility data, it is not recommended if accurate data are required outside the temperature range within which experimental results are available.

1-Hexanol; $C_6H_{14}O$; [111-27-3]
1-Heptanol; $C_7H_{16}O$; [110-70-6]
1-Octanol; $C_8H_{18}O$; [111-87-5]

Only the data of Boyer and Bircher (2) are available for the solubilities of ethene at an ethene partial pressure of 101.3 kPa in 1-hexanol, 1-heptanol and 1-octanol at 298.15 K and in the latter solvent at 308.15 K as well. The data of Boyer and Bircher appear entirely consistent with those of other researchers when comparisons are possible. Hence these data are classified as tentative.

Since extrapolation to other temperatures is often required, equations will be provided based on the temperature coefficient of solubility in 1-butanol:

For 1-hexanol:

$$\log x_1 = 543.6/(T/\mathrm{K}) - 3.794 \qquad (7)$$

For 1-heptanol:

$$\log x_1 = 543.6/(T/\mathrm{K}) - 3.755 \qquad (8)$$

For 1-octanol

$$\log x_1 = 543.6/(T/\mathrm{K}) - 3.718 \qquad (9)$$

It is emphasized that the above equations are approximate only, and are based on few data and uncertain temperature coefficients of solubility.

Figure 2 is shown for three reasons. First it summarizes most of the available data for the solubilities of ethene in the normal alcohols at low pressure. Next it emphasizes the scarcity of the data for most temperatures above and below the ambient even in these common solvents. Finally, Figure 2 shows the diagrammatic representation of the extrapolating equations, Equations 2 to 9, that are listed in this Critical Evaluation.

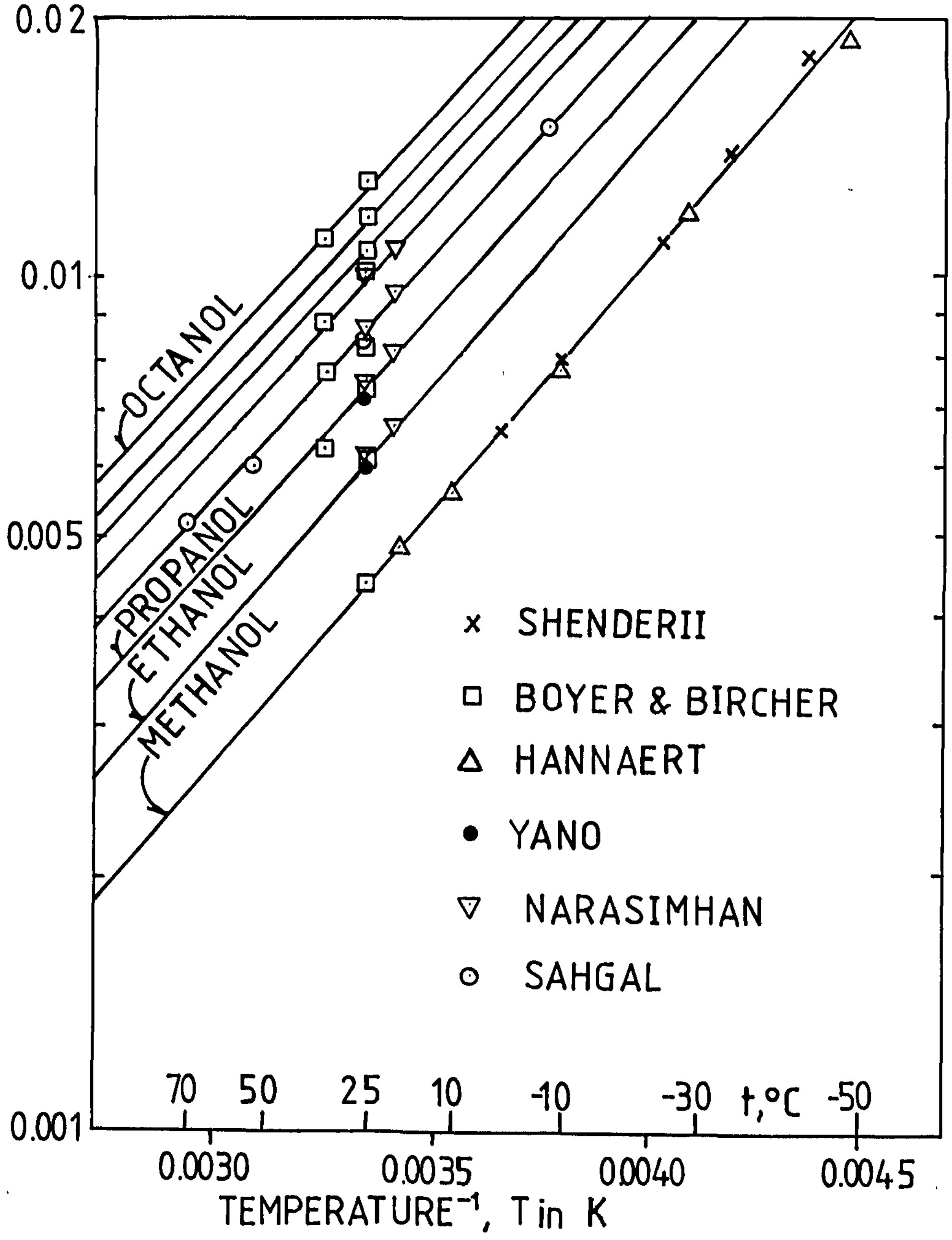
2-Propanol (isopropanol); C_3H_8O; [67-63-0]

Ethene solubilities in 2-propanol were reported for three temperatures, 273.15, 298.15 and 323.15 K, by Sahgal et al. (7). The solubilities in this branch-chained alcohol are some 11% lower than in the straight-chained alcohol, 1-propanol. The temperature span is sufficient to calculate an equation for interpolating or extrapolating the data:

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alkanols; pressures less than 0.2 MPa (2 atm)	W. Hayduk Chemical Engineering University of Ottawa Canada K1N 6N5 June, 1992

CRITICAL EVALUATION:

Fig. 2 Ethene solubility in alkanols for an ethene partial pressure of 101.3 KPa as a function of temperature.



COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alcohols; pressures less than 0.2 MPa (2 atm)	W. Hayduk Chemical Engineering University of Ottawa Ottawa, Ontario Canada K1N 6N5 June, 1992

CRITICAL EVALUATION:

$$\log x_1 = 581.7/(T/K) - 4.1247 \qquad (10)$$

The above equation should not be considered accurate beyond the temperature range for which it was developed. Calculated values of solubility based on equation (10) are listed in Table 4. These data are classified as tentative.

Table 4: Ethene solubilities in 2-propanol for a gas partial pressure of 101.3 kPa as calculated using equation (1)

t, °C	T, K	x_1, Mole fraction ethene
0	273.15	0.0101
10	283.15	0.00851
20	293.15	0.00724
25	298.15	0.00671
30	303.15	0.00623
40	313.15	0.00541
50	323.15	0.00474

Cyclohexanol; $C_6H_{12}O$; [108-93-0]

Cauquil's (8) single value for the ethene solubility in cyclohexanol is rejected for two reasons. It is most unlikely that the solubility in cyclohexanol will be only about one tenth that in 1-hexanol. Also Clever (13) found that the value reported by Cauquil for the solubility of methane in cyclohexanol was only one half that found by reliable researchers.

1,2-Ethanediol (ethylene glycol); $C_2H_5O_2$; [107-21-1]

Two groups of researchers measured the solubility of ethene in 1,2-ethanediol. These were Sahgal et al. (7) at 298.15 K and Hannaert et al. (6) at 303.15 K. The value of Hannaert et al. is less than half that of Sahgal et al., a most unlikely reduction in solubility for an increase in temperature of 5 K. Since the work was conducted under my supervision, I am aware of the care that was taken to ensure saturation of this viscous solvent and, therefore, believe the higher solubility to be correct. The value of Hannaert et al. was measured by a gas chromatographic method which in many instances has been subject to errors. The former value is classified as tentative.

2,2-[1,2 Ethanediylbis (oxy)] bis-ethanol, (triethylene glycol); $C_6H_{14}O_4$; [112-27-6]

The solubility of ethene in triethylene glycol was measured by Hannaert et al. for a temperature of 303.15 K. There is some doubt as to the accuracy of the chromatographic method used by these workers (see above) for viscous solvents, but no real comparison is possible in this case. Therefore, the value reported is classified as tentative.

Propanol, oxybis-, (Dipropylene glycol); $C_6H_{14}O_3$; [25265-71-8]
Phenol; C_6H_6O; [108-95-2]
Benzenemethanol (benzyl alcohol); C_7H_8O; [100-51-6]

Lenoir et al. (9) reported ethene solubility data for the solvents oxybispropanol, phenol and benzenemethanol. Their method of measurement involved gas chromatography at very low gas partial pressures with the

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alcohols; pressures less than 0.2 MPa (2 atm)	W. Hayduk Chemical Engineering University of Ottawa Ottawa, Ontario Canada K1N 6N5 June, 1992

CRITICAL EVALUATION:

result that extrapolation of the data to pressures in the order of 101.3 kPa is considered to involve significant errors. Because there are not other comparable results,these data are classified as tentative.

1-Butanol and 1,2-Ethanediol (ethylene glycol) solutions; $C_4H_{10}O$; [71-36-3] and $C_2H_5O_2$; [107-21-1]

Sahgal and Hayduk (10) reported solubilities of ethene at 101.3 kPa pressure at 298.15 K in the two-component solvent solutions composed of 1-butanol and 1,2-ethanediol (ethylene glycol). All compositions from pure 1-butanol to pure 1,2-ethanediol were used. These results are consistent with those for the pure solvents and are classified as tentative.

References

1. Shenderei, E.R.; Zel'venskii, Ya. D.; Ivanovskii, F.P. *Russian J. Appl. Chem.* 1962, *35*, 669-672. (or *Zhur. Prikl. Khim.*, 690-693).

2. Boyer, F.L.; Bircher, L.J. *J. Phys. Chem.* 1960, *64*, 1330-1331.

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13. Clever, H.L.; Young, C.L.; Eds. METHANE, Solubility Data Series, 1987, Vol. 27/28, 637, Pergamon Press Ltd., Oxford and New York.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methanol; CH_4O: [67-56-1]

ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii,
Ya.D.; Ivanovskii, F.P.
Russian J. Appl. Chem. <u>1962</u>, *35*,
669-672. (*Zhur. Prikl. Khim.*, 690-693.)

VARIABLES:

T/K = 217-273

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Henry's Constant H/atm(mole fraction)$^{-1}$	Mole Fraction[1] Ethene, x_1	Partial Molal Volume Ethene v_1 /cm^3(mole)$^{-1}$
0	273.15	152.2	0.00657	--
-10	263.15	126.3	0.00792	--
-25	248.15	91.5	0.0109	62.5
-35	238.15	72.5	0.0138	59.0
-45	228.15	56.3	0.0178	55.0
-56	217.15	42.3	0.0236	--

The authors expressed the effect of temperature on H by:

$$\log H = 4.336 + 590(T/K)^{-1}$$

Partial molal volume of ethylene dissolved in methanol at low temperatures are also given.

[1] Calculated by compiler for an ethylene partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with a magnetic stirrer. Pressure measured with a Bourdon gauge. Samples of liquid analyzed by stripping out ethene. The solubilities were measured at several pressures below atmospheric and Henry's constant was determined. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial ethene was purified by absorption and complex formation at 0°C under pressure in cuprous chloride. Impurities were not absorbed. The ethylene was regenerated at 60°C, condensed, and analyzed by GC.
2. Distilled.

Actual purities not given.

ESTIMATED ERROR:

$\delta H/H = \pm 0.02$

(Estimated by compiler)

REFERENCES:

1. Shenderei, E.R.; Zel' venskii, Ya.D.; Ivanovskii, F.P. *Khim. Prom.* <u>1960</u>, 370.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene; C_2H_4; [74-85-1] (2) Methanol; CH_3OH; [67-56-1]	Boyer, F. L.; Bircher, L. J. *J. Phys. Chem.* 1960, *64*, 1330 - 1331.

VARIABLES:	PREPARED BY:
T/K: 298.15 P/kPa: 101.325 (1 atm)	M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^4 x_1$	Bunsen Coefficient[1] α	Ostwald Coefficient $L/cm^3\ cm^{-3}$
298.15	43.9	2.41	2.63 ± 0.02

[1] $\alpha/cm^3(STP)\ cm^{-3}\ atm^{-1}$

The Bunsen coefficient was calculated by the compiler.

The mole fraction solubility was taken from Boyer's thesis (1).

The author's observed a linear relationship between the logarithm of the mole fraction solubility and the number of linear alcohol carbon atoms. Boyer's thesis gives the equations:

$$\log x_1 = -2.387 + 0.543 \log C \text{ for } 298.15 \text{ K}$$

$$\log x_1 = -2.474 + 0.580 \log C \text{ for } 308.15 \text{ K}$$

where C is the number of alcohol carbon atoms. Most of the mole fraction solubility values given in Table II of the paper were calculated from the equation for 298.15 K.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) Methanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

$\delta T/K = \pm 0.01$

$\delta L/cm^3 = \pm 0.02$

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.
2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Methanol; C_1H_4O; [67-56-1]	Ohgaki, K.; Nishii, H.; Katayama, T. *J. Chem. Eng. (Japan)* <u>1983</u>, *16*, 72-73.
VARIABLES: T/K = 298.15 ± 0.01 P/kPa = 60.8 - 97.0	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

Total Pressure P/kPa	Liquid Mole fraction $(10^3)x_1$	Gas Mole fraction y_1	Henry's Constant, MPa $H = p_1/x_1$
60.771	1.568	0.7103	27.26
61.564	1.573	0.7140	27.68
87.980	2.541	0.7986	27.30
97.007	2.842	0.8169	27.50
			Average = 27.43

The solubility calculated by compiler for an ethylene partial pressure of 101.325 kPa is x_1 = 0.00369 mole fraction ethylene.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A small (20 cm^3) magnetically stirred absorption vessel was connected to a larger (100 cm^3) gas reservoir at higher pressure in a constant temperature bath. The volumes of lines, valves and vessels were accurately determined. A quartz Bourdon gauge was used to measure the system pressure. A known mass of deaerated solvent was charged to the absorption vessel and the amount of vapor released on charging was estimated. Gas was charged incrementally to maintain a constant pressure until no additional gas was required. The change in pressure in the gas supply reservoir was used to determine the quantity consumed.

SOURCE AND PURITY OF MATERIALS:

1. Ethene, min. purity 99.95%.
2. Methanol, spectrograde, actual purity unspecified.

ESTIMATED ERROR:

δT/K = ± 0.01

$\delta x_1/x_1$ = ± 0.5% (authors)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Methanol; CH_4O; [67-56-1]	Narasimhan, S.; Natarajan, G.S.; Nageshwar, G.D. *Indian J. Technol.* 1981, *19*, 298-299.
VARIABLES: T/K = 293.15, 298.15 P/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

		Mole Fraction Ethene for		[1]Ostwald Coefficient
t/C	T/K	P = 101.325, x	$^1p_1$ = 101.325, x_1	L/cm^3 gas(cm^3 solvent)$^{-1}$
20	293.15	0.00484	0.00554	3.29
25	298.15	0.00422	0.00505	3.03

[1]Calculated by compiler. It is assumed that the mole fraction solubility, x, as originally given, is for a total pressure of 101.325 kPa although not specifically so stated in the paper. The mole fraction solubility is calculated for a partial pressure of 101.325 kPa.

Gas molar volumes of 23910, and 24330 cm^3/mole were used for the temperatures 293.15 K, and 298.15 K, respectively, and for a pressure of 101.325 kPa when calculating L.

It was confirmed by private communication with Dr. Nageshwar that x was for a total pressure of one atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. Methanol was treated for the removal of aldehydes and ketones and then distilled twice in a packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$
(Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A. *Anal. Chem.* 1948, *20*, 624.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Methanol; CH_4O; [67-56-1]	Yano, T.; Kidaka, T. Miyamoto, H.; Murakami, T. *Proc. Soc. Chem. Engrs. Japan (Osaka)*, <u>Oct. 14</u>, <u>1968</u>, 89-90.
VARIABLES: T/K = 298.15 P/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

		Mole Fraction Ethene, x_1 For:			
t/C	T/K	P=101.325 kPa	[1]p_1=101.325 kPa	[1] Ostwald Coefficient L/cm^{3}gas(cm^3 solvent)$^{-1}$	[1]Henry's Constant H/atm (mole fraction)$^{-1}$
25.0	298.15	0.00408	0.00488	2.93	204.8

[1]Calculated by compiler.

Although not specifically stated in paper it was assumed by the compiler that the reported solubility was for a total pressure of 101.325 kPa; therefore, the solubility for a partial pressure of 101.325 kPa was calculated assuming Henry's law and an ethene molar volume of 24320 cm^3/mole at 298.15 K and 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.	1. Source and purity not given. 2. Source and purity not given.
	ESTIMATED ERROR: $\delta x_1/x_1 = \pm\ 0.03$ (Compiler)
	REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

$T/K = 223.15 - 293.15$

$p_1/kPa = 101.3$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Mole Fraction Ethene, x_1
-50	223.15	0.0187
-30	243.15	0.0117
-10	263.15	0.0078
10	283.15	0.0056
20	293.15	0.0048

[1] Mole fraction solubility calculated by compiler for a gas partial pressure of 101.3 kPa using the equation developed by the authors with $\nu = 1$, for the applicable temperature range:

$$\log(K\pi\nu) = 4.21 - (\Delta H/\text{cal mol}^{-1})/(2.3R(T/K))$$

The authors' definitions are:

$\Delta H = 2{,}530$ cal mol^{-1}, Enthalpy of dissolution

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π / atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}/\text{atm} = (f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the least accurate.

The apparatus is of glass and consists of a burette in which the gas is confined over mercury, two bulbs for the solvent, one above the other, a mercury manometer and a constant temperature bath. A measured volume of solvent is degassed in the top bulb at ambient temperature and charged to the absorption bulb in the bath. Gas is charged to the desired pressure. The quantity of gas added at constant pressure is measured. Agitation is manual.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%.

2. Methanol. Merck and Co. At 20°C density specified as $\rho = 0.7944$ g cm^{-3} and refractive index n(D) = 1.3285.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm$ 10 to 15% (authors)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene; C_2H_4; [74-85-1] (2) Ethanol; C_2H_5OH; [64-17-5]	Boyer, F. L.; Bircher, L. J. *J. Phys. Chem.* 1960, *64*, 1330 - 1331.
VARIABLES: T/K: 298.15 P/kPa: 101.325 (1 atm)	**PREPARED BY:** M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient[1] α	Ostwald Coefficient $L/\text{cm}^3\ \text{cm}^{-3}$
298.15	61.4	2.34	2.56 ± 0.02

[1] $\alpha/\text{cm}^3(\text{STP})\ \text{cm}^{-3}\ \text{atm}^{-1}$

The Bunsen coefficient was calculated by the compiler.

The mole fraction solubility was taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) Ethanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

$\delta T/K = \pm 0.01$

$\delta L/\text{cm}^3 = \pm 0.02$

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.
2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Yano, T.; Kidaka, T. Miyamoto, H.;
Murakami, T.
Proc. Soc. Chem. Engrs. Japan (Osaka),
Oct. 14, 1968, 89-90.

VARIABLES:

T/K = 298.15
P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1 For: P=101.325 kPa	P_1=101.325 kPa	[1]Ostwald Coefficient L/cm^{3}gas(cm^3 solvent)$^{-1}$	[1]Henry's Constant H/atm (mole fraction)$^{-1}$
25.0	298.15	0.00558	0.00605	2.52	165.2

[1]Calculated by compiler.

Although not specifically stated in paper it was assumed by the compiler that the reported solubility was for a total pressure of 101.325 kPa; therefore, the solubility for a partial pressure of 101.325 kPa was calculated assuming Henry's law and an ethene molar volume of 24320 cm^3 / mole at 298.15 K and 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.

SOURCE AND PURITY OF MATERIALS:

1. Source and purity not given.
2. Source and purity not given.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm$ 0.03 (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Natarajan, G.S.;

Nageshwar, G.D.

Indian J. Technol. 1981, *19*, 298-299.

VARIABLES: $T/K = 293.15, 298.15$

$P/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t /C	T/K	Mole Fraction Ethene for $P = 101.325/x$	Mole Fraction Ethene for $^1p = 101.325/x_1$	^{1}Ostwald Coefficient L/cm^3 gas(cm^3 solvent)$^{-1}$
20	293.15	0.00633	0.00671	2.77
25	298.15	0.00575	0.00624	2.60

[1] Calculated by compiler. It is assumed that the mole fraction solubility, x, as originally given, is for a total pressure of 101.325 kPa although not specifically so stated in the paper. The mole fraction solubility is calculated for a partial pressure of 101.325 kPa.

Gas molar volumes of 23910, and 24330 cm^3/mole were used for the temperatures 293.15 K, and 298.15 K, respectively, and for a pressure of 101.325 kPa when calculating L.

It was confirmed by private communication with Dr. Nageshwar that x was for a total pressure of one atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. Ethanol was treated for the removal of aldehydes and ketones and then distilled twice in a packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$
(Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A.

Anal. Chem. 1948, *20*, 624.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 1-Propanol; C_3H_7OH; [71-23-8]

ORIGINAL MEASUREMENTS:

Boyer, F. L.; Bircher, L. J.

J. Phys. Chem. 1960, *64*, 1330 - 1331.

VARIABLES:

T/K: 298.15, 308.15
P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient[1] α	Ostwald Coefficient $L/cm^3\ cm^{-3}$
298.15	73.6	2.21	2.41 ± 0.01
308.15	62.7	1.95	2.20 ± 0.08

[1] $\alpha/cm^3(STP)\ cm^{-3}\ atm^{-1}$

The Bunsen coefficients were calculated by the compiler.

The mole fraction solubilities were taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) 1-Propanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

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

$\delta L/cm^3 = \pm\ 0.01$ (at 298.15 K)
$\pm\ 0.08$ (at 308.15 K)

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.
2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1- Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Natarajan, G.S.;

Nageshwar, G.D.

Indian J. Technol. 1981, *19*, 298-299.

VARIABLES: T/K = 293.15, 298.15

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene for P = 101.325/x	^1p = 101.325/x_1	^{1}Ostwald Coefficient L/cm^3 gas.(cm^3 solvent)$^{-1}$
20	293.15	0.00804	0.00820	2.64
25	298.15	0.00737	0.00758	2.47

[1] Calculated by compiler. It is assumed that the mole fraction solubility, x, as originally given, is for a total pressure of 101.325 kPa although not specifically so stated in the paper. The mole fraction solubility is calculated for a partial pressure of 101.325 kPa.

Gas molar volumes of 23910, and 24330 cm^3/mole were used for the temperatures 293.15 K, and 298.15 K, respectively, and for a pressure of 101.325 kPa when calculating L.

It was confirmed by private communication with Dr. Nageshwar that x was for a total pressure of one atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. 1-Propanol was treated for the removal of aldehydes and ketones and then distilled twice in a packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$
(Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A.
Anal. Chem. 1948, *20*, 624.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Yano, T.; Kidaka, T. Miyamoto, H.;
Murakami, T.
Proc. Soc. Chem. Engrs. Japan (Osaka),
Oct. 14, 1968, 89-90.

VARIABLES:

$T/\mathrm{K} = 298.15$
$P/\mathrm{kPa} = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene/x_1 For: P=101.325 kPa	$^1p_1$=101.325 kPa	^{1}Ostwald Coefficient L/cm^{3}gas(cm^3 solvent)$^{-1}$	^{1}Henry's Constant H/atm (mole fraction)$^{-1}$
25.0	298.15	0.00697	0.00717	2.34	139.6

^{1}Calculated by compiler.

Although not specifically stated in paper it was assumed by the compiler that the reported solubility was for a total pressure of 101.325 kPa; therefore, the solubility for a partial pressure of 101.325 kPa was calculated assuming Henry's law and an ethene molar volume of 24320 cm^3/mole at 298.15 K and 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus was employed in which the uptake of gas by a known volume of solvent in a dissolution cell was volumetrically determined. The gas was displaced by mercury as the gas dissolved at constant pressure. A magnetically operated gas circulating pump and bubbling tip were provided for bubbling the gas through the solvent in the dissolution cell.

SOURCE AND PURITY OF MATERIALS:

1. Source and purity not given.
2. Source and purity not given.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm\ 0.03$ (Compiler)

REFERENCES:

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 1-Butanol; C_4H_9OH; [71-36-3]

ORIGINAL MEASUREMENTS:

Boyer, F. L.; Bircher, L. J.

J. Phys. Chem. 1960, *64*, 1330 - 1331.

VARIABLES:

T/K: 298.15, 308.15
P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient[1] α	Ostwald Coefficient $L/\text{cm}^3\ \text{cm}^{-3}$
298.15	82.4	2.07	2.26 ± 0.01
308.15	77.3	1.87	2.11 ± 0.02

[1] $\alpha/\text{cm}^3(\text{STP})\ \text{cm}^{-3}\ \text{atm}^{-1}$

The Bunsen coefficients were calculated by the compiler.

The mole fraction solubilities were taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) 1-Butanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

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

$\delta L/\text{cm}^3 = \pm\ 0.01$ (at 298.15 K)
$\pm\ 0.02$ (at 308.15 K)

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.

2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES:

T/K = 264-343

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene x_1	Ostwald Coefficient L/ cm^{3}gas (cm^3 solvent)$^{-1}$
-9.2	263.95	0.0149	3.62
25	298.15	0.00834	2.23
49	322.15	0.00596	1.67
70	343.15	0.00511	1.50

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. 1-Butanol was from Fisher of 99.0 mole % minimum purity.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 2%

δT/K = ± 0.05

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. 1- Butanol; $C_4H_{10}O$; [71-36-3]	Narasimhan, S.; Natarajan, G.S.; Nageshwar, G.D. *Indian J. Technol.* 1981, *19*, 298-299.
VARIABLES: $T/K = 293.15, 298.15$ $P/kPa = 101.325$	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

		Mole Fraction Ethene, x_1, for		[1]Ostwald Coefficient
t/C	T/K	$P = 101.325$	[1]$p_1 = 101.325$	L/cm^3 gas (cm^3 solvent)$^{-1}$
20	293.15	0.00950	0.00956	2.52
25	298.15	0.00864	0.00871	2.32

[1]Calculated by compiler. It is assumed that the mole fraction solubility, x_1 as originally given, is for a total pressure of 101.325 kPa although not specifically so stated in the paper. The mole fraction solubility is calculated for a partial pressure of 101.325 kPa.

Gas molar volumes of 23910, and 24330 cm^3/mole were used for the temperatures 293.15 K, and 298.15 K, respectively, and for a pressure of 101.325 kPa when calculating L.

It was confirmed by private communication with Dr. Nageshwar that x_1 was for a total pressure of one atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. 1-Butanol was treated for the removal of aldehydes and ketones and then distilled twice in a packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$
(Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A.
Anal. Chem. 1948, *20*, 624.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Pentanol; $C_5H_{12}O$; [71-41-0]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Natarajan, G.S.; Nageshwar, G.D.

Indian J. Technol. 1981, *19*, 298-299.

VARIABLES: $T/K = 293.15, 298.15$

$P/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1, for $P = 101.325$	Mole Fraction Ethene, x_1, for $^1p_1 = 101.325$	^{1}Ostwald Coefficient L/cm^3 gas $(cm^3$ solvent$)^{-1}$
20	293.15	0.01082	0.01083	2.42
25	298.15	0.00995	0.00996	2.25

^{1}Calculated by compiler. It is assumed that the mole fraction solubility, x_1 as originally given, is for a total pressure of 101.325 kPa although not specifically so stated in the paper. The mole fraction solubility is calculated for a partial pressure of 101.325 kPa.

Gas molar volumes of 23910, and 24330 cm^3/mole were used for the temperatures 293.15 K, and 298.15 K, respectively, and for a pressure of 101.325 kPa when calculating L.

It was confirmed by private communication with Dr. Nageshwar that x_1 was for a total pressure of one atmosphere.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. 1-Pentanol was treated for the removal of aldehydes and ketones and then distilled twice in a packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$
(Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A. *Anal. Chem.* 1948, *20*, 624.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 1-Pentanol; $C_5H_{11}OH$; [71-41-0]

ORIGINAL MEASUREMENTS:

Boyer, F. L.; Bircher, L. J.

J. Phys. Chem. 1960, *64*, 1330 - 1331.

VARIABLES:

T/K: 298.15, 308.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction $10^4 x_1$	Bunsen Coefficient[1] α	Ostwald Coefficient L/cm^3 cm^{-3}
298.15	100.4	2.04	2.23 ± 0.03
308.15	88.7	1.82	2.05 ± 0.01

[1] α/cm^3(STP) cm^{-3} atm^{-1}

The Bunsen coefficients were calculated by the compiler.

The mole fraction solubilities were taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) 1-Pentanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm\ 0.01$

$\delta L/\mathrm{cm}^3 = \pm\ 0.03$ (at 298.15 K)
$\pm\ 0.01$ (at 308.15 K)

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.

2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 1-Hexanol; $C_6H_{13}OH$; [111-27-3]

ORIGINAL MEASUREMENTS:

Boyer, F. L.; Bircher, L. J.

J. Phys. Chem. 1960, *64*, 1330 - 1331.

VARIABLES:

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

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient[1] α	Ostwald Coefficient $L/\text{cm}^3\ \text{cm}^{-3}$
298.15	106.9	1.91	2.08 ± 0.03

[1] $\alpha/\text{cm}^3(\text{STP})\ \text{cm}^{-3}\ \text{atm}^{-1}$

The Bunsen coefficient was calculated by the compiler.

The mole fraction solubility was taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) 1-Hexanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

$\delta T/\text{K} = \pm 0.01$

$\delta L/\text{cm}^3 = \pm 0.03$

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.
2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 1-Heptanol; $C_7H_{15}OH$; [111-70-6]

ORIGINAL MEASUREMENTS:

Boyer, F. L.; Bircher, L. J.

J. Phys. Chem. 1960, *64*, 1330 - 1331.

VARIABLES:

T/K: 298.15

P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient[1] α	Ostwald Coefficient L/cm^3 cm^{-3}
298.15	117.0	1.88	2.05 ± 0.02

[1] α/cm^3(STP) cm^{-3} atm^{-1}

The Bunsen coefficient was calculated by the compiler.

The mole fraction solubility was taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) 1-Heptanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

δT/K = ± 0.01

δL/cm^3 = ± 0.02

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.

2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 1-Octanol; $C_8H_{17}OH$; [111-87-5]

ORIGINAL MEASUREMENTS:

Boyer, F. L.; Bircher, L. J.

J. Phys. Chem. 1960, *64*, 1330 - 1331.

VARIABLES:

T/K: 298.15, 308.15
P/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient[1] α	Ostwald Coefficient L/cm^3 cm^{-3}
298.15	129.0	1.75	1.91 ± 0.03
308.15	110.0	1.56	1.76 ± 0.02

[1] α/cm^3(STP) cm^{-3} atm^{-1}

The Bunsen coefficients were calculated by the compiler.

The mole fraction solubilities were taken from Boyer's thesis (1).

See the methanol data sheet for the equations relating the mole fraction solubility and the number of normal alcohol carbon numbers.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A commercial Van Slyke blood gas apparatus (E. H. Sargent Co.) was modified by the authors.

The total pressure of the gas and the solvent vapor in the solution chamber was adjusted to a pressure of one atm. The pressure was maintained at one atm during the solution process. The saturated solution was transferred to a bulb below the lower stopcock of the extraction vessel and sealed off. The gas and solvent vapor were then brought to volume over mercury. See (2) for details of the extraction procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Matheson Co. Stated to be 99.5 mol per cent.

(2) 1-Octanol. Source not given. Treated by standard methods to remove aldehydes and ketones, then dried and distilled.

ESTIMATED ERROR:

δT/K = ± 0.01
δL/cm^3 = ± 0.03 (at 298.15 K)
± 0.02 (at 308.15 K)

REFERENCES:

1. Boyer, F. L., Ph.D. thesis, 1959, Vanderbilt Univ., Nashville, TN.

2. Peters, J. P.; Van Slyke, D. D. *Quantitative Clinical Chemistry* Baltimore, MD, 1932, Volume II.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. 2-Propanol; C_3H_8O; [67-63-0]	Sahgal, A.; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354-357.
VARIABLES: T/K = 273-323 P/kPa = 101.325	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1	Ostwald Coefficient L/ cm^3gas (cm^3 solvent)$^{-1}$
0	273.15	0.0101	3.02
25	298.15	0.00673	2.14
50	323.15	0.00473	1.58

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. 2-Propanol was from J.T. Baker of 99.9 mole % purity.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene or ethylene; C_2H_4; [74-85-1] (2) Cyclohexanol; $C_6H_{12}O$; [108-93-0]	Cauquil, G. *J. Chim. Phys.* 1927, *24*, 53-55.
VARIABLES: $T/K = 299$ $p_1/kPa = 102$	PREPARED BY: H. L. Clever

EXPERIMENTAL VALUES:

The author states that one liter of cyclohexanol absorbs 301 cm^3 ethene at 26 ^0C and 766 mmHg.

The compiler calculates a Ostwald coefficient of $L/cm^3\ cm^{-3} = 0.301$ and a mole fraction solubility of $x_1 = 1.27 \times 10^{-3}$ at 299 K and a gas partial pressure of 101.325 kPa (1 atm).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus appears to be of the Bunsen type.

The initial and final volumes of gas in contact with the liquid were measured. The vapor pressure of the liquid was ignored.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. No information.

(2) Cyclohexanol. Distilled, boiling point 160.9 ^0C at 766 mmHg. Degassed and tested to be air free.

ESTIMATED ERROR:

$\delta L/L = \pm 0.05$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1,2-Ethanediol (ethylene glycol); $C_2H_5O_2$; [107-21-1]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, $10^4 x_1$	Ostwald Coefficient $L/\ cm^3 gas\ (cm^3\ solvent)^{-1}$
25	298.15	7.15	0.312

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. 1,2-Ethanediol was from Fisher Chemicals of 99.8 mole % purity.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. 1,2-Ethanediol (ethylene glycol); $C_2H_5O_2$; [107-21-1]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, 32, 156-164.

VARIABLES:

$T/K = 303.15$

$p_1/kPa = 101.3$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	$K\pi\nu$	[1]Mole Fraction Ethene, x_1
30	303.15	3,200	0.000313

[1]Mole fraction solubility calculated by compiler for a gas partial pressure of 101.3 kPa with $\nu = 1$.

The authors' definitions for $K\pi\nu$ are:

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π / atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}/\text{atm} = (f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the gas chromatographic method.

The stationary phase of the column was impregnated with a known mass of solvent. Nitrogen was used for determining the free volume of gas in the column. Various corrections were employed for dead volumes in the tubing and detector as well as for inlet and outlet pressures. Unfortunately the method could only be used with solvents of very low volatility.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%.

2. 1,2-Ethanediol. No information.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm$ 2 to 5% (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2,2 -[1,2-Ethanediylbis (oxy)] bis-ethanol, (triethylene glycol); $C_6H_{14}O_4$; [112-27-6]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*,

156-164.

VARIABLES:

T/K = 303.15

p /kPa = 101.3

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K		[1] Mole Fraction Ethene, x_1
30	303.15	550	0.00182

[1] Mole fraction solubility calculated by compiler for a gas partial pressure of 101.3 kPa with ν = 1.

The authors' definitions for $K\pi\nu$ are:

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π/ atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = (f_1/atm)/x_1 where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the gas chromatographic method.

The stationary phase of the column was impregnated with a known mass of solvent. Nitrogen was used for determining the free volume of gas in the column. Various corrections were employed for dead volumes in the tubing and detector as well as for inlet and outlet pressures. Unfortunately the method could only be used with solvents of very low volatility.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%.
2. Triethylene glycol. No information.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 2 to 5% (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Propanol, oxybis-, (Dipropylene glycol); $C_6H_{14}O_3$; [25265-71-8]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

$T/K = 298.2 - 343.2$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant $H_{C_2H_4}/atm$	Mole fraction at 1 atm* $x_{C_2H_4}$
298.2	204	0.00490
323.2	254	0.00394
343.2	295	0.00339

* Calculated by compiler assuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e., $x_{C_2H_4}(1\ atm) = 1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Phenol; C_6H_6O; [108-95-2]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

$T/K = 323.2$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant $H_{C_2H_4}/atm$	Mole fraction at 1 atm* $x_{C_2H_4}$
323.2	259	0.00386

* Calculated by compiler assuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e., $x_{C_2H_4}(1\ atm) = 1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene (Ethylene); C_2H_4; [74-85-1] 2. Benzenemethanol (Benzyl alcohol); C_7H_8O; [100-51-6]	Lenoir, J-Y.; Renault, P. Renon, H. *J. Chem. Eng. Data* 1971, *16*, 340-2.
VARIABLES: $T/K = 298.15$ $P/kPa = 101.32$	PREPARED BY: C.L. Young

EXPERIMENTAL VALUES:

T /K	Henry's constant $H_{C_2H_4}$/atm	Mole fraction at 1 atm* $x_{C_2H_4}$
298.15	160	0.00625

* Calculated by compiler assuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e. $x_{C_2H_4}$ (1 atm) = $1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta H/atm = \pm 6\%$

(estimated by compiler).

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Butanol; $C_4H_{10}O$; [71-36-3]
3. 1,2-Ethanediol (ethylene glycol); $C_2H_5O_2$; [107-21-1]

ORIGINAL MEASUREMENTS:

Sahgal, A.; Hayduk, W.

J. Chem. Eng. Data 1979, *24*, 222-227.

VARIABLES:

T/K = 298.15
P/kPa = 101.325
x_3/Mole Fraction = 0-1.0

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Concentration of Solvent		Ethene Solubility	
t/C	T/K	z_3, Volume Fraction[1]	x_3, Mole Fraction[2]	Mole Fraction Ethene, x_1	Ostwald Coefficient L/cm^3 gas(cm^3 solvent)$^{-1}$
25	298.15	0(Butanol)	0	0.00834	2.23
		0.174	0.260	0.00611	1.82
		0.201	0.295	0.00570	1.72
		0.342	0.461	0.00456	1.48
		0.407	0.531	0.00384	1.31
		0.490	0.615	0.00334	1.17
		0.790	0.860	0.00151	0.604
		0.927	0.956	0.00106	0.450
		1.0(Glycol)	1.000	0.000715	0.312

[1] Volume fraction is based on volumes of two liquid components before mixing.

[2] Mole fraction is shown on a gas-free basis.

Values for pure solvents were previously given (in reference 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus utilized a continuous flow of deaerated solvent injected into a glass absorption spiral tube by means of a calibrated syringe pump. The mixed solvent was prepared volumetrically then deaerated and a sample analyzed by a density measurement. A mercury lift device was used for continuously adjusting the residual volume at constant pressure in a gas storage burette. Solvent injection and gas consumption rates were used to calculate solubilities. This paper also includes solution densities and refractive indices as well as ethene molecular diffusivities in the solutions.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson with minimum purity of 99.5 mole %. Molar volume used at 298.15 K and 101.325 kPa was 24,326 cm^3/mole.
2. 1-Butanol was from Fisher; purity 99.0 mole %.
3. 1,2-Ethanediol was from Fisher; purity 99.8 mole %.

ESTIMATED ERROR:

$T/K = \pm 0.05$ $\delta P/P = \pm 0.01$

$\delta z_3 = \pm 0.001$ $\delta x_1/x_1 = \pm 0.02$

REFERENCES:

1. Sahgal, A.; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alkanols, pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 November, 1993

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Alkanol Solvents for Pressures greater than 0.2 MPa (2 atm)

Four groups of researchers (1-4) reported solubilities of ethene in methanol, ethanol, 1-propanol and 1-octanol for temperatures ranging from 228.15 K to 498.15 K and pressures ranging from 0.10 MPa to 10.9 MPa. No data are available for the numerous other alkanols and alcohols.

The data of Konobeev and Lyapin (1) for three of the alkanols are listed for total pressures of their experiments; hence, it was necessary to use the solvent vapor pressure to estimate the corresponding ethene partial pressure. Further, these data are entirely self-consistent so that the effect of both temperature and pressure can be expressed by a simple equation of the form:

$$\log x_p = A/(T/K) + B \log (p/\text{MPa}) - C \qquad (1)$$

The above equation is useful over small temperature ranges when log x_p is proportional to the inverse of absolute temperature, and when Henry's law is obeyed or therefore, when log x_p is proportional to log p with the constant, B, being approximately equal to one.

Ethene solubilities in the individual solvents are discussed in detail below:

Methanol; CH_4O; [67-56-1]

Konobeev and Lyapin (1) reported ethene solubilities for a range of pressures in methanol at temperatures of 293.15 K, 313.15 K and 333.15 K, and Shenderei et al. (2) reported solubilities at low temperatures, 248.15 K, 238.15 K and 228.05 K. Both of these sets of data obey Henry's law for mole fraction solubilities of less than 0.08. The data of Shenderei et al. are approximately consistent with low pressure data (at 0.1013 MPa) and are classified as tentative. On the other hand, when extrapolated to a pressure of 0.1013 MPa, the data of Konobeev and Lyapin fall below those of other workers by about 16%. With this caution concerning the data of Konobeev and Lyapin, these data are also classified as tentative.

The data of Konobeev and Lyapin are described by the following equation up to an ethene partial pressure of 2 MPa with an average deviation from the data of 2.1% and a maximum deviation of 8.0%:

$$\log x_p = 538.17/(T/K) - 3.2071 + 1.026 \log (p/\text{MPa}) \qquad (2)$$

The data of Shenderei et al. are described by the following equation with average, and maximum deviations, of 3.0%, and 8.9%, respectively, and to a maximum pressure of 0.6 MPa:

$$\log x_p = 810.59/(T/K) - 4.2434 + 1.032 \log (p/\text{MPa}) \qquad (3)$$

The temperature effects expressed in the above two equations are sufficiently different so that a single, simple equation cannot successfully describe the data from both sources. Nor should the equations be used outside the temperature and pressure ranges for which they were developed. Figure 1 shows the experimental data and the equations discussed above.

Ethanol; C_2H_6O; [64-17-5]

Ellis et al. (3) reported solubilities of ethene in ethanol at 348.15 K (75°C) and for gas partial pressures from 1.46 MPa to 10.9 MPa. When

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. Alkanols, pressures greater than 0.2 MPa (2 atm)

EVALUATOR:

Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, ON
Canada K1N 6N5

November, 1993

CRITICAL EVALUATION:

the data were plotted on log-log coordinates, the relationship between mole fraction solubility and ethene partial pressure was found to be consistent and linear up to a pressure of 7 MPa. For this linear subset of data, the equation of the line best representing the data is:

$$\log x_p = 1.0094 \log (p/\mathrm{MPa}) - 1.5067 \qquad (4)$$

In the above equation p represents the ethene partial pressure in MPa. This equation represents the reduced data (4 points) with an average deviation of 1.8%, and a maximum deviation of 3.0%.

The data of Ellis et al. (3) are classified as tentative.

1-Propanol; C_3H_8O; [71-23-8]

Two groups of researchers have reported solubilities of ethene in 1-propanol at high pressures; these are Konobeev and Lyapin (1) for the temperatures 293.15 K, 313.15 K and 333.15 K, and Pryanikova et al. (4) for temperatures from 373.15 K to 498.15 K. The latter researchers reported their results only in graphical form. The results of the former researchers will be discussed first.

The data of Konobeev and Lyapin cover a pressure range from 0.29 MPa to 3.26 MPa. The conventional temperature dependence for the solubility is observed, and at the same time, the relatively simple dependence for varying gas partial pressures is also observed.

These solubility data for 1-propanol are represented by the following equation:

$$\log x_p = 487.93/(T/\mathrm{K}) + 1.051 \log (p/\mathrm{MPa}) - 2.8356 \qquad (5)$$

Equation (5) represents the solubility data with an average deviation of 3.1% and a maximum deviation of 10.0%. It is cautioned, however, that while the equation and data are self-consistent, when the equation is extrapolated to 0.1013 MPa pressure, a value much lower (about 25%) than that actually measured at that lower pressure is obtained. Hence, extrapolation beyond the indicated temperatures and pressures is liable to produce large errors.

The graphical, high temperature, high pressure results of Pryanikova et al. (4) were enlarged and readings obtained from the enlargement. Hence, these results are not equivalent to the data formerly discussed. However, when the results of the two research groups are compared directly it is found that the solubilities at 373.15 K of Pryanikova et al. correspond approximately, and even exceed in magnitude the results of Konobeev and Lyapin at 333.15 K, a most unlikely event. The mole fraction solubilities are expected to decrease with an increase in temperature. It is considered, therefore, that the results of Pryanikova et al. are somewhat too high and/or those of Konobeev and Lyapin are somewhat too low. It is not possible to unequivocally indicate which data are the more reliable although the latter data appear self-consistent and numerical values are reported.

Both sets of results are classified as tentative.

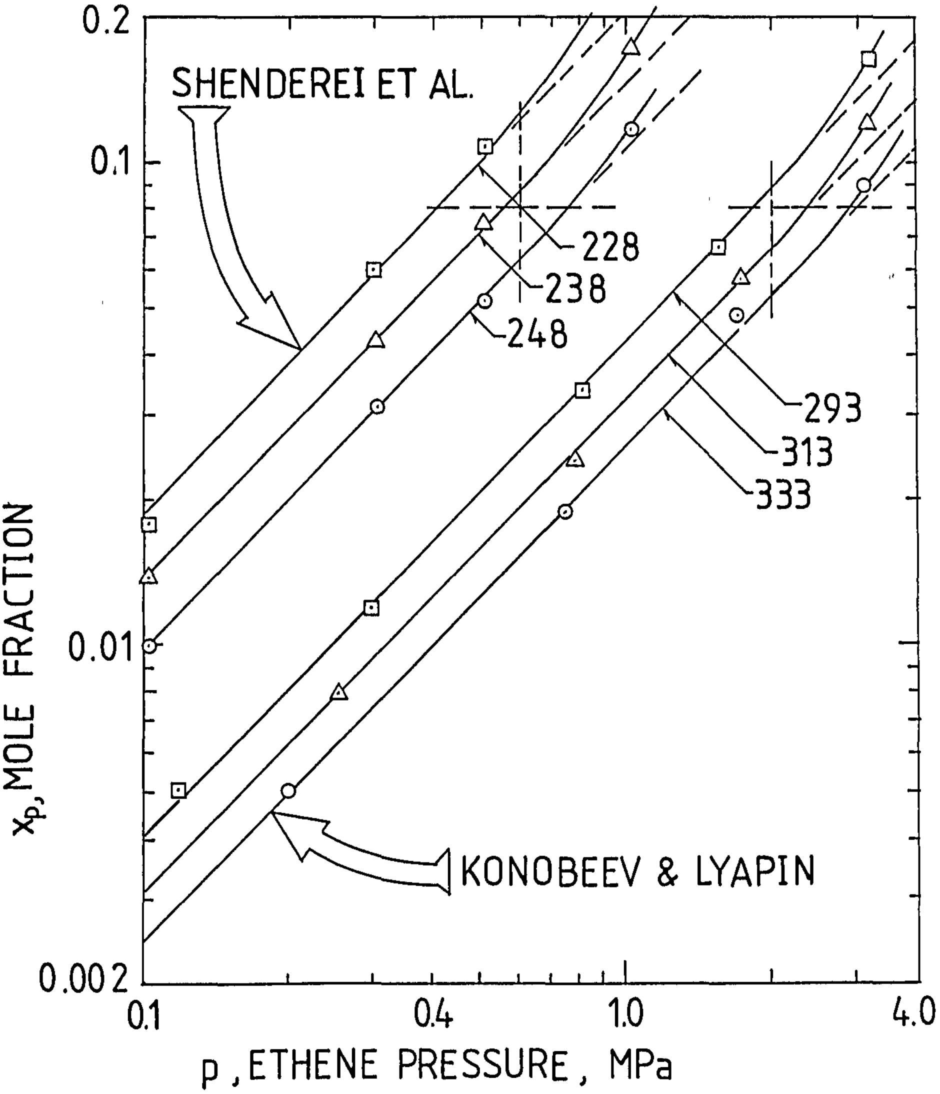
1-Octanol; $C_8H_{18}O$; [111-87-5]

Only the data of Konobeev and Lyapin (1) are available for solubilities at high pressure in 1-octanol and these are for the temperatures 293.15 K, 313.15 K and 333.15 K and for a pressure range from 0.28 MPa to 3.24 MPa. As for the previous solvent, 1-propanol, the temperature and

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alkanols, pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 November, 1993

CRITICAL EVALUATION:

Fig. 1 Ethene Solubility in Methanol as a function of Temperature and Pressure



pressure dependence for these data are well represented by the following equation:

$$\log x_p = 489.62/(T/\mathrm{K}) + 1.002 \log (p/\mathrm{MPa}) - 2.6590 \qquad (6)$$

The above equation represents the solubility data with an average deviation of 3.0% and a maximum deviation of the 12 data points of 6.1%. It is cautioned for this solvent also, that while the equation and data are self-consistent, when the equation is extrapolated to 0.1013 MPa pressure, a value much lower (about 33%) than that actually measured at that lower pressure is obtained. Hence, extrapolation beyond the indicated temperature and pressure ranges is liable to produce large errors.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Alkanols, pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 November, 1993

CRITICAL EVALUATION:

The data of Konobeev and Lyapin for 1-octanol solvent are classified as tentative.

References

1. Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-6.
2. Shenderei, E.R.; Zel'venskii, Ya. D.; Ivanovskii, F.P. *Russian J. Appl. Chem.* 1962, *35*, 669-672. (*Zhur. Prikl. Khim.* 1962, 690-693).
3. Ellis, S.R.M.; Valteris, R.L.; Harris, G.J. *Chem. Eng. Prog. Symp. Ser.*, 1968, *64*, 16-21.
4. Pryanikova, R.O.; Efremova, G.D.; Malikov, D.A.; Zagorets, P.A.; Shostenko, A.G.; Dodonov, A.M. *Tr. Mosk. Khim. Theknol. Inst.* 1973, *75*, 78-80.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Methanol; CH_3OH; [67-56-1]

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967, *43*, 114-6.

VARIABLES:

$T/K = 293.15 - 333.15$

$P/MPa = 0.13 - 3.22$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5 Pa$	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	1.317	0.005
	3.080	0.012
	8.197	0.034
	15.71	0.067
	32.12	0.165
313.15	2.888	0.008
	8.248	0.024
	17.83	0.057
	32.22	0.120
333.15	2.888	0.005
	8.288	0.019
	17.93	0.048
	32.22	0.089

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.
2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$ $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4 ; [74-85-1]

2. Methanol; CH_4O: [67-56-1]

ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii,

Ya.D.; Ivanovskii, F.P.

Russian J. Appl. Chem. 1962, *35* ,

669-672. (*Zhur. Prikl. Khim.*, 690-693.)

VARIABLES:

T/K = 228-248

P/MPa = 0.10-1.82, (1-18 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T^1/K	t/C	Total Pressure P/Atm	 P^1/MPa	Solubility^2 Mole fraction, x_1	 s /cm^3(g)$^{-1}$
248.15	-25.0	1	0.1013	0.0100	7.74
		3	0.3040	0.0311	22.29
		5	0.5066	0.0520	38.23
		10	1.013	0.1181	92.81
		12	1.216	0.1552	127.85
		15	1.520	0.2163	192.11
		18	1.824	0.3103	313.10
238.15	-35.0	1	0.1013	0.0138	9.75
		3	0.3040	0.0430	31.32
		5	0.5066	0.0751	56.51
		10	1.013	0.1750	147.84
		12	1.216	0.2265	203.51
		15	1.520	0.3631	397.19
228.05	-45.1	1	0.1013	0.0177	10.39
		3	0.3040	0.0600	44.48
		5	0.5066	0.1100	86.14
		10	1.013	0.3051	305.87
		12	1.216	0.5700	920.11

[1] Calculated by compiler.

[2] Solubility, s, expressed as cm^3 ethene at NTP per g of solvent.

It is noted that solubilities listed in this paper for a pressure of 101.3 kPa using a low pressure apparatus are up to 9% higher than those using the high pressure apparatus (see low pressure data).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with a magnetic stirrer. Pressure measured with a Bourdon gauge. Samples of liquid analyzed by stripping out ethene. The solubilities were measured at several pressures below atmospheric and Henry's constant was determined. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Commercial ethene was purified by absorption and complex formation at 0°C under pressure in cuprous chloride. Impurities were not absorbed. The ethylene was regenerated at 60°C, condensed, and analyzed by GC.

2. Distilled.

   Actual purities not given.

ESTIMATED ERROR:

$\delta x_1 / x_1$ = ± 2%

(Estimated by compiler)

REFERENCES:

1. Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P. *Khim. Prom.* 1960, *5*, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Ellis, S.R.M.; Valteris, R.L.;
Harris, G.J.

Chem. Eng. Prog. Symp. Ser.,
1968, *64*, 16-21.

VARIABLES:

T/K = 348.15

P/MPa = 1.5 - 10.9 (14-108 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

P/atm	Partial pressure[1]		Mole fraction ethene	
	p/atm	p/MPa	in liquid, x_1	in vapor, y_1
15.1	14.4	1.46	0.045	0.956
27.2	26.2	2.65	0.084	0.962
40.1	38.9	3.94	0.128	0.970
62.9	61.2	6.20	0.192	0.973
88.1	85.0	8.61	0.297	0.965
106.5	99.8	10.1	0.373	0.937
119.7	107.8	10.9	0.458	0.901

[1] Calculated by compiler

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A static method with a 500 cm stainless steel vessel equipped with a plunger, perforated-cup stirrer was used. The perforated cup was attached to a soft iron rod which was raised up by means of an electromagnet, and dropped downward under its own weight. Ethylene was displaced from a reservoir by mercury using a volumetric piston pump to the desired pressure. After equilibration, samples of gas and liquid were withdrawn for analysis. During the sampling process, an equivalent volume of mercury was allowed to flow from the sample bomb back to the equilibration vessel. The liquid portion of the samples was condensed at atmospheric pressure using dry-ice and acetone whereas the gas portion was aspirated volumetrically over water. Analysis was by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.03$ T/K = ± 2

$\delta P/P = \pm 0.01$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Pryanikova, R.O.; Efremova, G.D.; Malikov, D.A.; Zagorets, P.A.; Shostenko, A.G.; Dodonov, A.M.

Tr. Mosk. Khim. Theknol. Inst. 1973, *75*, 78-80.

VARIABLES:

T/K = 448.15 - 498.15

p_1/MPa = 1.19 - 4.98

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	[1]Total Pressure P/atm	[2]Ethene Partial Pressure p_1/MPa	Composition Mole Fraction Propanol, x_3	Composition Mole Fraction Ethene, x_1'	[2] Henry's Constant H/MPa(mol fraction)$^{-1}$ (x_1)
498.15	65.2	4.32	0.85	0.15	28.8
(225 C)	52.5	2.90	0.90	0.10	(0.00352)
	39.5	1.44	0.95	0.05	
473.15	62.5	4.98	0.80	0.20	24.8
(200 C)	51.0	3.73	0.85	0.15	(0.00408)
	39.3	2.46	0.90	0.10	
	28.0	1.23	0.95	0.05	
448.15	55.5	4.83	0.80	0.20	23.9
(175 C)	43.7	3.59	0.85	0.15	(0.00424)
	32.4	2.39	0.90	0.10	
	21.0	1.19	0.95	0.05	

[1] Only graphical results were presented in this paper in the form of total pressure (P) as a function of mole fraction propanol (x_3). Values were read from an enlarged graph by the compiler.

[2] The ethene partial pressure (p_1) was estimated using Raoult's law, and the Henry's law constant (H) as well as the mole fraction solubility for an ethene partial pressure of 0.101325 MPa (x_1) were calculated by the compiler.

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in reference 1. The equilibration device is a capillary tube containing an internal mixer which is moved up and down by means of an external, motor-driven magnet. The capillary tube is sealed in a vertical position and connected to a gas and liquid charging system, pressure gauges, as well as a volume regulator to maintain a constant pressure and to determine the volume of gas charged.

Molar volumes of liquid solutions are also given as a function of solution compositions, temperatures and pressures.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

T /K = ± 1.0

$\delta x_1/x_1$ = ± 3.0% (compiler)

REFERENCES:

1. Kritchevskii, I.R.; Efremova, G.D.

   Zhur. Fiz. Chim 1956, *30*, 1877.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Pryanikova, R.O.; Efremova, G.D.; Malikov, D.A.; Zagorets, P.A.; Shostenko, A.G.; Dodonov, A.M.

Tr. Mosk. Khim. Theknol. Inst. 1973, *75*, 78-80.

VARIABLES:

$T/K = 373.15 - 423.15$

$p_1/MPa = 1.08 - 4.68$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

....continued

T/K	[1] Total Pressure P/atm	[2] Ethene Partial Pressure p_1/MPa	Composition Mole Fraction Propanol, x_3	Ethene, x_1	[2] Henry's Constant $H/MPa(mol\ fraction)^{-1}$ (x_1)
423.15	50.5	4.68	0.80	0.20	23.4
(150 C)	39.1	3.51	0.85	0.15	(0.00434)
	27.7	2.32	0.90	0.10	
	16.5	1.15	0.95	0.05	
373.15	43.0	4.37	0.80	0.20	21.4
(100 C)	32.6	3.21	0.85	0.15	(0.00473)
	22.1	2.14	0.90	0.10	
	11.7	1.08	0.95	0.05	

[1] Only graphical results were presented in this paper in the form of total pressure (P) as a function of mole fraction propanol (x_3). Values were read from an enlarged graph by the compiler.

[2] The ethene partial pressure (p_1) was estimated using Raoult's law, and the Henry's law constant (H) as well as the mole fraction solubility for an ethene partial pressure of 0.101325 MPa (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in reference 1. The equilibration device is a capillary tube containing an internal mixer which is moved up and down by means of an external, motor-driven magnet. The capillary tube is sealed in a vertical position and connected to a gas and liquid charging system, pressure gauges, as well as a volume regulator to maintain a constant pressure and to determine the volume of gas charged.

Molar volumes of liquid solutions are also given as a function of solution compositions, temperatures and pressures.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$T/K = \pm 1.0$

$\delta x_1/x_1 = \pm 3.0\%$ (compiler)

REFERENCES:

1. Kritchevskii, I.R.; Efremova, G.D.

Zhur. Fiz. Chim. 1956, *30*, 1877.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. 1-Propanol; C_3H_7OH; [71-23-8]

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967, *43*, 114-6.

VARIABLES:

T/K = 293.15 - 333.15

P/MPa = 0.29 - 3.26

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5$Pa	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.090	0.019
	8.167	0.055
	15.81	0.109
	32.32	0.237
313.15	2.888	0.012
	8.288	0.042
	17.93	0.094
	32.63	0.180
333.15	2.888	0.011
	8.309	0.034
	17.93	0.082
	32.63	0.147

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$; $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. 1-Octanol; $C_8H_{17}OH$; [111-87-5]	Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-6.
VARIABLES: T/K = 293.15 - 333.15 P/MPa = 0.28 - 3.24	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5$Pa	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.131	0.034
	8.288	0.083
	13.88	0.141
	32.22	0.344
313.15	2.837	0.022
	8.258	0.066
	17.73	0.138
	32.42	0.253
333.15	2.857	0.018
	8.278	0.052
	17.83	0.121
	32.22	0.214

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

δT/K=±0.1; δP=±0.5%; $\delta x_{C_2H_4}$ =±0.002

(estimated by compiler)

REFERENCES:

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

Critical evaluation of the solubility of ethene at a partial pressure not greater than 101.3 kPa in organic halides

In general mole fraction solubility in organic halides is lower than in alkanes but higher than in solvents containing oxygen or nitrogen. Consistent measurements in several organic halides have been obtained by more than one group. This enables a more reliable characterisation of the solubility pattern in organic halides than in oxygen or nitrogen compounds.

Tetrachloromethane; CCl_4; [56-23-5]

Solubility in tetrachloromethane at a partial pressure of 101.3 kPa has been reported by Horiuti (1), Narasimhan and Nageshwar (2), Sahgal *et al.*(3), Leites and Ivanovskii (4), Hannaert *et al.*(5), Brückl and Kim (6), and by Jadot (7). From the information available the single measurement by Narasimhan appears to be inconsistent with other measurements and must be ignored. The 19 data points from other sources can be fitted to the equation

$$\ln x_1 = -20.598 + 1773.8/(T/K) + 1.8277 \ln(T/K)$$

where x_1 is the mole fraction solubility at p_1 = 1.013 kPa

standard deviation in values of $x_1 = 3.1 \times 10^{-4}$

This equation is recommended for the temperature range 253-323 K.

Trichloromethane; $CHCl_3$; [67-66-3]

Solubility in trichloromethane was measured by Leites and Ivanovskii (4) at 243.15 K and by Camacho Rubio *et al.*(8) at 293-308 K. In each case data was presented in graphical form only. Data points from the two graphs fit the equation

$$\ln x_1 = -9.4327 + 1525.5/(T/K)$$

where x_1 is the mole fraction solubility at p_1 = 1.013 kPa

standard deviation in values of $x_1 = 3.1 \times 10^{-4}$

This equation is based on 5 data points and corresponds to a solubility curve which differs from the pattern of curves shown by most of the other halocompounds for which corresponding data is available (see fig 1). It should be accepted on a tentative basis for the temperature range 253-323 K pending further measurements on the system.

Chloroethene; C_2H_3Cl; [75-01-4]

Solubility in chloroethene was measured by Hannaert *et al.*(5) over the temperature range of 213.15-243.15 K. Results were published in the form of an equation for Henry's constant over this temperature range. Mole fraction solubility can be assumed to vary linearly with pressure to at least 101.3 kPa. Extrapolation of the mole fraction solubility to 298.15 K gives a value of 0.0183, close to the solubility in octane and appreciably greater than that in tetrachloro and trichloromethane. There is no reason to doubt Hannaert's measurements but they must be accepted on a tentative basis until they are confirmed by other measurements.

1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Hannaert *et al.*(5) also measured solubility in 1,2-dichloroethane in the temperature range 273.15-313.15 K. Choudhari and Doraiswami (9) measured solubility in the range 280-300.5 K. There is poor agreement between the two sets of measurements. The mole fraction solubility at 292.5 K from Hannaert's data is 0.00934 compared with Choudhari's value of 0.00804.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

The evaluator cannot determine which is likely to be the more reliable measurements. Data from the two sources can be fitted to the equation

$$\ln x_1 = -279.08 + 12799/(T/K) + 40.604 \ln x_1$$

where x_1 is the mole fraction solubility at p_1 = 1.013 kPa
standard deviation in values of $x_1 = 7.3 \times 10^{-4}$

The variation in solubility with change in temperature as indicated by this equation is inconsistent with the variation in solubility in other halocompounds (see fig.1). This equation should not be used outside the temperature range 273-313 K. Further measurements are needed on this system.

1,1,2,2-Tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Velichko *et al.*(10) reported solubility in 1,1,2,2-tetrachloroethane over a partial pressure range to 101.3 kPa at three temperature from 273.15 to 298.15 K. Mole fraction solubilities at a partial pressure of 101.3 kPa fit the equation

$$\ln x_1 = -11.562 + 1977.3/(T/K)$$

where x_1 is the mole fraction solubility at p_1 = 1.013 kPa
standard deviation in values of $x_1 = 5.2 \times 10^{-4}$

As can be seen in fig 1 the measurements indicate a much steeper change in mole fraction solubility with change in temperature as compared with most other chlorocompounds for which data are available. The change is similar to that apparent from the measurements on trichloromethane in the temperature range 293.15-308.15 K but needs confirmation by further work.

Chlorobenzene; C_6H_5Cl; [108-90-7]
Bromobenzene; C_6H_5Br; [108-86-1]

Solubility in chlorobenzene at a partial pressure of 101.3 kPa has been measured by Lopez *et al.*(11), Horiuti (1), and by Sahgal *et al.*(3) Measurements cover the temperature range 263.15 to 363.15 K and are consistent with one another. Data can be fitted to the equation

$$\ln x_1 = -26.1311 + 1950.0/(T/K) + 2.6600 \ln(T/K)$$

where x_1 is the mole fraction solubility at p_1 = 1.013 kPa
standard deviation in values of $x_1 = 6.7 \times 10^{-5}$
This equation is recommended by the evaluator for the temperature range 263.15 to 363.15 K.

Solubility in bromobenzene was also measured by Lopez *et al.*(11) in the temperature range 263.15 to 303.15 K. Mole fraction solubility at a partial pressure of 101.3 kPa may be fitted to the equation

$$\ln x_1 = -25.783 + 1910.4/(T/K) + 2.5971 \ln(T/K)$$

where x_1 is the mole fraction solubility at p_1 = 1.013 kPa
standard deviation in values of $x_1 = 1.2 \times 10^{-5}$
This equation fits the experimental data slightly better than the one given by the authors. There is no reason to doubt the validity of these measurements but they should be accepted on a tentative basis until confirmed by further measurements.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]
Bromocyclohexane; $C_6H_{11}Br$; [108-85-0]

Lopez *et al.*(12), measured the solubility in chlorocyclohexane and in bromocyclohexane in the temperature range 263.15 to 303.15 K. Mole fraction solubility in chlorocyclohexane is greater than in bromocyclohexane and also greater than in chlorobenzene. Mole fraction solubility in cyclohexylamine is similarly greater than that in benzenamine.

The evaluator has found that the data for solubility in chlorocyclohexane at a partial pressure of gas of 101.3 kPa fits the equation
$\ln x_1 = -9.8501 + 1275.4/(T/K) + 0.2262 \ln(T/K)$
where x_1 is the mole fraction solubility at p_1 = 1.013 kPa
standard deviation in values of $x_1 = 1.0 \times 10^{-5}$; temp. range 263-303 K
This equation gives better fit than the one given by the authors.

Data for bromocyclohexane may be fitted to the equation
$\ln x_1 = -28.775 + 2045.2/(T/K) + 3.0748 \ln(T/K)$
where x_1 is the mole fraction solubility at p_1 = 1.013 kPa
standard deviation in values of $x_1 = 2.2 \times 10^{-5}$; temp. range 263-303 K
This equation gives better fit than the one given by the authors.

There is no reason to doubt the measurements of solubility in these two solvents and they can be accepted on a tentative basis until confirmed by other workers.

Mixed solvents

Trichloromethane; $CHCl_3$; [67-66-3] + 2-propanone; C_3H_6O; [67-64-1]
methylbenzene; C_7H_8; [108-88-3]

Leites and Ivanovskii (4) measured solubility in mixtures of trichloromethane with 2-propanone and with methylbenzene at 243.15 K. No other data for these mixtures are available for comparison. The solubility in pure trichloromethane is consistent with measurements at higher temperatures. The value of the solubility in pure 2-propanone differs by about 8% from that calculated from Hannaert's data. Data for the mixture of trichloromethane and 2-propanone may be accepted on a tentative basis, bearing in mind the uncertainty in the data for pure 2-propanone. Leites and Ivanovskii also measured solubility in pure methylbenzene at 213.15, 223.15 and 243.15 K. The value at 243.15 K differs by about 6% from the value calculated from an equation published by Hannaert *et al.*(5). The solubility in mixtures of trichloromethane and methylbenzene may be accepted on a tentative basis.

Tetrachloromethane; CCl_4; [56-23-5] + heptane; C_7H_{16}; [142-82-5]

Leites and Ivanovskii measured solubility in mixtures of tetrachloromethane and heptane at 253.15 K. Their value for the solubility in pure tetrachloromethane at 253.15 K is consistent with data at higher temperatures from other workers. In addition their measurements of solubility in pure heptane from 213.15 to 253.15 K are consistent with measurements by other workers (3,7) at higher temperatures. The data for solubility in mixtures of tetrachloromethane and heptane may be accepted on a tentative basis.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

Tetrachloromethane; CCl_4; [56-23-5] + benzene; C_6H_6; [71-43-2]

Narasimham & Nageshwar (2) measured solubility in mixtures of tetrachloromethane and benzene at 293.15 K. Mole fraction solubilities corrected to a partial pressure of 101.3 kPa vary linearly with mole fraction of benzene. There is some uncertainty concerning corrections for the partial pressure of solvent (see compilation sheet). The solubility in pure tetrachloromethane at a partial pressure of 101.3 kPa, as estimated by the compiler from data reported in the same paper, has been rejected by the evaluator in favour of measurements by other workers. The value of the solubility in pure benzene which they reported is about 4% greater than that reported by Horiuti (1).

References

1. Horiuti, J. *Sci. Pap. Inst. Phys. Chem. Res. (Jpn)* 1931/32, *17*, 125-256.
2. Narasimhan, S.; Nageshwar, G.W. *Chem. Petro-Chem. J. (India)* 1979, *10*, 13-15.
3. Sahgal, A.; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354-357.
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5. Hannaert, H.; Haccuria, M.; Mathieu, M.P. *Ind. Chim. Belge* 1967, *32*, 156-164.
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9. Choudhari, R.V.; Doraiswami, L.K. *J. Chem. Eng. Data* 1972, *17*, 428-432.
10. Velichko, S.M.; Treger, Yu.A.; Flid, R.M. *Russian J. Phys. Chem.* 1973, *47*, 1620-1621.
11. Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1988, *43*, 183-189.
12. Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C. *J. Chem. Eng. Data* 1989, *34*, 198-200.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Organic halides

EVALUATOR:

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

November, 1993

CRITICAL EVALUATION:

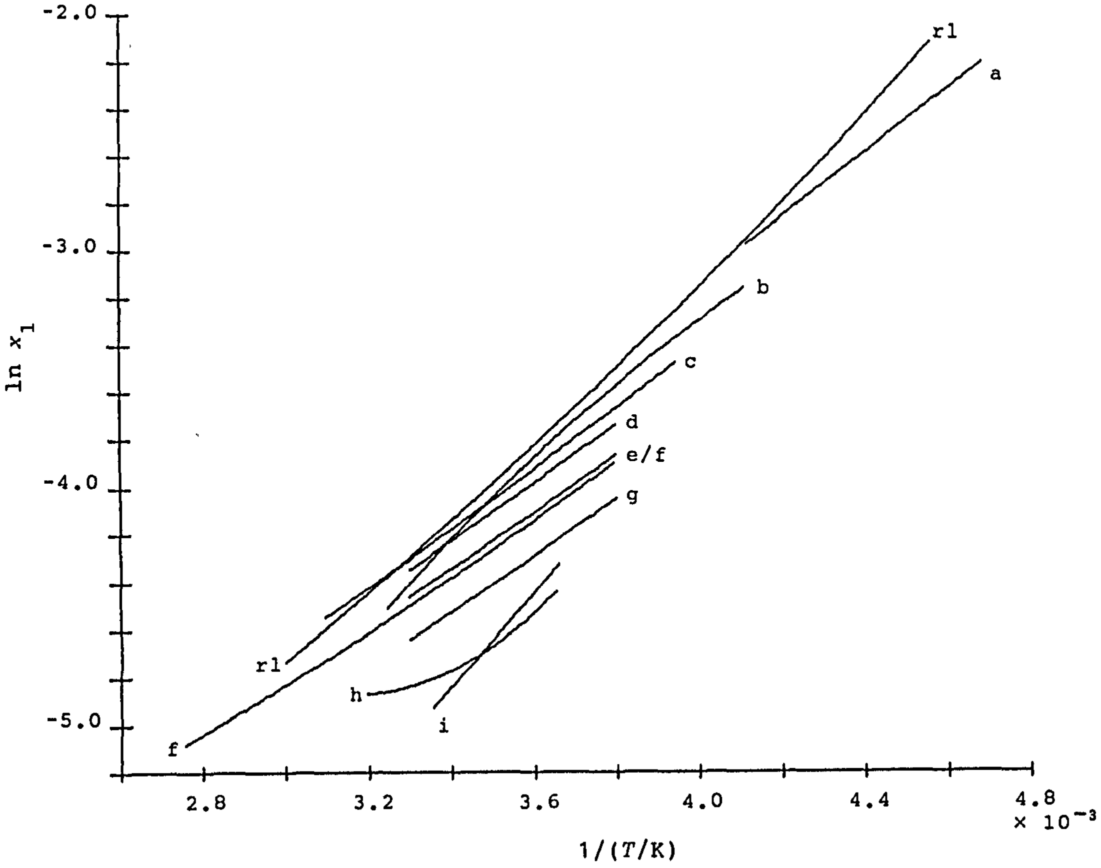


Figure 1 The solubility of ethene at a partial pressure of 101.3 kPa in organic halides

a	Chloroethene	f	Chlorobenzene
b	Trichloromethane	g	Bromobenzene
c	Tetrachloromethane	h	1,2-Dichloroethene
d	Chlorocyclohexane	i	1,1,2,2-Tetrachloroethane
e	Bromocyclohexane	rl	reference line based on Raoult's law equation.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Tetrachloromethane or carbon tetrachloride; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, *17*, 125 - 256.

VARIABLES:

T/K: 273.15 - 313.15

p_1/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick

H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^2x_1	Bunsen Coefficient $\alpha/\text{cm}^3(\text{STP})\text{cm}^{-3}\text{atm}^{-1}$	Ostwald Coefficient $L/\text{cm}^3\text{cm}^{-3}$
273.15	2.069	5.027	5.027
278.15	1.910	4.605	4.689
283.15	1.779	4.259	4.415
288.15	1.659	3.942	4.159
293.15	1.549	3.654	3.922
298.15	1.451	3.400	3.711
303.15	1.360	3.164	3.511
308.15	1.282	2.962	3.341
313.15	1.203	2.759	3.163

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

Smoothed Data: For use between 273.15 and 313.15 K.

$$\ln x_1 = -8.0980 + 11.5219/(T/100\text{K})$$

The standard error about the regression line is 2.62×10^{-5}.

T/K	Mol Fraction 10^2x_1
273.15	2.065
283.15	1.780
288.15	1.658
293.15	1.549
298.15	1.450
303.15	1.361
313.15	1.205

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) Ethene. Prepared by dropping ethanol into orthophosphoric acid. The gas was cooled, passed through several wash solutions, dried, and fractionated from liquid air several times.

(2) Tetrachloromethane. Kahlbaum. Dried over P_2O_5 and distilled. Boiling point (760 mmHg) 76.74°C.

ESTIMATED ERROR:

$\delta T/\text{K} = 0.05$

$\delta x_1/x_1 = 0.01$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Nageshwar, G.W.

Chem. Petro-Chem. J. (India)

1979, *10*, 13-15.

VARIABLES:

$T/K = 293.15$

$p/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene for: [1]$P/kPa = 101.325$	[2]$P_1/kPa = 101.325$	[2] Ostwald Coefficient L/cm^3 gas$(cm^3$ solvent$)^{-1}$
20	293.15	0.01612	0.01827	4.613

[1] Although not specifically stated in the paper, it is assumed that the mole fraction solubility is for a total pressure of 101.325 kPa.

[2] Calculated by compiler; a gas molar volume of 23910 $cm^3/mole$ was used at 293.15 K and 101.325 kPa for the calculation of L, and Henry's law was assumed to apply for the calculation of x_1.

It was confirmed by personal communication that the solubilities were measured at atmospheric pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400°C and analyzed by chromatography. Purity not given.
2. Tetrachloromethane was distilled twice in a laboratory packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A.

Anal. Chem. 1948, *20*, 624.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES: T/K = 273-323

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1	Ostwald Coefficient L/ cm^3 gas (cm^3 solvent)$^{-1}$
0	273.15	0.0208	5.02
25	298.15	0.0146	3.72
50	323.15	0.0103	2.74

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. Tetrachloromethane was from J.T. Baker of 99.9 mole % purity.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

$T/K = 253.15$,

$p_1/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] $\log_{10}$ (H'/mmHg)	[2] Henry's Constant, H/atm (mole fraction)$^{-1}$	[2] Mole Fraction Ethene, x_1
-20	253.15	4.391	32.37	0.0309

This result was part of a study for the behavior of solubilities in two-component solvent solutions.

[1] Only graphical results were available in this paper; a value of log of Henry's constant (H') was read from an enlarged graph by the compiler.

[2] Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and controlled to a temperature to ± 0.05 K. The equilibrium cell was mounted in the cryostat. The solvent was purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Tetrachloromethane was distilled and analyzed by chromatography. Actual purity not given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 258.15 - 293.15

p_1/kPa = 101.3

PREPARED BY:

W. Hayduk
H.L. Clever

EXPERIMENTAL VALUES:

t/C	T/K	[1]Mole Fraction Ethene, x_1
-15	258.15	0.0285
-10	263.15	0.0259
10	283.15	0.0184
20	293.15	0.0158

[1]Mole fraction solubility calculated by compilers for a gas partial pressure of 101.3 kPa using the equation developed by the authors with ν = 1, for the applicable temperature range:

$$\log(K\pi\nu) = 3.69 - (\Delta H/\text{cal mol}^{-1})/(2.3R(T/\text{K}))$$

The authors' definitions are:

ΔH = 2,530 cal mol^{-1}, Enthalpy of dissolution

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π / atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = $(f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the least accurate.

The apparatus is of glass and consists of a burette in which the gas is confined over mercury, two bulbs for the solvent, one above the other, a mercury manometer and a constant temperature bath. A measured volume of solvent is degassed in the top bulb at ambient temperature and charged to the absorption bulb in the bath. Gas is charged to the desired pressure. The quantity of gas added at constant pressure is measured. Agitation is manual.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%
2. Tetrachloromethane. Merck. Vapor pressures at -15 °C and 20 °C are 14 and 90 mm Hg. Purity not given.

ESTIMATED ERROR:

$\delta x_1/x_1$ = ± 10 to 15% (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane (Carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Brückl, N.; Kim, J. I.

Z. Phys. Chem. (Wiesbaden)

1981, *126*, 133-150.

VARIABLES:

$T/K = 298.2$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

$\ln H/\text{atm}$	Mole fraction of ethene in liquid[†], $x_{C_2H_4}$
4.23	0.01455

[†] at a partial pressure of 1 atmosphere, calculated by compiler, assuming $x_{C_2H_4} = 1/H$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined by a volumetric method described as "the Ostwald method". No other details given.

SOURCE AND PURITY OF MATERIALS:

1. Linde Co. sample, purity 99.8 volume per cent.
2. Uvasol or analytical grade.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta H = \pm 1.25\%$.

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Jadot, R.

J. Chim. Phys. 1972, *69*, 1036-40

VARIABLES:

T/K = 298.15

P/kPa = 101.3

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	Henry's Law Constant, H/atm	Mole fraction$^+$ at partial pressure of 101.3 kPa, $x_{C_2H_4}$	#ΔH^∞ /cal mol^{-1} (/J mol^{-1})
298.15	67.55	0.01480	598 (2502)

+ Calculated by compiler assuming $x_{C_2H_4} = 1/H$.

\# Excess partial molar enthalpy of solution at infinite dilution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The conventional gas chromatographic technique was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since no allowance was made for surface adsorption.

SOURCE AND PURITY OF MATERIALS:

No details given.

ESTIMATED ERROR:

δT/K = ±0.05; δH = ±2%

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

$T/K = 243.15$,

$p_1/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]$\log_{10}(H'/\mathrm{mmHg})$	[2]Henry's Constant, H/atm (mole fraction)$^{-1}$	[2]Mole Fraction Ethene, x_1
-30	243.15	4.257	23.67	0.0422

This result was part of a study for the behavior of solubilities in two-component solvent solutions.

[1] Only graphical results were available in this paper; a value of log of Henry's constant (H') was read from an enlarged graph by the compiler.

[2] Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and controlled to a temperature to ± 0.05 K. The equilibrium cell was mounted in the cryostat. The solvent was purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Trichloromethane was distilled and analyzed by chromatography. Actual purity not given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Camacho Rubio, F.; Delgado Diaz, S.; Alvaro Alvarez, R.

Revista Ing. Quim. (Spain) 1980, *12*, 83-87.

VARIABLES:

T/K = 293.15 - 308.15

p_1/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] $\log_{10} K_S$ K_S/mm Hg (mol/l)$^{-1}$	[2] Henry's Constant, H/atm (mol fraction)$^{-1}$	[2] Ethene Mole Fraction, x_1
20	293.15	3.602	66.62	0.0150
25	298.15	3.651	74.07	0.0135
30	303.15	3.699	82.10	0.0122
35	308.15	3.746	90.66	0.0110

The ethene solubility in chloroform is shown as a straight-line graph only, with log K_S versus $1/T$ for an applicable temperature range from 293.15 to 308.15 K.

[1] Values of log K_S were taken from an enlarged graph and fitted to an equation by the compiler as follows:

$$\log_{10} K_S = 6.5583 - 866.67\ (T/\mathrm{K})^{-1}$$

K_S = a form of Henry's constant, mm Hg pressure (mol/l)$^{-1}$.

[2] A more common Henry's constant (H) and mole fraction ethene solubility for a partial pressure of 101.3 kPa were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass vessel, 100 cm in volume, equipped with three ports and submerged in a constant temperature bath, is used for solubility determinations. One port is connected to a gas burette from which a known volume of gas can be charged using a mercury levelling bottle. Another port is for evacuation and the third is for temperature measurement. A magnetic stirrer is employed. A drying tube is used to ensure that the ethene is dry. Care is also taken to ensure that the purified solvent is not exposed to air.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Neither source nor purity specified.
2. Trichloromethane. The 1.5 parts ethanol stabilizer per 100 parts solvent (v/v) were removed by adsorption on activated silica. Purity not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 4\%$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Chloroethene (vinyl chloride); C_2H_3Cl; [75-01-4]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

$T/K = 213.15 - 243.15$

$p_1/kPa = 101.3$

PREPARED BY:

W. Hayduk
H.L. Clever

EXPERIMENTAL VALUES:

t/C	T/K	[1]Mole Fraction Ethene, x_1
-60	213.15	0.110
-50	223.15	0.0829
-40	233.15	0.0641
-30	243.15	0.0507

[1] Mole fraction solubility calculated by compilers for a gas partial pressure of 101.3 kPa using the equation developed by the authors with $\nu = 1$, for the applicable temperature range:

$$\log (K\pi\nu) = 3.68 - (\Delta H /\text{cal mol}^{-1})/(2.3R(T/K))$$

The authors' definitions are:

$\Delta H = 2{,}650$ cal mol^{-1}, Enthalpy of dissolution

$$K = Y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π/atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu/atm$, is equivalent to a Henry's constant in the form $H_{1,2}/atm = (f_1/atm)/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors described several methods used; the one used in this case was considered the most accurate.

The apparatus was of glass and consisted of a burette in which the gas was confined over mercury, an absorption vessel agitated electromagnetically, a turbine for circulating the gas, a mercury manometer and a constant temperature bath. The exposed tubing was minimized. The quantity of gas introduced into the absorption vessel was measured volumetrically. Solvent was degassed by repeated freezing and evacuation.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%
2. Chloroethene. BASF. Densities at -40°C and -60°C reported as 1.016 and 1.0485 g cm^{-3}. Specified purity 99.9%.

ESTIMATED ERROR:

$T/K = \pm 0.2$

$\delta x_1/x_1 = \pm 2$ to 5%

$p/\text{mm Hg} = \pm 0.1$ (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 273.15 - 313.15

p_1/kPa = 101.3

PREPARED BY:

W. Hayduk
H.L. Clever

EXPERIMENTAL VALUES:

t/C	T/K	[1] Mole Fraction Ethene, x_1
0	273.15	0.0113
10	283.15	0.0102
20	293.15	0.0093
25	298.15	0.0089
40	313.15	0.0079

[1] Mole fraction solubility calculated by compilers for a gas partial pressure of 101.3 kPa using the equation developed by the authors with $\nu = 1$, for the applicable temperature range:

$$\log (K\pi\nu) = 3.166 - (\Delta H /\text{cal mol}^{-1})/(2.3R(T/K))$$

The authors' definitions are:

ΔH = 1,520 cal mol^{-1}, Enthalpy of dissolution

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π/ atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = $(f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case was considered the most accurate.

The apparatus was of glass and consisted of a burette in which the gas was confined over mercury, an absorption vessel agitated electromagnetically, a turbine for circulating the gas, a mercury manometer and a constant temperature bath. The exposed tubing was minimized. The quantity of gas introduced into the absorption vessel was measured volumetrically.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. Specified purity 99.9%
2. 1,2-Dichloroethane. Produced by synthesis. Distilled and fractionally crystallized. Density at 20°C is 1.2627 g cm^{-3}. Purity > 99.9% by spectroscopy and gas chromatography.

ESTIMATED ERROR:

T/K = ± 0.2
$\delta x_1/x_1$ = ± 2 to 5%
p/mm Hg = ± 0.1 (authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethane, 1,2-Dichloro- (Ethylenedichloride); $C_2H_4Cl_2$; [107-06-2]

ORIGINAL MEASUREMENTS:

Choudhari, R.V.; Doraiswami, L.K.

J. Chem. Eng. Data 1972, *17*, 428-432.

VARIABLES:

T/K = 280.0-300.5

P/kPa = 94.23

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Solubility at P =94.23 (0.93 atm) s /g(l)$^{-1}$	[1] Solubility at p = 101.325 kPa Mole Fraction,x_1	[1] Henry's Constant H/atm/(mole fraction)$^{-1}$
280	3.67	0.01139	87.8
287	2.66	0.00854	117.1
292.5	2.43	0.00804	124.4
300.5	2.05	0.00718	139.2

[1] Calculated by compiler; x_1 is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The glass absorption vessel was equipped with a stainless steel stirrer and a jacket through which constant temperature water was circulated. A volume of 400-500 cm^3 of solvent was charged into the vessel, thermal equilibrium was established and then gas was bubbled through the solvent. Samples were withdrawn at 10-15 min. intervals for analysis using a chemical analysis for the olefin content. When the concentrations remained constant, equilibrium was considered established. Precautions were taken to exclude water vapor from the air from entering the vessel. Experiments were performed at atmospheric pressure, 0.93 atm (at Poona, India). Reference 1 refers to the method of olefin analysis.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 99.0%.
2. 1,2-Dichloroethane purity 99.0%.

ESTIMATED ERROR:

T/K = ± 0.05

$\delta s/s$ = ± 2%

REFERENCES:

1. Thomas, C.L.; Block, H.S.; Hockstra, J. *Ind. Eng. Chem. Anal. Ed.* 1938, *10*, 153.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1,1,2,2-Tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

ORIGINAL MEASUREMENTS:

Velichko, S.M.; Treger, Yu.A.; Flid, R.M.

Russian J. Phys. Chem. 1973, *47*, 1620-1621.

VARIABLES:

T/K = 273.15 - 298.15

p_1/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Solubility, c, Moles per litre	[2] Mole Fraction Ethene, x_1	[2]Ostwald Coefficient L/cm^3 gas(cm^3 solvent)$^{-1}$
0	273.15	0.250	0.0137	5.56
10	283.15	0.175	0.0097	4.04
25	298.15	0.132	0.0074	3.21

[1] Only graphical results were available in this paper; the solubility, c, was shown as a function of partial pressure, p_1, up to a partial pressure of 101.3 kPa showing that Henry's law was obeyed. Values of c for a partial pressure of 101.3 kPa were read from an enlarged graph by the compiler.

[2] Calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known quantity of solvent was charged into a thermostated saturation vessel attached to a mechanical mixer. Ethene gas admixed with argon was allowed to flow into the saturation vessel at a controlled rate. The composition of the gas was monitored by chromatography. Saturation of the solvent continued until the content of ethene entering and leaving the saturation vessel was the same. The gas analysis was by means of chromatography using a thermal conductivity detector. Samples of saturated solution were withdrawn by means of a syringe and analyzed also by chromatography but using a flame ionization detector.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not given.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 4\%$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Chlorobenzene; C_6H_5Cl
   [108-90-7]

ORIGINAL MEASUREMENTS:

Lopez, M.C.; Gallardo, M.A.;
Urieta, J.S.; Gutierrez Losa,C.
Rev. Acad. Cienc. (Zaragoza)
1988, *43*, 183-189.

VARIABLES:

T/K = 263.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction $10^4\ x_1$	[1]Ostwald Coefficient L/cm^3 cm^{-3}	[1]Bunsen Coefficient α/cm^3(STP) cm^{-3} atm^{-1}
263.15	202	4.46	4.63
273.15	171	3.88	3.88
283.15	146	3.39	3.27
293.15	126.5	3.01	2.80
303.15	110.5	2.69	2.42

[1] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data to the equation:

$$\ln x_1 = - 10.1836 + 1274.115(T/\mathrm{K}) + 0.2581 \ln (T/\mathrm{K})$$

They also obtained ΔH/kJ mol^{-1} = -9.95 and ΔS/J K^{-1} mol^{-1} = -70 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was similar to that used by Ben Naim and Baer (ref.1) and is described in ref.2. The apparatus consists of a burette system for the gas, a mercury manometer and a solution vessel. The mole fraction of dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of the solvent in the solution vessel determined by weighing.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Español del Oxigeno. Specified purity 99.9%.
2. Chlorobenzene. Merck. Specified purity 99.5%

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.01$ (authors)

REFERENCES:

1. Ben Naim, A.; Baer, S. *Trans. Far. Soc.* 1963, *59*, 2735.
2. Carnicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1979, *34*, 115.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene or ethylene; C_2H_4; [74-85-1] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Horiuti, J. *Sci. Pap. Inst. Phys. Chem. Res. (Jpn)* 1931/32, *17*, 125 - 256.
VARIABLES: T/K: 273.15 - 363.15 p_1/kPa: 101.325 (1 atm)	**PREPARED BY:** M. E. Derrick H. L. Clever

EXPERIMENTAL VALUES:

See following page

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) Ethene. Prepared by dropping ethanol into orthophosphoric acid. The gas was cooled, passed through several wash solutions, dried, and fractionated from liquid air several times.

(2) Chlorobenzene. Kahlbaum. Dried and distilled. Boiling point (760 mmHg) 131.96°C.

ESTIMATED ERROR:

$\delta T/K = 0.05$

$\delta x_1/x_1 = 0.01$

REFERENCES:

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, *17*, 125 - 256.

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^3x_1	Bunsen Coefficient α/cm³ (STP) cm⁻³ atm⁻¹	Ostwald Coefficient L/cm³ cm⁻³
273.15	16.99	3.882	3.882
278.15	15.74	3.575	3.640
283.15	14.63	3.304	3.425
288.15	13.60	3.053	3.221
293.15	12.60	2.812	3.018
298.15	11.92	2.645	2.887
303.15	11.08	2.445	2.714
308.15	10.41	2.283	2.576
313.15	9.838	2.146	2.460
318.15	9.339	2.026	2.360
323.15	8.876	1.915	2.265
328.15	8.380	1.798	2.160
333.15	8.009	1.709	2.084
338.15	7.639	1.621	2.007
343.15	7.288	1.538	1.932
348.15	6.989	1.467	1.870
353.15	6.725	1.404	1.815
358.15	6.459	1.341	1.758
363.15	6.218	1.284	1.707

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

Smoothed Data: For use between 273.15 and 363.16 K.

$$\ln x_1 = -13.9824 + 19.6322/(T/100\text{K}) + 2.7104 \ln (T/100\text{K})$$

The standard error about the regression line is 3.75×10^{-5}.

T/K	Mol Fraction 10^3x_1
273.15	17.05
288.15	13.56
298.15	11.83
308.15	10.45
318.15	9.33
333.15	8.00
348.15	7.00
363.15	6.21

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES:

T/K = 273-323

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Mole Fraction Ethene, x_1	Ostwald Coefficient L/ cm^3gas /cm^3 solvent
0	273.15	0.0173	3.92
25	298.15	0.0120	2.90
50	323.15	0.00893	2.27

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. Chlorobenzene was from Fisher of 99.9 mole % purity.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Bromobenzene; C_6H_5Br; [108-86-1]

ORIGINAL MEASUREMENTS:

Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C.

Rev. Acad. Cienc. (Zaragoza) 1988, *43*, 183-189.

VARIABLES:

T/K = 263.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction $10^4\ x_1$	[1]Ostwald Coefficient L/cm^3 cm^{-3}	[1]Bunsen Coefficient α/cm^3(STP) cm^{-3}atm^{-1}
263.15	174	3.70	3.84
273.15	147	3.21	3.21
283.15	126.2	2.83	2.73
293.15	109.4	2.52	2.34
303.15	96.5	2.27	2.05

[1] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data to the equation:

$$\ln x_1 = -17.9492 + 1581.0929\,(T/\mathrm{K})^{-1} + 1.4158\ \ln(T/\mathrm{K})$$

They also obtained ΔH/kJ mol^{-1} = -9.64 and ΔS/J K^{-1}mol^{-1} = -70 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus was similar to that used by Ben Naim and Baer (ref.1) and is described in ref.2. The apparatus consists of a burette system for the gas, a mercury manometer and a solution vessel. The mole fraction of dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of the solvent in the solution vessel determined by weighing.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Espanol del Oxigeno. Specified purity 99.9%.
2. Bromobenzene. Fluka. Specified purity 99.5%

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.01$ (authors)

REFERENCES:

1. Ben Naim, A.; Baer, S. *Trans. Far. Soc.* 1963, *59*, 2735.
2. Carnicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1979, *34*, 115.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]

ORIGINAL MEASUREMENTS:

Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C.

J. Chem. Eng. Data 1987, *32*, 472-474.

VARIABLES:

T/K = 263.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction $10^4\ x_1$	[1] Ostwald Coefficient L/cm^3 cm^{-3}	[1] Bunsen Coefficient α/cm^3(STP) cm^{-3}atm^{-1}
263.15	237	4.51	4.68
273.15	200	3.90	3.90
283.15	171	3.42	3.30
293.15	148	3.03	2.82
303.15	129	2.70	2.43

[1] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data to the equation:

$$\ln x_1 = -11.6539 + 1348.0(T/\mathrm{K})^{-1} + 0.5004 \ln(T/\mathrm{K})$$

x_1/mole fraction; T/K

They also obtained ΔH/kJ mol^{-1} = -9.98 and ΔS/J K^{-1} mol^{-1} = -69 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus used is similar to that used by Ben Naim and Baer (ref.1) and is described in detail elsewhere (ref.2). It consists of a system of burettes, a mercury manometer and a solution vessel. The mole fraction of the dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of solvent in the solution vessel determined by weighing.

Density and vapor pressure of the solvent were measured:

$$\rho/\mathrm{g\ cm^{-3}} = 1.2856 - 0.000977.T/\mathrm{K}$$

$$\ln(p_2/\mathrm{kPa}) = -5240.7\ (T/\mathrm{K})^{-1} + 13.07$$

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Español del Oxigeno. Specified purity 99.9%.
2. Chlorocyclohexane. Merck. Purity checked by GLC to be $\geq$ 98.5%.

ESTIMATED ERROR:

δT/K = $\pm$ 0.1 (authors)

$\delta x_1/x_1$ = $\pm$ 2% (compiler)

REFERENCES:

1. Ben Naim, A.; Baer, S.F.; *Trans. Far. Soc.* 1963, *59*, 2735.
2. Carnicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1979, *34*, 115.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Bromocyclohexane; $C_6H_{11}Br$; [108-85-0]

ORIGINAL MEASUREMENTS:

Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa,C.

J. Chem. Eng. Data 1989, *34*, 198-200.

VARIABLES:

T/K = 263.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction $10^4\ x_1$	[1]Ostwald Coefficient L/cm^3 cm^{-3}	[1]Bunsen Coefficient α/cm^3 (STP) cm^{-3} atm^{-1}
263.15	209	3.84	3.99
273.15	176	3.32	3.32
283.15	151	2.92	2.82
293.15	131.7	2.61	2.43
303.15	115.6	2.43	2.11

[1] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data to the equation:

$$\ln x_1 = -17.0486 + 1545.9236(T/K)^{-1} + 1.3105 \ln(T/K)$$

They also obtained ΔH/kJ mol^{-1} = -9.44 and ΔS/J K^{-1} mol^{-1} = -68 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is described elsewhere (ref.1); it is based on that proposed by Ben Naim and Baer (ref.2). The set-up consists of a burette system, a mercury manometer and a solution vessel. Mole fraction of the dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of liquid in the solution vessel determined by weighing.

Density and vapor pressure of the solvent were measured and correlated:

$$\rho/\text{kg m}^{-3} = -1.222(T/K) + 1693$$

$$\ln (p_2/\text{kPa}) = -5714.3(T/K)^{-1} + 18.2730$$

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Español del Oxigeno. Specified purity 99.9%.
2. Bromocyclohexane. Fluka. Purity checked by GLC to be >99%.

ESTIMATED ERROR:

δT/K = ± 0.01

$\delta x_1 / x_1$ = ± 0.01 (authors)

REFERENCES:

1. Cornicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1979, *34*, 115.
2. Ben Naim, A.; Baer, S. *Trans. Far. Soc.* 1963, *59*, 2735.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Trichloromethane (chloroform); $CHCl_3$; [67-66-3]
3. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

T/K = 243.15,
p_1/kPa = 101.325
x_1 = 0 - 1.0

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Solvent Composition, x_3, Mole Fraction Toluene	[2] $\log_{10}H'$, H'/mm Hg	[3]Henry's Constant H/atm (mole fraction)$^{-1}$	[3]Mole Fraction Ethene, x_1
-30	243.15	0 (chloroform)	4.257	23.78	0.0421
		0.25	4.384	31.86	0.0314
		0.50	4.439	36.16	0.0277
		0.75	4.446	36.74	0.0272
		1.0 (acetone)	4.423	34.85	0.0287

[1] Compositions of two-component solvent solutions are given on a solute-free basis.

[2] Only graphical results were available; values of log Henry's constant (H') were read from an enlarged graph by the compiler.

[3] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and the temperature was controlled to ± 0.05 K. The equilibration cell was mounted in the cryostat. The solvents were purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Trichloromethane was distilled and analyzed by chromatography. Purity not specified.
3. Propanone was distilled and analyzed by chromatography. Purity not specified.

ESTIMATED ERROR:

δT/K = ± 0.05

$\delta x_1/x_1$ = ± 0.01 (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Trichloromethane (chloroform); $CHCl_3$; [67-66-3]
3. Methylbenzene (toluene); C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9* , 653-657.

VARIABLES:

$T/K = 243.15,$
$p_1/kPa = 101.325$
$x_3 = 0 - 1.0$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Solvent Composition, x_3, Mole Fraction Toluene	[2] log H', H'/mm Hg	[3] Henry's Constant H/atm (mole fraction)$^{-1}$	[3]Mole Fraction Ethene, x_1
-30	243.15	0 (chloroform)	4.257	23.67	0.0432
		0.25	4.295	25.95	0.0385
		0.50	4.319	27.43	0.0365
		0.75	4.324	27.75	0.0360
		1.0 (toluene)	4.304	26.50	0.0377

[1] Compositions of two-component solvent solutions are given on a solute-free basis.

[2] Only graphical results were available; values of log Henry's constant (H') were read from an enlarged graph by the compiler.

[3] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and the temperature was controlled to ± 0.05 K. The equilibration cell was mounted in the cryostat. The solvents were purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Trichloromethane was distilled and analyzed by chromatography. Purity not specified.
3. Methylbenzene was distilled and analyzed by chromatography. Purity not specified.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]
3. Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

$T/K = 253.15$,
$p_1/kPa = 101.325$
$x_3 = 0 - 1.0$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Solvent Composition, x_3, Mole Fraction	[2] $\log_{10}H'$, $H'/mm\ Hg$	[3] Henry's Constant $H/atm\ (mole\ fraction)^{-1}$	[3] Mole Fraction Ethene, x_1
-20	253.15	0 (CCl_4)	4.391	32.37	0.0309
		0.25	4.319	27.43	0.0365
		0.50	4.282	25.19	0.0397
		0.75	4.258	23.83	0.0420
		1.0 (heptane)	4.243	23.02	0.0434

[1] Compositions of two-component solvent solutions are given on a solute-free basis.

[2] Only graphical results were available; values of log Henry's constant (H') were read from an enlarged graph by the compiler.

[3] Values of Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and the temperature was controlled to ± 0.05 K. The equilibration cell was mounted in the cryostat. The solvents were purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. Tetrachloromethane was distilled and analyzed by chromatography. Purity not specified.
3. Heptane was distilled and analyzed by chromatography. Purity not specified.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$

$\delta x_1/x_1 = \pm 0.01$ (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzene; C_6H_6; [71-43-2]
3. Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Narasimhan, S.; Nageshwar, G.W.

Chem. Petro-Chem. J. (India)

<u>1979</u>, *10*, 13-15.

VARIABLES:

$T/K = 293.15$
$P/kPa = 101.325$
Concentration/x_3 = 0.1-0.9

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	Mole Fraction CCl_4 in Mixed Solvent, x_3	Ethene Solubility for: [1]$P/kPa=101.325$	[2]$p/kPa=101.325$	[2]Ostwald Coefficient L/cm^3 gas/cm^3 solvent
20	0.1059	0.01266	0.01406	3.80
	0.2054	0.01279	0.01444	3.87
	0.3030	0.01332	0.01486	3.96
	0.4141	0.01366	0.01528	4.03
	0.5006	0.01402	0.01572	4.12
	0.6201	0.01446	0.01625	4.22
	0.7002	0.01480	0.01666	4.29
	0.8107	0.01521	0.01717	4.38
	0.9046	0.01570	0.01776	4.51

[1] Although not specifically stated in the paper, it is assumed that the mole fraction solubility, x, is for a total pressure of 101.325 kPa.

[2] Calculated by compiler; a gas molar volume of 23910 cm^3/mole was used at 293.15 K and 101.325 kPa for the calculation of L, and Henry's law was assumed to apply for the calculation of x_1.

It was confirmed by personal communication that the solubilities were measured at atmospheric pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solvent was held in a jacketed burette. Constant temperature water was circulated through the jacket. Gas was bubbled through the solvent until saturated. The dissolved gas content was determined by an electrometric dead-stop titration technique which yielded the bromine number. The electrometric titrator was based on a design given in reference 1.

The burettes containing the mixed solvent were saturated with gas in series. Thus evaporation of solvent from the second burette was minimized.

Actual purities and sources of solvents not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene prepared by catalytic dehydration of ethanol over activated alumina at 350-400 °C and analyzed by chromatography. Purity not given.

2. Benzene was distilled twice in a laboratory packed column.

3. Tetrachloromethane was distilled twice in a laboratory packed column.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (Estimated by compiler)

REFERENCES:

1. Dubois, H.D.; Skoog, D.A. *Anal. Chem.* <u>1948</u>, *20*, 624.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides, pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 January, 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Organic Halides (mainly Alkyl Halides) for Pressures greater than 0.20 MPa

Ethene solubilities in organic halide solvents were reported by seven groups of researchers (1-7) for pressures ranging from 0.2 MPa to 11.7 MPa. For these data, in every case, only one research group reported their results for any one solvent; hence, a comparison of data from two or more sources was not possible. Instead, it was only possible to check the consistency of the data. For that purpose graphs of log *x* (mole fraction solubility) versus log *p* (gas partial pressure) were drawn with the solubilities shown as a function of temperature as a parameter. For several of the solvents it was possible to express the data, especially for relatively low pressures, using an equation of the form shown below, with the constant C being nearly equal to one when Henry's law applied:

$$\log x_p = A + B/T + C \log p \qquad (1)$$

The solubilities in the individual solvents will now be considered.

Bromochloromethane; CH_2BrCl; [74-97-5]

Lebedeva et al. (1) reported ethene solubilities in bromochloromethane at 323.15 K, 373.15 K and 423.15 K at pressures ranging from 1.013 MPa to 11.73 MPa. At the lower pressures, up to 10 MPa, Henry's law is approximately obeyed and the corresponding Henry's constants have been tabulated on the data sheet. There are a number of apparently anomalous results.

These data are classified as tentative.

Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

The solubilities of ethene in trichloromethane were reported by Shim and Kohn (2) for pressures ranging from 1.013 MPa to the critical pressures and for five temperatures ranging from 273.15 K to 373.15 K. Except for one result at a temperature of 373.15 K and a pressure of 1.013 MPa, the data appear consistent. They are well represented by the following correlating equation which relates the mole fraction ethene at equilibrium, the temperature, and ethene partial pressure:

$$\log x_p = 522.32(T/\mathrm{K})^{-1} + 0.9600 \log (p/\mathrm{MPa}) - 2.5371 \qquad (2)$$

Equation (2) is limited to pressures $0.6 \text{ MPa} < p < 6.0 \text{ MPa}$. For the indicated pressure range it yields an average, and a maximum deviation from the data of 3.1%, and 9.2%, respectively. Equation (2) and the data on which it is based, are shown in Figure 1. It is noted that equation (2) yields a value about 35% too high when extrapolated to 0,1013 MPa pressure at 298.15 K; hence, it is evident that this equation cannot be used outside the range of the data on which it is based.

The results of Shim and Kohn (2) are classified as tentative.

Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

Konobeev and Lyapin (3) reported solubility data for ethene in tetrachloromethane at 293.15 K, 313.15 K and 333.15 K and pressures from 0.29 MPa to 3.18 MPa. For the purpose of estimating the partial pressure of ethene in the gas phase, Raoult's law was assumed and the pure solvent vapor pressures of 0.0122, 0.0284 and 0.059 MPa were used for the temperatures of 293.15, 313.15 and 333.15 K, respectively. The solubilities over the temperature and pressure range of the data are then well represented by the following equation:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Organic halides, pressures greater than 0.2 MPa (2 atm)

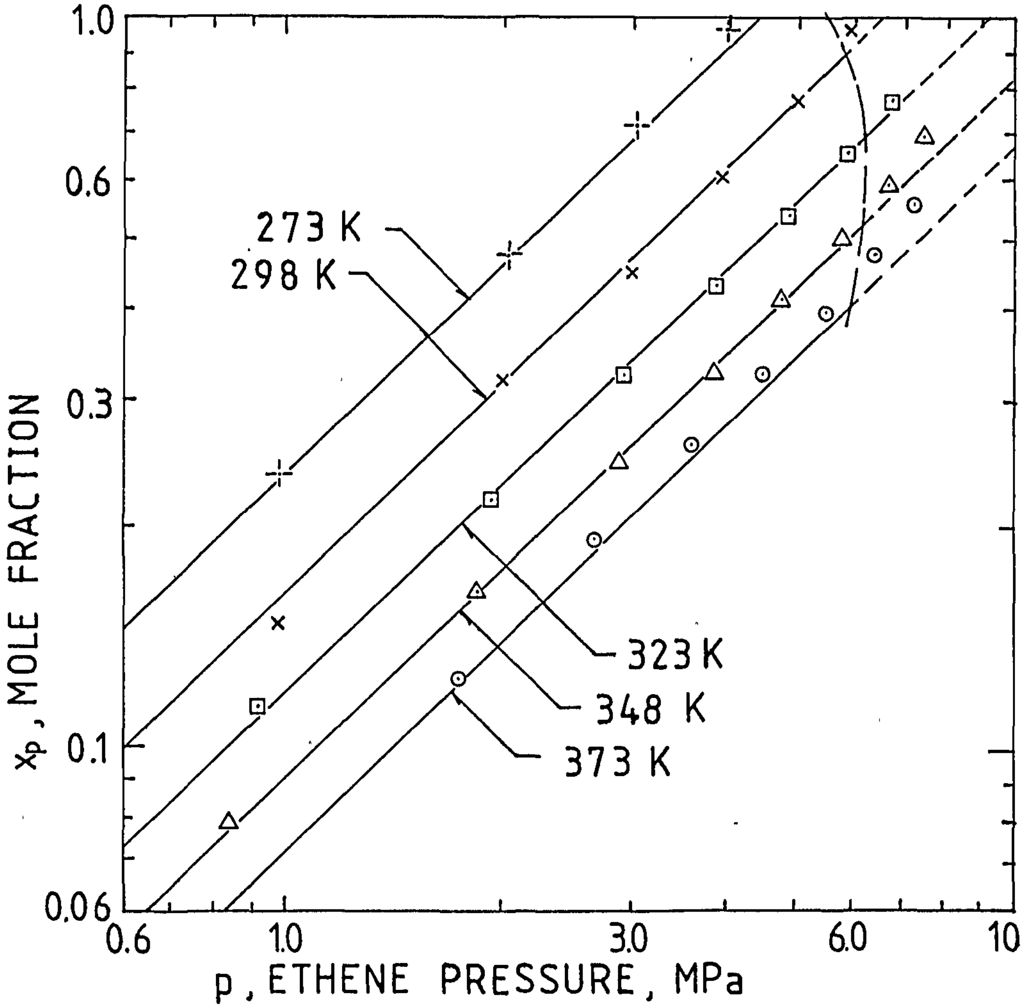
EVALUATOR:

Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, ON
Canada K1N 6N5

January, 1994

CRITICAL EVALUATION:

Fig. 1 Ethene Solubility in Trichloromethane as a Function of Temperature and Pressure; Shim and Kohn (2)



$$\log x_p = 521.68(T/\mathrm{K})^{-1} + 1.047 \log (p/\mathrm{MPa}) - 2.6314 \qquad (3)$$

Equation (3) has average, and maximum deviations from the experimental results of 3.9%, and 9.9%, respectively. Here also, it is cautioned that equation (3) cannot be accurately extrapolated for solubilities at 0.1013 MPa pressure; deviations of approximately 20% are observed.

The data of Konobeev and Lyapin for solubilities in tetrachloromethane are classified as tentative.

1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Konobeev and Lyapin (3) also provided ethene solubilities in 1,2-dichloroethane for pressures ranging from 0.29 MPa to 3.11 MPa and for the temperatures 293.15 K, 313.15 K and 333.15 K. As for the solvent tetrachloromethane, the pure solvent vapor pressures were used along with Raoult's law to estimate ethene partial pressures. The resulting relation between ethene partial pressure, (p), temperature, T, and the mole

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides, pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 January, 1994

CRITICAL EVALUATION:

fraction, x_p, is entirely consistent and is well expressed by the following equation:

$$\log x_p = 446.77(T/K)^{-1} + 1.052 \log (p/MPa) - 2.5285 \qquad (4)$$

The average, and maximum deviations of the data from the correlating equation are 2.1%, and 4.5%, respectively.

The data of Konobeev and Lyapin for solubilities in 1,2-dichloroethane are classified as tentative.

Ethane, 1,1,2-trichloro- 1,2,2-trifluoro-(Freon 113); $C_2Cl_3F_3$; [76-13-1]

Sokolov and Konshin (4) reported data for ethene solubilities in Freon 113 at the temperatures, 300.15 K, 343.15 K and 363.15 K for pressures ranging from 0.20 MPa to 1.11 MPa. No gas phase compositions were available; hence, Raoult's law was used to estimate the solvent partial pressure in the gas phase. It became apparent that the gas contained significant concentrations of solvent vapor especially at the two higher temperatures, estimated to be more than 50% for a number of the results. Thus, because highly accurate results are difficult to obtain with volatile solvents there are some inconsistencies in these results.

Omitting the data point corresponding to a total pressure of 0.31 MPa at 343.15 K, an equation for the remaining data was derived:

$$\log x_p = 531.24\ (T/K)^{-1} + 1.070 \log (p/MPa) - 2.4376 \qquad (5)$$

The average, and maximum deviations of the data from equation (5) are 3.4%, and 10%, respectively. It is cautioned that the application of Raoult's law is unlikely to be accurate at high vapor concentrations, so that equation (5) is approximate only.

The data of Sokolov and Konshin for ethene solubilities in Freon 113 are classified as tentative.

3,3,3-Trifluoro, 1-propene (trifluoropropylene); $C_3H_3F_3$; [677-21-4]

Zernov et al. (5) reported solubilities in 3,3,3-trifluoro 1-propene at temperatures from 283.1 K to 363.1 K and pressures from 0.393 MPa to 5.88 MPa. Henry's law is only approximately obeyed for the temperatures below 333.1 K. The data at the higher temperatures (at 353.1 K and 363.1 K) appear to be inconsistent with those at the lower temperature.

These data are classified as tentative.

Acetic acid, trichloro-ethyl ester (ethyltrichloroacetate); $C_4H_5Cl_3O_2$; [515-84-4]

The results of Kristesashvili et al. (6) for solubilities in acetic acid, trichloro-ethyl ester were shown for the temperatures 363.15 K and 373.15 K and pressures up to 8.1 MPa only in graphical form. Approximate Henry's constants were obtained from the graphs.

These data for acetic acid, trichloro-ethyl ester are classified as tentative.

1-Propene,1,1,2,3,3-pentafluoro-3 trifluoroethenyloxy-(perfluoropropylene vinyl ether); C_5F_8O; [64080-43-9]

Sokolov and Konshin (4) reported solubilities of ethene in 1,1,2,3,3-pentafluoro-3 trifluoroethenyloxy-1-propene at temperatures ranging from

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic halides, pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 January, 1994

CRITICAL EVALUATION:

298.15 K to 353.15 K and pressures from 0.20 MPa to 1.11 MPa. These data were reported as distribution constants in the form of ratios of concentrations in the liquid phase to those in the gas phase. In addition, the solubilities were expressed in moles per litre and as Henry's constants. It was not possible to calculate mole fraction solubilities because neither solution densities nor gas phase compositions could be estimated. Nor could the tabulated results be checked for consistency.

These data are classified as tentative.

Propane, 1,1,1,3- Tetrachloro-; $C_3H_4Cl_4$; [1070-78-6]
Pentane, 1,1,1,5- Tetrachloro-; $C_5H_8Cl_4$; [2467-10-9]
Heptane, 1,1,1,7- Tetrachloro-; $C_7H_{12}Cl_4$; [3922-36-9]
Nonane, 1,1,1,9- Tetrachloro-; $C_9H_{16}Cl_4$; [1561-48-4]

Efremova and Kovpakova (7) reported ethene solubilities in the four tetrachloroalkanes in graphical form only, for temperatures ranging from 273.35 K to 373.15 K and for pressures from about 1 MPa to the critical pressures. From these graphs approximate Henry's constants were estimated because Henry's law was obeyed for ethene concentrations of up to about 0.4 mole fraction. When tested for consistency with respect to temperature, it was noted that the ethene solubility in tetrachloropropane solvent was only marginally different than that in tetrachloropentane. It is not clear whether or not this is anomolous because no clear consistency test is available. One might have expected lower solubilities in tetrachloropropane to be consistent with those of the other three solvents.

These approximate results for solubilities in the tetrachloroalkanes are classified as tentative.

References

1. Lebedeva, E.S.; Kashirina, A.S.; Grokholskaya, V.P. *Ref. Zh. Khim. Abstr.* 1971, *No. 138777*, 92-100.
2. Shim, J.; Kohn, J.P. *J. Chem. Eng. Data*, 1964, *9*, 1-2.
3. Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-116.
4. Solokov, Yu. P.; Konshin, A.I. *Zh. Prikl. Khim.* 1989, *62*, 1395-1398.
5. Zernov, V.S.; Kogan, V.G.; Lyubetskii, S.G.; Duntov, F.I. *Zh. Prikl. Khim.* 1971, *44*, 683-686. (*English Translation* 693-696).
6. Kristesashvili, L.V.; Chkhubianshvili, N.G.; Tatenashvili, M.Kh. *Soobshch. Akad. Nauk Guz. SSR.* 1979, *93*, 365-368.
7. Efremova, G.D.; Kovpakova, P.F. *Zhur. Fiz. Khim.* 1958, *32*, 1231-1240.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Bromochloromethane; CH_2BrCl; [74-97-5]

ORIGINAL MEASUREMENTS:

Lebedeva, E.S.; Kashirina, A.S.; Grokholskaya, V.P.

Ref. Zh. Khim. Abstr. 1971, No.138777, 92-100.

VARIABLES:

$T/K = 323.15 - 423.15$

$P/MPa = 1.013 - 11.73$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Pressure		Mole Fraction Ethene in Liquid, and Gas, x_1, y_1 50°C		100°C		150°C	
P/atm	^{1}/MPa	x_1	y_1	x_1	y_1	x_1	y_1
10	1.013	0.005	0.920	0.020	0.740	0.005	0.410
20	2.027	0.010	0.940	0.040	0.835	0.040	0.410
30	3.040	0.015	0.950	0.065	0.885	0.065	0.595
40	4.053	0.040	0.955	0.110	0.890	0.100	0.670
50	5.066	0.280	0.945	0.160	0.900	0.130	0.725
^{2}56.2	5.694	0.900					
60	6.080			0.210	0.905	0.165	0.750
70	7.093			0.250	0.900	0.205	0.775
80	8.106			0.310	0.895	0.250	0.790
90	9.119			0.380	0.880	0.305	0.790
100	10.32			0.500	0.845	0.375	0.780
^{2}106.5	10.79			0.770			
110	11.15					0.470	0.725
^{2}116	11.73					0.620	

Only interpolated or smoothed data above, given in this paper.

[1] Calculated by compiler.

[2] Critical conditions.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments are described in reference 1. A steel vessel was used along with a heating block, thermostat and pressure gauge for measuring the P - T - x data. Approximate Henry's constants and ethene solubilities, corresponding to a gas partial pressure of 101.3 kPa were calculated by the compiler for pressures to 2.9 MPa at 50°C, and 5.0 MPa at 100°C and 150°C.

t/C	50	100	150
H/atm mol fraction^{-1}	1900	408.5	272
x_1/mole fraction	0.00053	0.0029	0.0037

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Source and purity not specified.
2. Bromochloromethane. Source and purity not specified. Densities and vapor pressures given in paper. Approximate equation for vapor pressures (compiler) based on data given:

$$\log (P/\text{atm}) = 4.4726 - 1521.3/(T/K)$$

ESTIMATED ERROR:

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

$\delta x_1/x_1 = \pm 2\%$ (compiler)

REFERENCES:

1. Lebedeva, E.S.; Khodeva, S.M.; *Zh. Fiz. Khim.* 1961, *35*, 2608.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Shim, J.; Kohn, J.P.

J. Chem. Eng. Data 1964, *9*, 1-2.

VARIABLES: T/K = 273-373

P/MPa = 1.0-10.2 (10-100 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Total Pressure /atm	Total Pressure [1]P/MPa	Partial Pressure [1]p_1/MPa	Liquid Phase Ethene Mole Fraction, x_1	Gas Phase Ethene Mole Fraction, y_1
0	273.15	10	1.013	1.013	0.236	1
		20	2.027	2.027	0.475	1
		30	3.040	3.040	0.708	1
		40	4.053	4.053	0.964	1
25	298.15	10	1.013	0.9859	0.148	0.973
		20	2.027	2.000	0.297	0.987
		30	3.040	3.018	0.448	0.993
		40	4.053	4.050	0.606	0.999
		50	5.066	5.061	0.771	0.999[2]
		60	6.080	5.946	0.968	0.978
		60.2[3]	6.100	5.911	0.969	0.969
50	323.15	10	1.013	0.9150	0.114	0.903
		20	2.027	1.929	0.220	0.952
		30	3.040	2.936	0.324	0.966
		40	4.053	3.931	0.431	0.970
		50	5.066	4.924	0.539	0.972
		60	6.080	5.909	0.654	0.972[2]
		70	7.093	6.802	0.777	0.959[2]
		76.8[3]	7.782	6.957	0.894	0.894

[1] Calculated by compiler. [2] Interpolated by authors.
[3] Critical conditions as indicated by authors.
Liquid phase and gas phase molar volumes also given in this paper.

continued ...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Calibrated borosilicate glass cells were used in two sizes: 12-cm^3 for pressures to 70 atm and 5-cm^3 for pressures from 70-100 atm. The cell was initially almost filled with solvent then evacuated to the solvent vapor pressure. The initial solvent volume was obtained. Gas was volumetrically charged from a high pressure reservoir by displacement with mercury. Gas absorption was facilitated using a magnetically actuated stainless steel ball. At the highest pressure the cell was essentially completely filled with solution. The change in solution volume was noted with each increment of gas. The corresponding gas phase compositions were obtained using separate experiments and measuring the small volume of solvent necessary to saturate the gas. Details in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson; purity 99.5%. Gas dried at 50 atm pressure using silica gel.
2. Chloroform was the spectro grade from Matheson Coleman Bell; no purity given.

ESTIMATED ERROR:

$\delta P/P = \pm 0.01$ $\delta T/K = \pm 0.07$

$\delta x_1/x_1 = \pm 0.01$

REFERENCES:

1. Shim, J.; Kohn, J.P.

J. Chem. Eng. Data ,1962, *7*, 3.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Shim, J.; Kohn, J.P.

J. Chem. Eng. Data 1964, *9*, 1-2.

VARIABLES: $T/K = 273-373$

$P/MPa = 1.0-10.2$ (10-100 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Total Pressure /atm	Total Pressure [1]P/MPa	Partial Pressure [1]p_1/MPa	Liquid Phase Ethene Mole Fraction, x_1	Gas Phase Ethene Mole Fraction, y_1
75	348.15	10	1.013	0.8390	0.078	0.828
		20	2.027	1.834	0.164	0.905
		30	3.040	2.845	0.247	0.936
		40	4.053	3.838	0.328	0.947
		50	5.066	4.813	0.412	0.950
		60	6.080	5.776	0.500	0.950
		70	7.093	6.688	0.594	0.943[2]
		80	8.106	7.506	0.694	0.926[2]
		90	9.119	7.97	0.816	0.874[2]
		90.9[3]	9.210	7.645	0.830	0.830
100	373.15	10	1.013	0.6667	0.057	0.658
		20	2.027	1.688	0.124	0.833
		30	3.040	2.645	0.192	0.870
		40	4.053	3.591	0.260	0.886
		50	5.066	4.539	0.327	0.896
		60	6.080	5.484	0.398	0.902
		70	7.093	6.412	0.479	0.904[2]
		80	8.106	7.312	0.563	0.902[2]
		90	9.119	8.098	0.654	0.888[2]
		100	10.133	8.481	0.773	0.837[2]
		100.9[3]	10.224	8.148	0.797	0.797

[1] Calculated by compiler. [2] Interpolated by authors.

[3] Critical conditions as indicated by authors.

Liquid phase and has phase molar volumes also given in this paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Calibrated borosilicate glass cells were used in two sizes: 12-cm^3 for pressures to 70 atm and 5-cm^3 for pressures from 70-100 atm. The cell was initially almost filled with solvent then evacuated to the solvent vapor pressure. The initial solvent volume was obtained. Gas was volumetrically charged from a high pressure reservoir by displacement with mercury. Gas absorption was facilitated using a magnetically actuated stainless steel ball. At the highest pressure the cell was essentially completely filled with solution. The change in solution volume was noted with each increment of gas. The corresponding gas phase compositions were obtained using separate experiments and measuring the small volume of solvent necessary to saturate the gas. Details in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was from Matheson; purity 99.5%. Gas dried at 50 atm pressure using silica gel.
2. Chloroform was the spectro grade from Matheson Coleman Bell; no purity given.

ESTIMATED ERROR:

$\delta P/P = \pm 0.01$ $\delta T/K = \pm 0.07$

$\delta x_1/x_1 = \pm 0.01$

REFERENCES:

1. Shim, J.; Kohn, J.P.

J. Chem. Eng. Data 1962, *7*, 3.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Tetrachloromethane (Carbon Tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Konobeev, B.I.; Lyapin, V.V.

Khim. Prom. 1967, *43*, 114-6.

VARIABLES:

$T/K = 293.15 - 333.15$

$P/MPa = 0.29 - 3.18$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5 Pa$	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	2.857	0.036
	8.299	0.117
	12.77	0.187
	17.02	0.254
	17.63	0.250
	25.33	0.372
	31.11	0.642
313.15	2.878	0.026
	8.217	0.089
	14.19	0.158
	17.63	0.188
	18.95	0.216
	28.37	0.317
	31.61	0.342
333.15	2.998	0.020
	8.248	0.070
	15.20	0.139
	17.73	0.154
	28.27	0.254
	31.82	0.276

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.
2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$; $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]	Konobeev, B.I.; Lyapin, V.V. *Khim. Prom.* 1967, *43*, 114-6.
VARIABLES: T/K = 293.15 - 333.15 P/MPa = 0.29 - 3.11	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K	$P/10^5$Pa	Mole fraction of ethene in liquid $x_{C_2H_4}$
293.15	3.070	0.028
	8.177	0.078
	15.60	0.154
	17.53	0.179
	30.80	0.337
313.15	2.878	0.020
	8.217	0.060
	17.63	0.140
	31.11	0.267
333.15	2.888	0.015
	8.238	0.048
	17.83	0.116

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Static equilibrium cell fitted with magnetic stirrer. Samples analysed by gas chromatography. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. Purity better than 99.6 mole per cent.

2. No details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P = \pm 0.5\%$; $\delta x_{C_2H_4} = \pm 0.002$

(estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Ethane, 1,1,2-trichloro-1,2,2-trifluoro- (Freon 113); $C_2Cl_3F_3$; [76-13-1]	Sokolov, Yu. P.; Konshin, A.I. *Zh. Prikl. Khim.* **1989**, *62*, 1395-1398.
VARIABLES:	PREPARED BY:
T/K = 300.15 - 363.15 P/MPa = 0.20 - 1.11	W. Hayduk

EXPERIMENTAL VALUES:

t/°C	[1]T/K	Pressure P/MPa	Solubility C_1, mol/litre	Solubility [1]x_1, mol fraction	[2]Henry's Constant H/MPa(mol fraction)$^{-1}$
27	300.15	0.20	0.25	0.029	5.33
		0.31	0.47	0.054	
		0.51	0.87	0.095	
		0.71	1.51	0.154	
70	343.15	0.31	0.08	0.010	7.91
		0.51	0.29	0.037	
		0.71	0.51	0.064	
		0.91	0.79	0.097	
		1.11	1.01	0.123	
90	363.15	0.51	0.11	0.015	9.15
		0.71	0.30	0.040	
		0.91	0.47	0.062	
		1.11	0.64	0.083	

[1] Calculated by Compiler.

[2] Stated by authors to be $\lim_{x_1 \to 0} (p_1/x_1)$ for p_1 = partial pressure of gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubilities were measured using a stirred reactor with a magnetic drive having a volume of 250 cm^3 and equipped with a pressure gauge and a surrounding jacket for temperature control. Gas and sample handling systems were attached. A volume of 100-200 cm^3 of deaerated solvent was charged to the reactor and equilibrated. A small liquid sample chamber was used to confine a known volume of saturated solution. The sample was then completely evaporated into a much larger vessel. Helium carrier gas was used to increase the pressure of the vapor-gas mixture to about 0.12 MPa. The sample was then analyzed by gas chromatography. Details are in Ref. 1.

SOURCE AND PURITY OF MATERIALS:

No information about gas and solvent source or purity was supplied.

ESTIMATED ERROR:

$\delta C_1 = \pm 3\%$ (Compiler)

REFERENCES:

1. Sokolov, Yu. A.; Konshin, A.I. *Zh. Prikl. Khim.* **1987**, *60*, 2720.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 3,3,3-Trifluoro, 1-Propene (Trifluoropropylene); $C_3H_3F_3$; [677-21-4]

ORIGINAL MEASUREMENTS:

Zernov, V.S.; Kogan, V.B.;

Lyubetskii, S.G.; Duntov, F.I.

Zh. Prikl. Khim. 1971, *44*, 683-686,

(*J. App. Chem. USSR* 1971, *44*, 693-696).

VARIABLES: T/K = 283.1-363.1

P/Mpa = 0.393-5.88, (3.9-58.0 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Total Pressure P/Mpa	[1]Ethene Partial Pressure p_1/MPa	[1]Ethene Mole Fraction Liquid, x_1	Gas, y_1	Molar Volume/cm^3(mole)$^{-1}$ Liquid	Gas
283.1	0.393	0	0	0	100.6	5280
	0.980	0.483	0.065	0.493	100.9	1960
	1.57	0.989	0.133	0.630	101.2	1120
	2.94	2.558	0.364	0.870	102.0	510
	3.92	3.783	0.600	0.965	102.9	350
	4.90	4.753	0.902	0.970	113.5	160
293.1	0.546	0	0	0	100.9	3870
	0.980	0.392	0.044	0.400	101.1	2050
	1.57	0.879	0.102	0.560	101.5	1175
	2.94	2.387	0.280	0.812	102.4	542
	3.92	3.783	0.600	0.965	103.2	375
	4.90	4.655	0.695	0.950	105.0	240
303.1	0.734	0	0	0	101.7	2860
	0.980	0.294	0.020	0.300	101.9	2120
	1.57	0.735	0.068	0.468	102.3	1230

[1] Calculated by compiler; ethene partial pressure is based on the gas phase composition, y_1. Mole percent solvent was given in the paper.

The first pressure for each different temperature is the solvent vapor pressure.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of two graduated thick-walled glass tubes 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury could be independently charged to the bottom of each tube. The saturation tube was equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir was pressurized with nitrogen whose pressure could be regulated. Ethylene was stored in one tube, while the solvent was condensed in the equilibration tube. The ethylene was transferred to the solvent tube as required. The solubility method was thus a volumetric one.
The densities of the liquefied solvent as well as critical properties of the solutions are also given in the paper.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was 99.3 mole % pure.
2. Trifluoropropylene was 99.96% pure and had a normal boiling point of 248 K.

ESTIMATED ERROR:

δT/K = ± 0.05

$\delta x_1/x_1$ = ± 0.02 (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 3,3,3-Trifluoro, 1-Propene (Trifluoropropylene); $C_3H_3F_3$; [677-21-4]

ORIGINAL MEASUREMENTS:

Zernov, V.S.; Kogan, V.B.;

Lyubetskii, S.G.; Duntov, F.I.

Zh. Prikl. Khim. 1971, *44*, 683-686, (*J. App. Chem. USSR* 1971, *44*, 693-696).

VARIABLES: T/K = 283.1-363.1

P/MPa = 0.393-5.88, (3.9-58.0 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

T/K	Total Pressure P/MPa	[1]Ethene Partial Pressure p_1/MPa	[1]Ethene Mole Fraction Liquid, x_1	Gas, y_1	Molar Volume/$\text{cm}^3(\text{mole})^{-1}$ Liquid	Gas
303.1	2.94	2.181	0.222	0.742	103.3	560
	3.92	3.391	0.388	0.865	104.7	385
	4.90	4.508	0.585	0.920	107.7	280
313.1	0.980	0	0	0	102.9	2120
	1.57	0.606	0.042	0.386	103.4	1290
	2.94	1.902	0.170	0.647	104.7	570
	3.92	3.116	0.308	0.795	106.2	398
	4.90	4.190	0.490	0.855	107.9	278
	5.88	5.027	0.710	0.855	113.0	150
333.1	1.60	0	0	0	108.6	1230
	1.96	0.539	0.025	0.275	109.1	960
	2.94	1.338	0.102	0.455	110.9	620
	3.92	2.450	0.193	0.625	112.8	402
	4.90	3.528	0.330	0.720	116.1	290
	5.88	4.234	0.525	0.720	135.0	162

[1] Calculated by compiler; ethene partial pressure is based on the gas phase composition, y_1. Mole percent solvent was given in the paper.

The first pressure for each different temperature is the solvent vapor pressure.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of two graduated thick-walled glass tubes 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury could be independently charged to the bottom of each tube. The saturation tube was equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir was pressurized with nitrogen whose pressure could be regulated. Ethylene was stored in one tube, while the solvent was condensed in the equilibration tube. The ethylene was transferred to the solvent tube as required. The solubility method was thus a volumetric one.
The densities of the liquefied solvent as well as critical properties of the solutions are also given in the paper.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was 99.3 mole % pure.
2. Trifluoropropylene was 99.96% pure and had a normal boiling point of 248 K.

ESTIMATED ERROR: $\delta T/\text{K} = \pm 0.05$

$\delta x_1/x_1 = \pm 0.02$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 3,3,3-Trifluoro, 1-Propene (Trifluoropropylene); $C_3H_3F_3$; [677-21-4]

ORIGINAL MEASUREMENTS:

Zernov, V.S.; Kogan, V.B.;

Lyubetskii, S.G.; Duntov, F.I.

Zh. Prikl. Khim. 1971, *44*, 683-686,
(*J. App. Chem. USSR* 1971, *44*, 693-696).

VARIABLES: T/K = 283.1-363.1

P/MPa = 0.393-5.88, (3.9-58.0 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

T/K	Total Pressure P/MPa	[1]Ethene Partial Pressure p_1/MPa	[1]Ethene Mole Fraction Liquid, x_1	Gas, y_1	Molar Volume/cm^3 (mole)$^{-1}$ Liquid	Gas
353.1	2.50	0	0	0	118.5	725
	2.94	0.867	0.028	0.295	119.5	640
	3.92	1.646	0.093	0.420	122.1	415
	4.90	2.646	0.195	0.540	127.8	300
	5.88	3.263	0.350	0.555	139.0	172
363.1	2.92	0	0	0	127.7	570
	3.38	0.862	0.030	0.255	129.5	520
	3.92	1.250	0.060	0.319	131.4	422
	4.90	2.132	0.155	0.435	138.0	305
	5.88	2.56	0.310	0.435	153.5	180

[1]Calculated by compiler; ethene partial pressure is based on the gas phase composition, y_1. Mole percent solvent was given in the paper.

The first pressure for each different temperature is the solvent vapor pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of two graduated thick-walled glass tubes 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury could be independently charged to the bottom of each tube. The saturation tube was equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir was pressurized with nitrogen whose pressure could be regulated. Ethylene was stored in one tube, while the solvent was condensed in the equilibration tube. The ethylene was transferred to the solvent tube as required. The solubility method was thus a volumetric one.
The densities of the liquefied solvent as well as critical properties of the solutions are also given in the paper.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was 99.3 mole % pure.
2. Trifluoropropylene was 99.96% pure and had a normal boiling point of 248 K.

ESTIMATED ERROR: δT/K = ± 0.05

$\delta x_1/x_1$ = ± 0.02 (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. 1-Propene,1,1,2,3,3-pentafluoro-3-trifluoroethenyloxy- or perfluoro (propylene vinyl) ether; C_5F_8O; [64080-43-9]

ORIGINAL MEASUREMENTS:

Sokolov, Yu. P.; Konshin, A.I.

Zh. Prikl. Khim. <u>1989</u>, *62*,

1395-1398.

VARIABLES:

T/K = 298.15 - 353.15
P/MPa = 0.20 - 1.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/°C	[1]T/K	Pressure P/MPa	Solubility C_1/mol/litre	[2] Distribution Constant, K_d	[3] Henry's Constant H/MPa/mol fraction
25	298.15	0.20	0.08	3.40	5.79
		0.31	0.23		
		0.51	0.52		
		0.71	0.80		
		0.91	0.97		
		1.11	1.34		
		1.32	1.62		
50	323.15	0.51	0.31	2.76	7.11
		0.71	0.47		
		0.91	0.71		
		1.11	0.87		
		1.32	1.12		
70	343.15	0.71	0.37	2.64	8.58
		0.91	0.51		
		1.11	0.76		
		1.32	0.95		
80	353.15	0.71	0.23	1.66	11.30
		0.91	0.32		
		1.11	0.46		

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[1] Calculated by Compiler.
[2] Distribution constant $K_d = C_l/C_g$ where C_l = mol/litre in liquid, C_g = mol /litre in gas.
[3] Stated by authors to be $\lim_{x_1 \to 0} (p_1/x_1)$ for p_1 = partial pressure of gas.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubilities were measured using a stirred reactor with a magnetic drive having a volume of 250 cm^3 and equipped with a pressure gauge and a surrounding jacket for temperature control. Gas and sample handling systems were attached. A volume of 100-200 cm^3 of deaerated solvent was charged to the reactor and equilibrated. A small liquid sample chamber was used to confine a known volume of saturated solution. The sample was then completely evaporated into a much larger vessel. Helium carrier gas was used to increase the pressure of the vapor-gas mixture to about 0.12 MPa. The sample was then analyzed by gas chromatography. Details are in Ref. 1.

SOURCE AND PURITY OF MATERIALS:

No information about gas and solvent source or purity was supplied.

ESTIMATED ERROR:

$\delta C_1 = \pm$ 3% (Compiler)

REFERENCES:

1. Sokolov, Yu. A.; Konshin, A.I. *Zh. Prikl. Khim.* <u>1987</u>, *60*, 2720.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Propane, 1,1,1,3-Tetrachloro-; $C_3H_4Cl_4$; [1070-78-6]

ORIGINAL MEASUREMENTS:

Efremova, G.D.; Kovpakova, P.F.

Zhur. Fiz. Khim. 1958, *32*, 1231-1240.

VARIABLES:

T/K = 273.35 - 373.15

p_1/MPa = 1.013 - 10.13

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Henry's Constant, H/Atm (mole fraction)$^{-1}$	[1] Mole Fraction Ethene, x_1 for p_1 = 101.3 kPa
0.2	273.35	70	0.0143
25	298.15	104	0.0096
50	323.15	133	0.0075
75	348.15	160	0.0063
100	373.15	188	0.0053

[1] Henry's law constants and mole fraction solubilities at 101.3 kPa were evaluated by the compiler from enlarged graphs only; there were no numerical solubility data. Henry's law was observed to fit the data closely up to about 0.40 mole fraction ethene for all temperatures.

Phase equilibrium compositions of ethene in liquid solutions are graphically shown as a function of pressure over the complete ethene composition range to 99 mole percent ethene. Critical phenomena are reported for high concentrations of ethene at high pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in ref. 1. The equilibration device is a capillary tube 1 mm in diameter containing an internal mixer which is moved up and down by means of an external, motor-driven magnet. The capillary tube is sealed in a vertical position and connected to a gas and liquid charging system, pressure gauges, as well as a volume regulator to maintain a constant pressure and to determine the volume of gas charged.

Graphs of liquid solution molar volumes are also given as a function of solution compositions, including those for critical values at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 97.5% by analysis.
2. Tetrachloro-propane vacuum distilled. Actual purity not given. Density and refractive index at 20°C:

ρ = 1.4325 g cm^{-3},

n_D = 1.4806

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 4\%$ (compiler)

REFERENCES:

1. Kritchevskii, I.R.; Efremova, G.D.

Zhur. Fiz. Khim. 1956, *30*, 1877.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Pentane, 1,1,1,5-Tetrachloro-; $C_5H_8Cl_4$; [2467-10-9]	Efremova, G.D.; Kovpakova, P.F. *Zhur. Fiz. Khim.* 1958, *32*, 1231-1240.
VARIABLES: T/K = 273.35 - 373.15 p_1/MPa = 1.013 - 10.13	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Henry's Constant, H/Atm (mole fraction)$^{-1}$	[1] Mole Fraction Ethene, x_1 for p_1 = 101.3 kPa
0.2	273.35	74	0.0135
25	298.15	108	0.0093
50	323.15	133	0.0075
75	348.15	162	0.0062
100	373.15	192	0.0052

[1] Henry's law constants and mole fraction solubilities at 101.3 kPa were evaluated by the compiler from enlarged graphs only; there were no numerical solubility data. Henry's law was observed to fit the data closely up to about 0.40 mole fraction ethene for all temperatures.

Phase equilibrium compositions of ethene in liquid solutions are graphically shown as a function of pressure over the complete ethene composition range to 99 mole percent ethene. Critical phenomena are reported for high concentrations of ethene at high pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in ref. 1. The equilibration device is a capillary tube 1 mm in diameter containing an internal mixer which is moved up and down by means of an external, motor-driven magnet. The capillary tube is sealed in a vertical position and connected to a gas and liquid charging system, pressure gauges, as well as a volume regulator to maintain a constant pressure and to determine the volume of gas charged.

Graphs of liquid solution molar volumes are also given as a function of solution compositions, including those for critical values at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 97.5% by analysis.
2. Tetrachloro-pentane, vacuum distilled. Actual purity not given. Density and refractive index at 20°C:

ρ = 1.3455 g cm^{-3},

n_D = 1.4879

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 4\%$ (compiler)

REFERENCES:

1. Kritchevskii, I.R.; Efremova, G.D.

Zhur. Fiz. Khim. 1956, *30*, 1877.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Heptane, 1,1,1,7-Tetrachloro-; $C_7H_{12}Cl_4$; [3922-36-9]

ORIGINAL MEASUREMENTS:

Efremova, G.D.; Kovpakova, P.F.

Zhur. Fiz. Khim. 1958, *32*, 1231-1240.

VARIABLES:

T/K = 273.35 - 373.15

p_1/MPa = 1.013 - 10.13

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Henry's Constant, H/Atm (mole fraction)$^{-1}$	[1] Mole Fraction Ethene, x_1 for p_1 = 101.3 kPa
0.2	273.35	70	0.0143
25	298.15	93	0.0108
50	323.15	117	0.0085
75	348.15	139	0.0072
100	373.15	164	0.0061

[1] Henry's law constants and mole fraction solubilities at 101.3 kPa were evaluated by the compiler from enlarged graphs only; there were no numerical solubility data. Henry's law was observed to fit the data closely up to about 0.40 mole fraction ethene for all temperatures.

Phase equilibrium compositions of ethene in liquid solutions are graphically shown as a function of pressure over the complete ethene composition range to 99 mole percent ethene. Critical phenomena are reported for high concentrations of ethene at high pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in ref. 1. The equilibration device is a capillary tube 1 mm in diameter containing an internal mixer which is moved up and down by means of an external, motor-driven magnet. The capillary tube is sealed in a vertical position and connected to a gas and liquid charging system, pressure gauges, as well as a volume regulator to maintain a constant pressure and to determine the volume of gas charged.

Graphs of liquid solution molar volumes are also given as a function of solution compositions, including those for critical values at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 97.5% by analysis.
2. Tetrachloro-heptane, vacuum distilled. Actual purity not given. Density and refractive index at 20°C:

ρ = 1.2509 g cm^{-3},

n_D = 1.4843

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm$ 4% (compiler)

REFERENCES:

1. Kritchevskii, I.R.; Efremova, G.D.

Zhur. Fiz. Khim. 1956, *30*, 1877.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Nonane, 1,1,1,9-Tetrachloro-; $C_9H_{16}Cl_4$; [1561-48-4]	Efremova, G.D.; Kovpakova, P.F. *Zhur. Fiz. Khim.* 1958, *32*, 1231-1240.
VARIABLES:	PREPARED BY:
T/K = 273.35 - 373.15 p_1/MPa = 1.013 - 10.13	W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1] Henry's Constant, H/Atm (mole fraction)$^{-1}$	[1] Mole Fraction Ethene, x_1 for p_1 = 101.3 kPa
0.2	273.35	63	0.0159
25	298.15	82	0.0122
50	323.15	105	0.0095
75	348.15	129	0.0078
100	373.15	154	0.0065

[1] Henry's law constants and mole fraction solubilities at 101.3 kPa were evaluated by the compiler from enlarged graphs only; there were no numerical solubility data. Henry's law was observed to fit the data closely up to about 0.40 mole fraction ethene for all temperatures.

Phase equilibrium compositions of ethene in liquid solutions are graphically shown as a function of pressure over the complete ethene composition range to 99 mole percent ethene. Critical phenomena are reported for high concentrations of ethene at high pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in ref. 1. The equilibration device is a capillary tube 1 mm in diameter containing an internal mixer which is moved up and down by means of an external, motor-driven magnet. The capillary tube is sealed in a vertical position and connected to a gas and liquid charging system, pressure gauges, as well as a volume regulator to maintain a constant pressure and to determine the volume of gas charged.

Graphs of liquid solution molar volumes are also given as a function of solution compositions, including those for critical values at high pressures.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 97.5% by analysis.
2. Tetrachloro-nonane, vacuum distilled. Actual purity not given. Density and refractive index at 20 °C:

   ρ = 1.1913 g cm^{-3},

   n_D = 1.4827

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 4\%$ (compiler)

REFERENCES:

1. Kritchevskii, I.R.; Efremova, G.D.

   Zhur. Fiz. Khim. 1956, *30*, 1877.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Acetic acid, trichloro-ethyl ester (ethyltrichloroacetate); $C_4H_5Cl_3O_2$; [515-84-4]

ORIGINAL MEASUREMENTS:

Kristesashvili, L.V.;
Chkhubianishvili, N.G ;
Tatenashvili, M.Kh.

Soobshch. Akad. Nauk. Gruz. SSR 1979, *93* , 365-368.

VARIABLES:

$T/K = 363.15, 373.15$

$p_1/MPa = 0.1 - 8.1$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

[1]Henry's Constants

t/C	T/K	$H'/atm (mole fraction)^{-1}$	$H/MPa (mol fraction)^{-1}$	[1]Mole Fraction Ethene, x_1
90	363.15	117.5	11.9	0.0085
100	373.15	140	14.2	0.0071

Only a graph showing ethene mole fractions as a function of ethene partial pressure to pressures up to 80 atm (8.11 MPa) was available. Henry's law was stated to be followed.

[1] Henry's constants and mole fractions solubility for an ethene partial pressure of 101.3 kPa (x_1) were calculated by the compiler based on an enlarged graph showing the data.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equipment consisted of a stainless steel autoclave containing a magnetic stirrer and immersed in a constant temperature bath. The autoclave was attached to a second stainless steel vessel, in a constant temperature bath, used as a gas supply vessel. Attached also was a vacuum system and a pressure gauge. A known quantity of solvent was degassed. The drop in pressure in the second vessel was used as a measure of the quantity of ethene dissolved.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 3\%$ (compiler)

REFERENCES:

COMPONENTS: 1. Ethene; C_2H_4; [74-85-1] 2. Solvents, other than alcohols, containing carbon, oxygen and hydrogen	EVALUATOR: Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

Critical evaluation of the solubility of ethene at a partial pressure not greater than 101.3 kPa in solvents, other than alcohols, containing carbon, oxygen and hydrogen.

It is often helpful to compare experimental values of mole fraction solubilities x_1, of a gas at a particular temperature with reference values from the Raoult's law equation

$$x_1 = p_1/p_0$$

where p_0 is the vapour pressure of liquefied gas at the temperature in question. The variation with temperature of p_1/p_0 provides a reference line for comparison of solubilities. The critical temperature of ethene is 282.4 K but it is convenient to extrapolate the vapour pressure of ethene to temperatures above the critical temperature to calculate a reference line and hence facilitate qualitative comparison of experimental solubilities. Mole fraction solubilities in most solvents containing oxygen fall below the reference line and are low compared with solubility in straight chain hydrocarbons.

2-Propanone; C_3H_6O; [67-64-1]

Solubility in 2-propanone has been measured by Horiuti (1), Hannaert *et al.*(2), Leites and Ivanovskii (3), and by McDaniel (4). McDaniel's values for a partial pressure of 101.3 kPa fall appreciably below those given by Horiuti and can be disregarded because other measurements by McDaniel have been found to be significantly lower than measurements carried out more recently. Solubility values calculated from equations given by Hannaert for 283.15 K and 293.15 K are, respectively, about 18% and 14% above values given by Horiuti. Horiuti's data for the temperature range of 273.15 to 313.15 K are likely to be the more reliable. Measurements carried out by this author on other systems is often in close agreement with more recent precision measurements. Horiuti's data can be fitted to the equation:

$$\ln x_1 = -1.3472 + 795.05/(T/K) - 1.0247 \ln(T/K)$$

where x_1 is the mole fraction solubility at $p_1 = 101.3$ kPa

standard deviation in values of $x_1 = 2.0 \times 10^{-5}$ temp. range 273-313 K

This equation may be accepted on a tentative basis.

The following equation is based upon Horiuti's measurements from 273.15 to 313.15 K, on Hannaert's measurements from 243.15 to 293.15 K and on the single value at 243.15 K given by Leites and Ivanovskii.

$$\ln x_1 = -8.5070 + 1195.3/(T/K)$$

standard deviation in values of $x_1 = 8.5 \times 10^{-4}$ temp. range 243-313 K

This equation is recommended on a tentative basis for temperatures below 273 K.

Methyl acetate; $C_3H_6O_2$; [79-20-9]

Horiuti (1) also measured solubility in methyl acetate. Mole fraction solubilities at a partial pressure of 101.3 kPa fit the equation

$$\ln x_1 = 3.2620 + 569.63/(T/K) - 1.6935 \ln(T/K)$$

standard deviation in values of $x_1 = 3.4 \times 10^{-5}$ temp. range 273-313 K

Horiuti's data for methyl acetate are classified as tentative.

Cyclopentanone; C_5H_8O; [120-92-3]
Cyclohexanone; $C_6H_{10}O$; [108-94-1]
2-Methylcyclohexanone; $C_7H_{12}O$; [583-60-8]
2,6-Dimethylcyclohexanone; $C_8H_{14}O$; [2816-57-1]
Cycloheptanone; $C_7H_{12}O$; [502-42-1]

Solubility in cyclic ketones has been measured by Gallardo and co-workers (5-9) at a partial pressure of ethene of 101.3 kPa in the temperature range 273.15 to 303.15 K. Mole fraction solubilities at the same temperature in

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Solvents, other than Alcohols, containing Carbon, Oxygen and Hydrogen

EVALUATOR:

Peter G.T. Fogg
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University of North London
Holloway Road, London, N7 8DB, U.K.

November, 1993

CRITICAL EVALUATION:

these solvents are in the order 2,6-dimethylcyclohexanone > 2-methylcyclohexanone > cycloheptanone > cyclohexanone > cyclopentanone. Sets of measurements are consistent with each other (see fig. 1) and all fall below the reference line based on Raoult's law in this temperature range.

Solubilities at a partial pressure of gas of 101.3 kPa may be fitted to the following equations derived by the evaluator. These give slightly better fit than equations given by the authors.

2,6-dimethylcyclohexanone

$\ln x_1 = -8.5574 + 1294.9/(T/K)$

standard deviation in values of $x_1 = 3.4 \times 10^{-5}$

2-methylcyclohexanone

$\ln x_1 = 41.885 - 980.94/(T/K) - 7.5339 \ln(T/K)$

standard deviation in values of $x_1 = 5.9 \times 10^{-5}$

cycloheptanone

$\ln x_1 = -22.106 + 1764.3/(T/K) + 2.0544 \ln(T/K)$

standard deviation in values of $x_1 = 2.4 \times 10^{-5}$

cyclohexanone

$\ln x_1 = 35.451 - 773.66/(T/K) - 6.5627 \ln(T/K)$

standard deviation in values of $x_1 = 2.9 \times 10^{-5}$

cyclopentanone

$\ln x_1 = 25.679 - 337.58/(T/K) - 5.1162 \ln(T/K)$

standard deviation in values of $x_1 = 1.4 \times 10^{-5}$

These equations may be accepted on a tentative basis for the temperature range 273.15 to 303.15 K.

4-Methyl-1,3-dioxolan-2-one (*propylene carbonate*); $C_4H_6O_3$; [108-32-7]

Henry's constants for dissolution of ethene in 4-methyl-1,3-dioxolan-2-one was measured by a chromatographic method at 298.2-343.2 K by Lenoir *et al.* (10). Mole fraction solubility at 298.2 K and a partial pressure of 101.3 kPa, calculated on the assumption of a linear variation of mole fraction solubility with partial pressure, is 0.00521 compared with 0.00421 from measurements by Brückl and Kim (11). Solubilities reported by Lenoir *et al.* for some of the other systems which they have studied are high compared with measurements by other groups. This is probably due to limitations of the chromatographic method. Further measurements on this system are required.

1,2-Epoxyhexane; $C_6H_{12}O$; [592-90-5]

Mole fraction solubilities measured by Gibanel *et al.*(12) at a partial pressure of 101.3 kPa in 1,2-epoxyhexane fall in between solubilities in 2-methylcyclohexanone and 2,6-dimethylcyclohexanone. The data may be fitted to the equation

$\ln x_1 = -50.928 + 3025.0/(T/K) + 6.4117 \ln(T/K)$

standard deviation in values of $x_1 = 2.9 \times 10^{-5}$ temp. range 273-303 K

This equation may be accepted on a tentative basis.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents, other than Alcohols, containing Carbon, Oxygen and Hydrogen	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

Solubility in the cyclic diether, 1,4-dioxane is low compared with that in cyclic ketones. Solubilities at a partial pressure of ethene of 101.3 kPa reported by Gallardo *et al.*(13) for the temperature range 285.15 to 303.15 K fit the equation

$$\ln x_1 = -1.2404 + 763.88/(T/K) - 1.0499 \ln(T/K)$$

standard deviation in values of $x_1 = 1.7 \times 10^{-5}$

This equation fits the data better than the one given by the authors and may be accepted on a tentative basis.

1,1'-[Methylenebis(oxy)]-bisethane; $C_5H_{12}O_2$

The mole fraction solubility reported by Lizano *et al.*(14) at a partial pressure of 101.3 kPa in the acetal, 1,1'-[methylenebis(oxy)]-bisethane, is higher than that in the cyclic ketones (see fig. 1). Values lie above the reference line based upon the Raoult's law equation. The data may be fitted to the equation

$$\ln x_1 = -17.138 + 1927.7/(T/K) + 1.1882 \ln(T/K)$$

standard deviation in values of $x_1 = 2.6 \times 10^{-5}$; temp. range 263-303 K

This equation may be accepted on a tentative basis

References

1. Horiuti, J. *Sci. Pap. Inst. Phys. Chem. Res. (Jpn)* 1931/32, *17*, 125-256.
2. Hannaert, H.; Haccuria, M.; Mathieu, M.P. *Ind. Chim. Belge* 1967, *32*, 156-164.
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4. McDaniel, A.S. *J. Phys. Chem.* 1911, *15*, 587-610.
5. Gallardo, M.A.; Lopez, M.C.; Urieta, J.S.; Gutierrez Losa, C. *Fluid Phase Equil.* 1989, *50*, 223-233.
6. Gallardo, M.A.; Melendo, J.M.; Urieta, J.S.; Gutierrez Losa, C. *Can. J. Chem.* 1987, *65*, 2198-2202.
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10. Lenoir, J-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data* 1971, *16*, 340-342.
11. Brückl, N.; Kim, J.I. *Z. Phys. Chem. (Wiesbaden)* 1981, *126*, 133-150.
12. Gibanel, F.; Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C. *Fluid Phase Equil.* 1988, *42*, 261-268.
13. Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C. *J. Chim. Phys. Phys.-Chim. Biol.* 1983, *80*, 621-625.
14. Lizano, L.P.; Lopez, M.C.; Royo, F.M.; Urieta, J.S. *J. Soln. Chem.* 1990, *19*, 721-728.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Solvents, other than alcohols, containing carbon, oxygen and hydrogen

EVALUATOR:

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

November, 1993

CRITICAL EVALUATION:

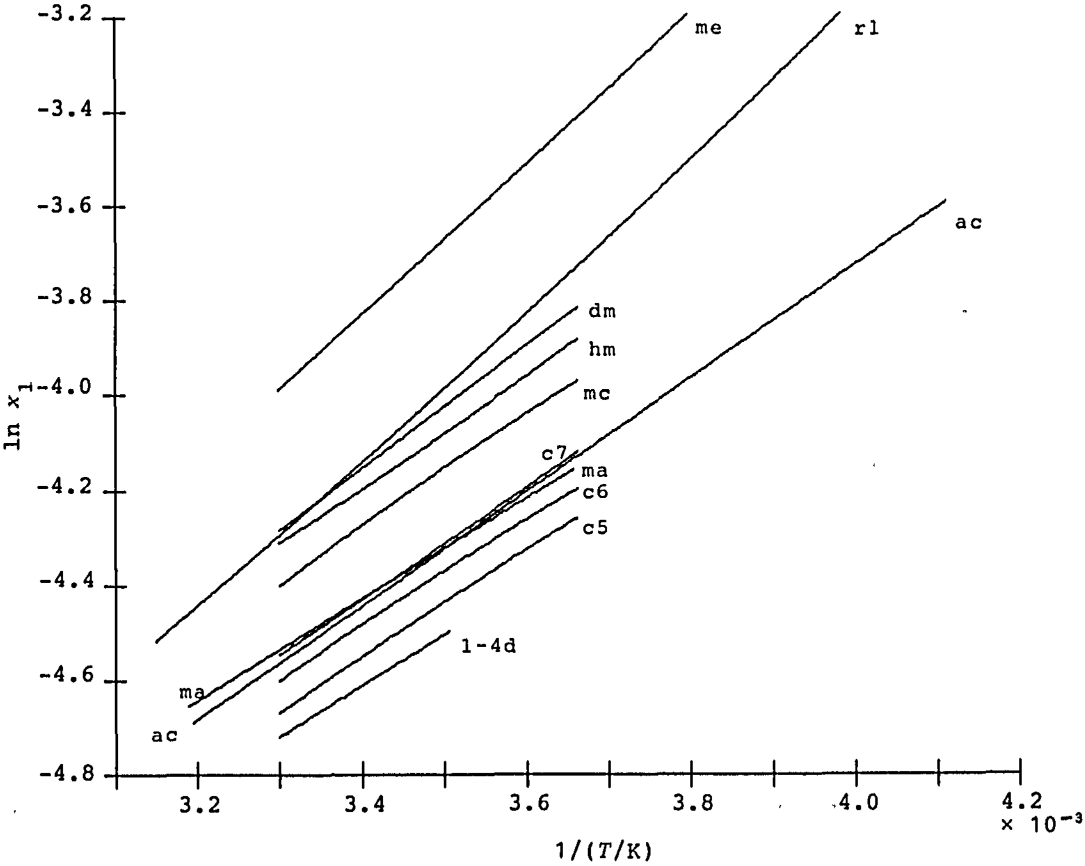


Figure 1 The solubility of ethene at a partial pressure of 101.3 kPa in compounds containing oxygen

me	1,1'-[Methylenebis(oxy)]bisethane	**ac**	2-Propanone (acetone)
dm	2,6-Dimethylcyclohexanone	**ma**	Methyl acetate
hm	1,2-epoxyhexane (hexamethylene oxide)	**c6**	Cyclohexanone
mc	2-Methylcyclohexanone	**c5**	Cyclopentanone
c7	Cycloheptanone	**1-4**	1,4-Dioxane

rl Reference line based upon the Raoult's law equation

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) 2-Propanone or acetone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn) 1931/32, *17*, 125 - 256.

VARIABLES:

T/K: 273.15 - 313.15
p_1/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^2x_1	Bunsen Coefficient α/cm^3(STP)cm^{-3}atm^{-1}	Ostwald Coefficient L/cm^{3}cm^{-3}
273.15	1.520	4.843	4.843
278.15	1.420	4.490	4.572
283.15	1.325	4.156	4.308
288.15	1.240	3.862	4.074
293.15	1.160	3.585	3.847
298.15	1.088	3.335	3.640
303.15	1.028	3.129	3.473
308.15	0.9641	2.912	3.285
313.15	0.9144	2.741	3.142

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

Smoothed Data: For use between 273.15 and 313.15 K.

$$\ln x_1 = -8.1906 + 10.9452/(T/100\mathrm{K})$$

The standard error about the regression line is 2.67 x 10^{-5}.

T/K	Mol Fraction 10^2x_1
273.15	1.524
283.15	1.323
288.15	1.237
293.15	1.160
298.15	1.089
303.15	1.025
313.15	0.914

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) Ethene. Prepared by dropping ethanol into orthophosphoric acid. The gas was cooled, passed through several wash solutions, dried, and fractionated from liquid air several times.

(2) Acetone. Nippon Pure Chemical Co. or Merck. Extra pure grade. Recrystallized with sodium sulfite and stored over calcium chloride. Fractionated, boiling point (760 mmHg) 56.09°C.

ESTIMATED ERROR:

δT/K = 0.05
$\delta x_1/x_1$ = 0.01

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4 ; [74-85-1]
2. 2-Propanone, (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M.P.

Ind. Chim. Belge 1967, *32* , 156-164.

VARIABLES:

T/K = 243.15 - 293.15

p_1/kPa = 101.3

PREPARED BY:

W. Hayduk
H.L. Clever

EXPERIMENTAL VALUES:

t/C	T /K	[1]Mole fraction Ethene, x_1
-30	243.15	0.0264
-10	263.15	0.0196
10	283.15	0.0152
20	293.15	0.0135

[1] Mole fraction solubility calculated by compilers for a gas partial pressure of 101.3 kPa using the equation developed by the authors with $\nu = 1$, for the applicable temperature range:

$$\log (K\pi\nu) = 3.28 - (\Delta H/\text{cal mol}^{-1})/(2.3R(T/K))$$

The authors' definitions are:

ΔH = 1,890 cal mol^{-1}, Enthalpy of dissolution

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}}$$

π/ atm = total pressure

ν = coefficient of fugacity

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = (f_1/atm)/ x_1 where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe several methods used; the one used in this case is the least accurate.

The apparatus is of glass and consists of a burette in which the gas is confined over mercury, two bulbs for the solvent, one above the other, a mercury manometer and a constant temperature bath. A measured volume of solvent is degassed in the top bulb at ambient temperature and charged to the absorption bulb in the bath. Gas is charged to the desired pressure. The quantity of gas added at constant pressure is measured. Agitation is manual.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Air Liquide. For narcosis, 99.9 per cent.
2. 2-Propanone. Merck and Co. Vapor pressure, p /mm Hg = 11 at -30°C and 184 at 20°C as specified by authors.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm$ 10 to 15%
(authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Leites, I.L.; Ivanovskii, F.P.

Khim. Prom. 1962, *9*, 653-657.

VARIABLES:

T/K = 243.15,

p_1/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t /C	T /K	[1] $\log_{10}$(H'/mmHg)	[2] Henry's Constant, H/atm (mole fraction)$^{-1}$	[2] Mole Fraction Ethene, x_1
-30	243.15	4.423	34.85	0.0287

This result was part of a study for the behavior of solubilities in two-component solvent solutions.

[1] Only graphical results were available in this paper; a value of log of Henry's constant (H') was read from an enlarged graph by the compiler.

[2] Henry's constant (H) and mole fraction solubility (x_1) were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A metal cryostat was cooled with dry-ice and acetone and controlled to a temperature to ± 0.05 K. The equilibrium cell was mounted in the cryostat. The solvent was purified by fractional distillation and analyzed by chromatography. Details were not given.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was stated to be 99.9%.
2. 2-Propanone was distilled and analyzed by chromatography. Actual purity not given.

ESTIMATED ERROR:

δT/K = ± 0.05

$\delta x_1/x_1$ = ± 0.01 (Authors)

REFERENCES:

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) 2-Propanone or acetone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

McDaniel, A. S.

J. Phys. Chem. 1911, *15*, 587-610.

VARIABLES:

T/K = 293.15 - 308.15

p_1/kPa = 101.3 (1 atm)

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature t/°C	Temperature T/K	Mol Fraction 10^2x_1	Bunsen Coefficient[a] α	Ostwald Coefficient[b] L/cm³ cm⁻³
20.0	293.15	0.780	2.2900	2.5709
25.0	298.15	0.746	2.2752	2.4834[c]
35.0	308.15	0.681	2.0460	2.3084

[a] Bunsen coefficient, α/cm³(STP) cm⁻³ atm⁻¹.

[b] Listed as absorption coefficient in the original paper. Interpreted to be equivalent to Ostwald coefficient by compiler.

[c] Ostwald coefficient (absorption coefficient) estimated as 298.15 K value by author.

[d] Mole fraction values calculated by compiler assuming ideal gas behavior.

EVALUATOR'S COMMENT: McDaniel's data should be used with caution. His values are often 20 percent or more too small when compared with more reliable data.

The values of the Bunsen Coefficient and Ostwald Coefficient (Absorption Coefficient) given by the author for 293.15 K are incompatible. The mole fraction solubility given above has been calculated from the Ostwald Coefficient.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is all glass. It consists of a gas buret connected to a contacting vessel. The solvent is degassed by boiling under reduced pressure. Gas pressure or volume is adjusted using mercury displacement. Equilibration is achieved at atm pressure by hand shaking, and incrementally adding gas to the contacting chamber. Solubility measured by obtaining total uptake of gas by known volume of the solvent.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Prepared by reaction of 1,2-dibromoethane with zinc-copper.

(2) 2-Propanone.

ESTIMATED ERROR:

$\delta L/L \geq -0.20$

REFERENCES:

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Acetic acid, methyl ester or methyl acetate; $C_3H_6O_2$; [79-20-9]

ORIGINAL MEASUREMENTS:

Horiuti, J.

Sci. Pap. Inst. Phys. Chem. Res. (Jpn) <u>1931/32</u>, *17*, 125 - 256.

VARIABLES:

T/K: 273.15 - 313.15

p_1/kPa: 101.325 (1 atm)

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^2x_1	Bunsen Coefficient $\alpha/\text{cm}^3\,(\text{STP})\,\text{cm}^{-3}\,\text{atm}^{-1}$	Ostwald Coefficient $L/\text{cm}^3\,\text{cm}^{-3}$
273.15	1.567	4.618	4.618
278.15	1.470	4.300	4.379
283.15	1.381	4.009	4.156
288.15	1.287	3.710	3.914
293.15	1.208	3.456	3.709
298.15	1.136	3.226	3.521
303.15	1.071	3.017	3.348
308.15	1.009	2.823	3.185
313.15	0.9581	2.660	3.049

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

Smoothed Data: For use between 273.15 and 313.15 K.

$$\ln x_1 = -8.0481 + 10.6457/(T/100\text{K})$$

The standard error about the regression line is 4.61×10^{-5}.

T/K	Mol Fraction 10^2x_1
273.15	1.575
283.15	1.373
288.15	1.286
293.15	1.208
298.15	1.136
303.15	1.071
313.15	0.958

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) Ethene. Prepared by dropping ethanol into orthophosphoric acid. The gas was cooled, passed through several wash solutions, dried, and fractionated from liquid air several times.

(2) Methyl acetate. Merck. Extra pure grade. Dried with P_2O_5. Distilled several times. Boiling point (760 mmHg) 57.12°C.

ESTIMATED ERROR:

$\delta T/\text{K} = 0.05$

$\delta x_1/x_1 = 0.01$

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. 1,3-Dioxolan-2-one,4-methyl- (Propylene carbonate); $C_4H_6O_3$; [108-32-7]	Brückl, N.; Kim, J. I. *Z. Phys. Chem. (Wiesbaden)* 1981, *126*, 133-150.
VARIABLES: T/K = 298.2 P/kPa = 101.3	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

T/K = 298.2

ln H	10^3 × Mole fraction of ethene in liquid†, $10^3 x_{C_2H_4}$
5.47	4.211

† at a partial pressure of 1 atmosphere, calculated by compiler, assuming $x_{C_2H_4} = 1/H$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined by a volumetric method described as "the Ostwald method". No other details given.

SOURCE AND PURITY OF MATERIALS:

1. Linde Co. sample, purity 99.8 volume per cent.
2. Uvasol and analytical grade.

ESTIMATED ERROR:

δT/K = ±0.1; δH = ±1.25%.

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1,3-Dioxolan-2-one,4-methyl- (Propylene carbonate); $C_4H_6O_3$; [108-32-7]

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

$T/K = 298.2 - 343.2$

$P/kPa < 101.3$ (low pressures)

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Henry's constant $H_{C_2H_4}/atm$	Mole fraction at 1 atm* $x_{C_2H_4}$
298.2	192	0.00521
323.2	235	0.00426
343.2	271	0.00369

* Calculated by compiler assuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e., $x_{C_2H_4}(1\ atm) = 1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene; C_2H_4; [74-85-1] (2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	Gallardo, M. A.; Urieta, J. S.; Gutierrez Losa, C. *J. Chim. Phys. Phys.-Chim. Biol.* 1983, *80*, 621-25.
VARIABLES:	**PREPARED BY:**
T/K = 285.15 - 303.15 p_1/kPa = 101	H. L. Clever

EXPERIMENTAL VALUES:

T/K	Mol Fraction 10^4x_1	Bunsen Coefficient α/ $cm^3(STP)cm^{-3}atm^{-1}$	Ostwald Coefficient $L/cm^3\ cm^{-3}$
285.15	111.6	2.995	3.125
289.15	105.6	2.820	2.985
293.15	100.7	2.675	2.870
298.15	94.81	2.505	2.730
303.15	89.08	2.335	2.595

The compiler calculated the Bunsen and Ostwald coefficients from the author's mole fraction values assuming ideal gas behavior. The values are rounded to the nearest 0.005.

The authors fitted their data to the equation:

$- \ln x_1 = 3.648 \ln (T/K) - 16.123$ from which they obtained

ΔH_1°/kJ mol^{-1} = -9.04, and ΔS_1°/J K^{-1} mol^{-1} = -69 for the transfer

of one mole of ethene from the gas phase at 101 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to that of Ben-Naim and Baer (ref 1). It was described in detail in an earlier paper (ref 2).

The apparatus consists of a gas buret, mercury manometer, and solution vessel. The solvent is degassed in the solution vessel. Measurements were carried out on the solvent vapor saturated gas.

Literature 1,4-dioxane vapor pressure data were fitted to the equation

$$\ln (p_2 /\text{kPa}) = -4591.3/(T/K) + 16.98.$$

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Sociedad Espanola del Oxigeno. Stated to be 99.90 %.

(2) 1,4-Dioxane. Merck and Co. Purity checked by GLC to be ≥ 99 %.

ESTIMATED ERROR:

δT/K = ± 0.1
δp_1/kPa = ± 1
$\delta x_1/x_1$ = ± 0.01

REFERENCES:

1. Ben Naim, A.; Baer, S. *Trans.Faraday Soc.* 1963, *59*, 2735-38.
2. Carniecer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa,C. *Rev. Acad. Ciencieas Zaragoza* 1979, *34*, 115-22.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Cyclopentanone; C_5H_8O; [120-92-3]

ORIGINAL MEASUREMENTS:

Gallardo, M.A.; Lopez, M.C.; Urieta, J.S.; Gutierrez Losa, C.

Fluid Phase Equil. 1989, *50*, 223-233.

VARIABLES:

T/K = 273.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	[1] Mole Fraction $10^4\ x_1$	[2] Ostwald Coefficient L/cm^3 cm^{-3}	[2] Bunsen Coefficient α/cm^3(STP) cm^{-3}atm^{-1}
273.15	141.3	3.67	3.67
283.15	123.1	3.28	3.16
293.15	107.1	2.92	2.72
298.15	100.1	2.76	2.53
303.15	93.83	2.62	2.36

[1] For a gas partial pressure of 101.325 kPa.

[2] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data as a Henry's constant, H/atm mole fraction^{-1}, to the following equation:

$$\ln H = 8.4036 - 1132.98(T/\mathrm{K})^{-1}$$

They also obtained ΔH/kJ mol^{-1} = -9.42 and ΔS/JK^{-1} mol^{-1} = -70 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is described in ref.1. It consists of a system of burettes for the gas, a mercury manometer and a solution vessel. The mole fraction of dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes and the mass of solvent in the solution vessel determined by weighing.

The solvent vapor pressure was also measured and correlated as follows:

$$\ln(P/\mathrm{kPa}) = -5067.57(T/\mathrm{K})^{-1} + 17.449$$

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Espanol del Oxigeno. Specified purity 99.9%.
2. Cyclopentanone. Fluka. Specified purity 99.5% Purity also checked with GLC and refractive index measurements.

ESTIMATED ERROR:

T/K = ± 0.2

$\delta x_1/x_1$ = ± 0.7% (authors)

REFERENCES:

1. Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C.
J. Chim. Phys. 1983, *80*, 621.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Hexane, 1,2-epoxy-, (Hexamethylene oxide) $C_6H_{12}O$; [592-90-5]

ORIGINAL MEASUREMENTS:

Gibanel, F.; Lopez, M.C.; Gallardo, M.A.; Urieta, J.S.; Gutierrez Losa, C.

Fluid Phase Equil. 1988, *42*, 261-268.

VARIABLES:

T/K = 273.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction $10^4\ x_1$	[1] Ostwald Coefficient L/cm^3 cm^{-3}	[1] Bunsen Coefficient α/cm^3(STP) cm^{-3} atm^{-1}
273.15	206	4.24	4.24
283.15	175	3.68	3.55
293.15	152	3.28	3.05
298.15	143	3.12	2.85
303.15	134	2.96	2.66

[1] The Bunsen and Ostwald coefficients were calculated by the compiler using a solvent density at 293.15K of 0.890 g cm^{-3}.

The authors fitted their data to the equation:

$$-\ln x_1 = 8.2306 - 1186.82\ (T/\mathrm{K})^{-1}$$

They also obtained ΔH/kJ mol^{-1} = -9.87 and ΔS/J K^{-1}mol^{-1} = -68 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is described elsewhere (ref.1); it is based on that proposed by Ben Naim and Baer (ref.2). The set-up consists of a burette system, a mercury manometer and a solution vessel. Mole fraction of the dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of liquid in the solution vessel by weighing.

The solvent vapor pressure was determined and fitted to the following equation:

$$\ln(P_2/\mathrm{kPa}) = -4{,}891.6\ (T/\mathrm{K})^{-1} + 17.3387$$

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Español del Oxigeno. Specified purity 99.9%.
2. Hexamethylene oxide. Merck. Specified purity 99%.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm\ 0.01$ (authors)

REFERENCES:

1. Cornicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1979, *34*, 115.
2. Ben Naim, A.; Baer, S. *Trans. Far. Soc.* 1963, *59*, 2735.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Cyclohexanone; $C_6H_{10}O$; [108-94-1]

ORIGINAL MEASUREMENTS:

Gallardo, M.A.; Melendo, J.M.; Urieta, J.S.; Gutierrez Losa, C.

Can. J. Chem. **1987**, *65*, 2198-2202.

VARIABLES:

T/K = 273.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction $10^4\ x_1$	[1] Ostwald Coefficient L /cm^3 cm^{-3}	[1] Bunsen Coefficient α/cm^3(STP) cm^{-3} atm^{-1}
273.15	150	3.33	3.33
283.15	131.5	2.99	2.88
293.15	114.5	2.67	2.49
298.15	106.9	2.52	2.31
303.15	100.5	2.40	2.16

[1] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data to the equation:

$$-\ln x_1 = 3.8489 \ln T - 17.393$$

They also obtained ΔH/kJ mol^{-1} = -9.54 and ΔS/J K^{-1} mol^{-1} = -70 for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus is described in an earlier paper (ref. 1). It consists of a system of burettes, a mercury manometer and a solution vessel. The mole fraction of the dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of solvent in the solution vessel determined by weighing.

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Espanol del Oxigeno, Specified purity 99.9%.
2. Cyclohexanone. Carlo Erba. Specified purity $\geq$ 99%.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 0.007$ (Authors)

REFERENCES:

1. Carnicer, J.; Gibanel, F.; Urieta, J.S; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* **1979**, *34*, 115.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Methylcyclohexanone; $C_7H_{12}O$; [583-60-8]

ORIGINAL MEASUREMENTS:

Gallardo, M.A.; Carmen Lopez, M.; Urieta, J.S.; Gutierrez Losa, C.

Can. J. Chem. 1989, *67*, 809-811.

VARIABLES:

T/K = 273.15 - 303.15

p_1/kPa = 101.32

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	Mole Fraction 10^4 x_1	[1] Ostwald Coefficient $L/\text{cm}^3\ \text{cm}^{-3}$	[1] Bunsen Coefficient $\alpha/\text{cm}^3(\text{STP})\ \text{cm}^{-3}\ \text{atm}^{-1}$
273.15	188	3.580	3.580
283.15	164	3.205	3.090
293.15	140.7	2.815	2.620
298.15	131.5	2.660	2.435
303.15	122.8	2.515	2.265

[1] The Bunsen and Ostwald coefficients were calculated by the compiler.

The authors fitted their data to the equation:

$$- \ln x_1 = 8.3232 - 1190.24\ (T/\text{K})^{-1}$$

They also obtained $\Delta H/\text{kJ mol}^{-1} = -9.9$ and $\Delta S/\text{J K}^{-1}\text{mol}^{-1} = -69$ for the transfer of one mole of ethene from the gas phase at 101.32 kPa to the hypothetical unit mole fraction solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental apparatus and method is described elsewhere (ref.1). It consists of a system of burettes, a mercury manometer and a solution vessel. The mole fraction of the dissolved gas is estimated from the volume change at constant pressure of saturated gas in the burettes, and the mass of solvent in the solution vessel determined by weighing.

The vapor pressure of the solvent was measured and fitted to the following equation:

$$\ln(P_2/\text{kPa}) = - 5552.37\ (T/\text{K})^{-1} + 18.046$$

SOURCE AND PURITY OF MATERIALS:

1. Ethene. Sociedad Español del Oxigeno. Specified purity 99.9%.
2. 2-Methylcyclohexanone. Merck. Purity checked by GLC to be $\geq$ 98.1%.

ESTIMATED ERROR:

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

$\delta x_1/x_1 = \pm 0.007$ (authors)

REFERENCES:

1. Cornicer, J.; Gibanel, F.; Urieta, J.S.; Gutierrez Losa, C. *Rev. Acad. Cienc. (Zaragoza)* 1979, *34*, 115.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) 2,6-Dimethylcyclohexanone;
$C_8H_{14}O$;
[2816-57-1]

ORIGINAL MEASUREMENTS:

Gallardo, M. A.; Lopez, M. C.;
Urieta, J. S.; Gutierrez-Losa, C.

Can. J. Chem.
1990, *68*, 435-439.

VARIABLES:

T/K = 273.15 - 303.15
p_1/kPa = 101.32

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Mole Fraction 10^4x_1	Bunsen Coefficient α/cm^3(STP) cm^{-3}atm^{-1}	Ostwald Coefficient L/cm^{3}cm^{-3}
273.15	220	3.72	3.72
283.15	186	3.10	3.22
293.15	159	2.62	2.81
298.15	148.4	2.43	2.66
303.15	137.3	2.24	2.48

The compiler calculated the Bunsen and Ostwald coefficients. Density data were calculated from the equation given in the source and ideal gas behavior was assumed.
The authors fitted the solubility data to the equation:

$$-\ln x_1 = 8.5532 - 1293.69/(T/\mathrm{K}).$$

The enthalpy and entropy of solution at 298.15 K and a partial pressure of 101.32 kPa were:

$$\Delta H = -10.76 \text{ kJ mol}^{-1} \text{ and } \Delta S = -0.071 \text{ J K}^{-1} \text{ mol}^{-1}.$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus, based on the design of Ben-Naim and Baer, was described earlier (ref 1). The essential parts were a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. The saturation and volumetric measurements were carried out using solvent saturated gas. It appears that the mole fraction solubility at one atm was estimated from the raw data by assuming Henry's law is obeyed and that the partial pressure of the solvent is given by Raoult's law.

SOURCE AND PURITY OF MATERIALS:

(1) Sociedad Española del Oxigeno sample; purity 99.90 mole per cent.

(2) Fluka sample; purity 98.2 mole per cent. Major impurities had similar gas solubilities.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.05$;
$\delta x/x = \pm 0.02$.

REFERENCES:

1. Carnicer, J.; Gibanel, F.; Urieta, J. S.; Gutierrez-Losa, C.
Rev. Acad. Ciencias Zaragoza
1979, *1340*, 115-22.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) Cycloheptanone; $C_7H_{12}O$; [502-42-1]

ORIGINAL MEASUREMENTS:

Gallardo, M. A.; Lopez, M. C.; Urieta, J. S.; Gutierrez-Losa, C.
Fluid Phase Equil.

1990, *58*, 159-172.

VARIABLES:

$T/K = 273.15 - 303.15$
$p/kPa = 101.32$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	Mole Fraction 10^4x_1	Bunsen Coefficient α /cm^3(STP) cm^{-3}atm^{-1}	Ostwald Coefficient L/cm^{3}cm^{-3}
273.15	162.4	32.00	32.00
283.15	138.7	27.03	28.02
293.15	120.9	23.31	25.01
298.15	113.2	21.71	23.69
303.15	105.9	20.20	22.42

The compiler calculated the Bunsen and Ostwald coefficients. Density data were calculated from the equation given in the source and ideal gas behavior was assumed.
The authors fitted the solubility data to the equation:

$$\ln x_1 = -8.4142 + 1172.26/(T/K).$$

The enthalpy and entropy of solution at 298.15 K and a partial pressure of 101.32 kPa were:

$$\Delta H = -9.75 \text{ kJ mol}^{-1} \text{ and } \Delta S = -0.070 \text{ J K}^{-1} \text{ mol}^{-1}.$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus, based on the design of Ben-Naim and Baer, was described earlier (ref 1). The essential parts were a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. The saturation and volumetric measurements were carried out using solvent saturated gas. It appears that the mole fraction solubility at one atm was estimated from the raw data by assuming Henry's law is obeyed and that the partial pressure of the solvent is given by Raoult's law.

SOURCE AND PURITY OF MATERIALS:

(1) Sociedad Española del Oxigeno sample; purity 99.90 mole per cent.

(2) Merck and Co. sample; purity 99.2 mole per cent.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$;
$\delta x/x = \pm 0.007$.

REFERENCES:

1. Carnicer, J.; Gibanel, F.; Urieta, J. S.; Gutierrez-Losa, C.
Rev. Acad. Ciencias Zaragoza 1979, *1340*, 115.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethene; C_2H_4; [74-85-1] (2) 1,1'-[Methylenebis(oxy)]bis-ethane (*formaldehyde diethyl acetal*); $C_5H_{12}O_2$; [462-95-3]	Lizano, L. P.; Lopez, M. C.; Royo, F. M.; Urieta, J. S. *J. Soln. Chem.* 1990, *19*, 721-728.
VARIABLES:	**PREPARED BY:**
T/K = 263.15 - 303.15 p/kPa = 101.32	C. L. Young

EXPERIMENTAL VALUES:

T/K	Mole Fraction 10^4x_1	Bunsen Coefficient α/cm^3(STP) cm^{-3}atm^{-1}	Ostwald Coefficient L/cm^{3}cm^{-3}
263.15	411	79.59	76.68
273.15	329	62.41	62.41
283.15	267	49.71	51.54
293.15	221	40.45	43.42
303.15	185	33.32	36.98

The compiler calculated the Bunsen and Ostwald coefficients. Density data were calculated from the equation given in the source and ideal gas behavior was assumed.
The authors fitted the solubility data to the equation:

$$\ln x_1 = -9.2184 + 1585.23/(T/\mathrm{K}).$$

The enthalpy and entropy of solution at 298.15 K and a partial pressure of 101.32 kPa were:

$$\Delta H = -13.18 \text{ kJ mol}^{-1} \text{ and } \Delta S = -0.077 \text{ kJ K}^{-1} \text{ mol}^{-1}.$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility apparatus, based on the design of Ben-Naim and Baer, was described earlier (ref 1). The essential parts were a gas buret, mercury manometer, and solution vessel. The solvent was degassed in the solution vessel. The saturation and volumetric measurements were carried out using solvent saturated gas.

SOURCE AND PURITY OF MATERIALS:

(1) Sociedad Española del Oxigeno sample; purity 99.90 mole per cent.

(2) Aldrich sample; purity better than 99 mole per cent.

ESTIMATED ERROR:

δT/K = ±0.05;
$\delta x/x$ = ±0.002.

REFERENCES:

1. Carnicer, J.; Gibanel, F.; Urieta, J. S.; Gutierrez-Losa, C. *Rev. Acad. Ciencias Zaragoza* 1979, *1340*, 115.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents containing oxygen excluding water and alcohols; pressures greater than 0.20 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 February, 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Oxygen-Containing Solvents excluding Water and Alcohols for Pressures greater than 0.20 MPa

Ethene solubilities were reported for elevated pressures in five solvents containing oxygen which are generally described as ketones, an organic carbonate, ester, and an organic acid. When possible, the consistency of the data was tested by plotting log *x* (mole fraction solubility) versus log *p* (ethene partial pressure) expecting to observe a linear relation for relatively low concentrations of ethene and for relatively low gas partial pressures. The simplest equation describing the effects of both temperature and pressure has been observed to have the following form:

$$\log x_p = A + B(T/K)^{-1} + C \log (p/\text{MPa}) \qquad (1)$$

For a wider range in temperature, a more accurate description of the temperature effect involving two terms has been sometimes used. Furthermore, when there is a consistent curvature in the log x_p - log p relation, a correction to equation (1) is introduced, thus describing the data over a larger range of pressure. With these modifications equation (1) becomes:

$$\log x_p = A + B\,(T/K)^{-1} + C \log (p/\text{MPa}) + D \log (T/K) + E(p/\text{MPa}) \qquad (2)$$

Equation (2) is warranted only when solubility data cover wide ranges of temperature and pressure.

The solubilities in the individual solvents will now be considered.

2-Propanone (acetone); C_3H_6O; [67-64-1]

Four research groups reported ethene solubilities in 2-propanone (1-4): Kiss et al. (1) and Shenderei et al. (2) for low temperatures, 228.15 K to 248.15 K and a range of pressures, and Voronkov et al.(3) and Hronec et al.(4) for a wide range of temperatures and pressures. Unfortunately, only the data of the former two groups are self-consistent and consistent with each other. On the other hand, the data of the latter two groups are entirely inconsistent and do not check one another even approximately for comparable temperatures and pressures. To be more specific, the data of Hronec et al. (4) do not even approximately approach Henry's law for low pressures, whereas the data for the other three groups of researchers do. The data of Voronkov et al. (3) cover a larger pressure range than the other data (to approximately 4 MPa). Unfortunately, the solubilities as recorded for Voronkov et al. for the temperatures of 323.15 K, 353.15 K and 373.15 K all are of the same order of magnitude, especially at higher pressures, a most unlikely possibility. Also the data for the lower temperature (263.15 K) does not even approach the higher values of Kiss et al. (1) and Shenderei et al. (2). It is considered that some serious errors were incorporated in the data of Voronkov et al. (3) and those of Hronec et al. (4) and, therefore, they are both rejected. Hence, there are no reliable solubility data at elevated pressures for 2-propanone at ambient and higher temperatures.

For low temperatures the data of Kiss et al. (1) and Shenderei et al. (2) are consistent and have been used to develop an equation to represent the data. It should be mentioned that the data of Kiss et al. as obtained for method B gave solubilities somewhat lower than those for method A, and hence were considered less accurate and were not used in the development of equation (3):

$$\log x_p = 716.29\,(T/K)^{-1} + 1.0053 \log (p/\text{MPa}) + 0.050\,p - 3.502 \qquad (3)$$

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents containing oxygen excluding water and alcohols; pressures greater than 0.20 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 February, 1994

CRITICAL EVALUATION:

In this case the combined data of both research groups were reasonably well represented for pressures from 0.1 MPa to 1.0 MPa with an average, and a maximum difference of 2.8%, and 7.0%, respectively. It is noted that a factor for the slight curvature in the log x_p - log p lines is included in equation (3).

These data for solubilities in 2- propanone at 228.15 K, 238.15 K, and 248.15 K are classified as tentative.

Propanoic acid (propionic acid); $C_3H_6O_3$; [79-09-4]

Ethene solubilities in propionic acid were reported only as Henry's constant by Efremova and Sokolova (5) for the temperatures of 323.15 K, 373.15 K and 423.15 K, although the pressure range for the measurements was reported to be from 2.53 MPa to 12.41 MPa. It is noted that one of the values on the data sheet (for ethene solubility at 423.15 K) is for a temperature above the normal boiling point of the solvent, or above 414 K.

These solubility results are classified as tentative.

Acetic acid, ethenyl ester (vinyl acetate); $C_4H_6O_2$; [108-5-4]

Only the data of Zernov et al. (6) are available for ethene solubilities in the ethenyl ester of acetic acid (vinyl acetate). When the consistency of these data is tested using the relation between log x and log p, three inconsistencies appear. First, at low pressures and for temperatures from 293.1 K to 353.1 K, the solubilities are all of the same order of magnitude, which appears to be a most unlikely behavior. Next, at pressures greater than 1 MPa for some of the data the solubilities form large irregular inflections in the solubility-pressure relation; again this appears most unlikely. Finally, the composition of the gas phase at equilibrium indicates a relatively constant vapor content of the gas phase with changing pressures over large pressure ranges. This also, appears unlikely.

Only because no other solubility results are available in this solvent for comparison, these solubility data are classified as tentative.

1,3-Dioxolan-2-one, 4-methyl-(propylene carbonate); $C_4H_6O_3$; [108-32-7]

Ethene solubilities in 1,3-dioxolan-2-one, 4-methyl (propylene carbonate) as reported by Shakhova et al. (7) are entirely consistent. An equation based on all the data for the complete pressure range was developed as follows:

$$\log x_p = 442.90\ (T/K)^{-1} + 0.9260 \log (p/MPa) - 2.8703 \qquad (4)$$

Vapor pressures for this solvent are not readily available but believed to be low. In the development of equation (4) it was assumed that the solvent vapor pressure was negligible. The average, and maximum, deviations for the data from the equation are 2.3%, and 6.4%, respectively. When extrapolated to 0.1013 MPa for a temperature of 298.15 K, a value of the ethene solubility of 0.00495 mole fraction ethene, is obtained.

Figure 1 shows these data for propylene carbonate solvent and the lines representing equation (4). These data are classified as tentative.

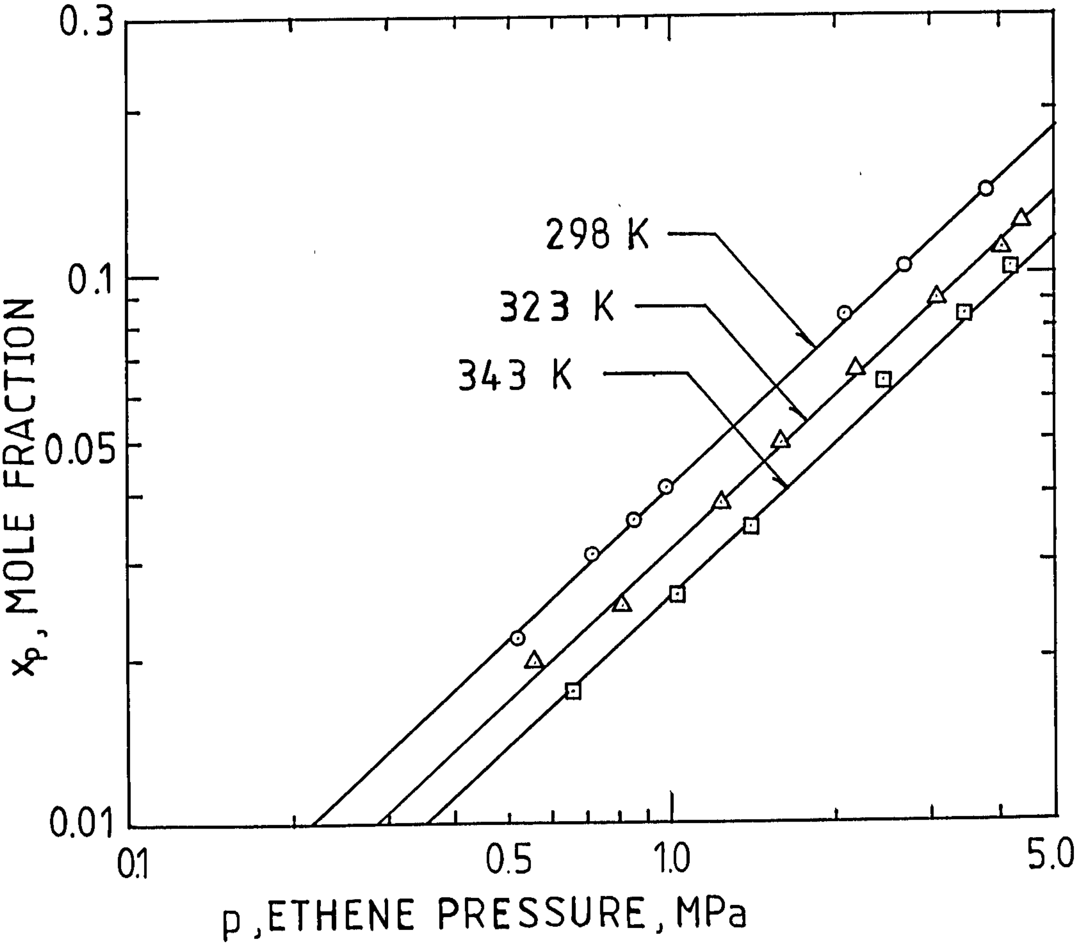
2-Butanone (methyl ethyl ketone); C_4H_8O; [74-93-3]

Ethene solubilities in 2-butanone for varying pressures at 223.15 K 238.15 K and 248.15 K as reported by Shenderei et al. (2) are entirely

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents containing oxygen excluding water and alcohols; pressures greater than 0.20 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 February, 1994

CRITICAL EVALUATION:

Fig. 1 Ethene Solubility in Propylene carbonate as a Function of Temperature and Pressure



consistent when plotted as log x versus log p. An equation based on the data for mole fraction solubilities (x_p) of less than 0.60 is as follows:

$$\log x_p = 553.24\ (T/\mathrm{K})^{-1} - 2.6964 + 1.074 \log (p/\mathrm{MPa}) \qquad (5)$$

The vapor pressure for 2-butanone at these low temperatures was considered to be negligibly low. The average, and maximum deviations of the data from equation (5) are 2.8%, and 8.8%, respectively. There are no low pressure solubility data for this solvent for comparison.

These data are classified as tentative.

References

1. Kiss, G.; Vanko, M.: Hagara, A.; Vanko, A. *Petrochem. (Czech.)* 1980, *20*, 132-137.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents containing oxygen excluding water and alcohols; pressures greater than 0.20 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 February, 1994

CRITICAL EVALUATION:

2. Shenderei, E.R.; Zel'venskii, Ya. D.; Ivanovskii, F.P. *Zhur. Fiz Khim.* 1962, *36*, 801-808.

3. Voronkov, A.P.; Mislavskaya, V.S.; Mushii, R. Ya.; Drygina, V.V. *Zh. Prikl. Khim.* 1979, *52*, 2642; *VINITI No. 458-79.*

4. Hronec, M.; Hagara, A.; Ilavsky, J. *Petrochem. (Czech.)* 1983, *23*, 111-115.

5. Efremova, G.D.; Sokolova, E.S. *Zh. Fiz. Khim.* 1973, *47*, 1228-9; *VINITI No. 6067-73.*

6. Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G. *J. Appl. Chem. (USSR)* 1971, *44*, 1837-1840. or *Zhur. Prikl. Khim.* 1971, 44, 1819-1823.

7. Shakhova, S.F.; Zubchenko, Yu P.; Rezina, O.A. *Khim. Prom.* 1973, *49*, 271.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Kiss, G.; Vanko, M.; Hagara, A.; Vanko, A.

Petrochemia (Czechoslovakia), 1980, *20*, 132-137.

VARIABLES:

$T/\mathrm{K} = 238.15, 248.15$

$P/\mathrm{MPa} = 0.101\text{-}1.013$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Partial Pressure p_1/MPa	Solubility s/cm^3 gas at NTP(g solvent)$^{-1}$	[1]Mole Fraction Ethene, x_1	[1]Henry's Constant H/atm(mole fraction)$^{-1}$
-35.0	238.15				
By method A:		0.152	20.08	0.0495	30.33
		0.203	27.21	0.0659	30.36
		0.304	42.38	0.0990	30.32
		0.405	58.55	0.1318	30.36
		0.507	77.21	0.1667	30.00
		0.608	100.80	0.2071	28.97
		0.709	126.85	0.2474	28.30
		0.811	166.87	0.3019	26.50
		0.912	197.88	0.3390	26.55
		1.013	242.87	0.3863	25.89
By method B:		0.101	11.8	0.0297	33.70
		0.203	24.8	0.0604	33.12
		0.405	58.3	0.1313	30.48

[1] Calculated by compiler.

Mole fraction ethylene at a gas partial pressure of 1 atm and 238.15 K is $x_1 = 0.0333$ as estimated by compiler assuming Henry's law.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Method A: The solubility cell is placed in a metal block surrounded by a cooling coil supplied by liquid nitrogen. Septum stoppers at the top and bottom permit sampling of the solution by means of a pressure microsyringe. The cell is initially charged with 2.5 cm^3 of solvent which is then saturated with gas by bubbling through a distribution ring containing 0.1 mm holes. The gas is continuously released through a pressure controlling manometer. The temperature is measured by miniature thermocouple. Analysis is by gas chromatography.

Method B: Apart from the explanation that a static method was used, no further description is provided.

SOURCE AND PURITY OF MATERIALS:

No information about the source and purity of gas or solvent is provided.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.1$

$\delta p/\mathrm{MPa} = \pm 0.001$

$\delta s/s = \pm 0.02$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Kiss, G.; Vanko, M.; Hagara, A.; Vanko, A.

Petrochemia (Czechoslovakia), 1980, *20*, 132-137.

VARIABLES:

T/K = 238.15,248.15

P/MPa = 0.101-1.013

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

...continued

t/C	T/K	Partial Pressure p_1/MPa	Solubility s/cm^3 gas at NTP(g solvent)$^{-1}$	[1]Mole Fraction Ethene, x_1	[1]Henry's Constant H/atm(mole fraction)$^{-1}$
-25.0	248.15				
By method A:		0.152	15.40	0.0384	39.09
		0.203	21.80	0.0535	37.40
		0.304	32.20	0.0770	38.95
		0.405	44.57	0.1035	38.63
		0.507	56.66	0.1280	30.05
		0.608	75.11	0.1629	36.83
		0.709	88.48	0.1865	37.53
		0.811	110.69	0.2229	35.89
		0.912	125.49	0.2454	36.68
		1.013	153.73	0.2849	35.10
By method B:		0.101	9.6	0.0243	41.20
		0.203	19.7	0.0486	41.18
		0.405	43.4	0.1011	39.57

[1]Calculated by compiler.

Mole fraction ethylene at a gas partial pressure of 1 atm and 248.15 K is 0.0256 as estimated by compiler assuming Henry's law.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Method A: The solubility cell is placed in a metal block surrounded by a cooling coil supplied by liquid nitrogen. Septum stoppers at the top and bottom permit sampling of the solution by means of a pressure microsyringe. The cell is initially charged with 2.5 cm^3 of solvent which is then saturated with gas by bubbling through a distribution ring containing 0.1 mm holes. The gas is continuously released through a pressure controlling manometer. The temperature is measured by miniature thermocouple. Analysis is by gas chromatography.

Method B: Apart from the explanation that a static method was used, no further description is provided.

SOURCE AND PURITY OF MATERIALS:

No information about the source and purity of gas or solvent is provided.

ESTIMATED ERROR:

δT/K = ± 0.1

δp/MPa = ± 0.001

$\delta s/s$ = ± 0.02(Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Hronec, M.; Hagara, A.; Ilavsky, J.

Petrochemia, (Czechoslovakia), <u>1983</u>, *23*, 111-115.

VARIABLES:

T/K = 238.15,308.15

P/kPa = 150-504

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Total Pressure P/kPa	[1]Partial Pressure p_1/kPa	Solubility s/cm^3 gas at NTP(g solvent)$^{-1}$	[1]Mole Fraction x_1	[1]Henry's Constant H/atm (mole fraction)$^{-1}$
-35	238.15	150	148.9	5.5	0.0141	104.6
		201	199.9	11.8	0.0300	66.5
		302	300.9	24.8	0.0604	49.2
		504	502.9	58.3	0.1311	37.8
-25	248.15	150	148.0	4.2	0.0108	135.7
		201	199.0	9.6	0.0243	80.9
		302	300.0	19.7	0.0486	61.0
		504	502.0	43.4	0.1011	49.0
-15	258.15	150	146.2	2.6	0.0067	215.6
		201	197.2	6.6	0.0168	115.7
		302	298.3	15.8	0.0393	74.8
		504	500.5	34.1	0.0812	60.8
5	278.15	150	137.9	0.9	0.0023	585
		201	189.0	3.0	0.0077	242
		302	290.2	8.4	0.0213	134
		504	492.5	19.8	0.0488	99.6
35	308.15	302	255.7	1.5	0.0039	652
		504	458.5	8.9	0.0225	201

[1]Calculated by compiler.

It is noted by the compiler that the results tabulated here appear to be inconsistent and in serious disagreement with results published earlier from the same laboratory: Kiss, Vanko, Hagara and Vanko, *Petrochemia*, <u>1980</u>, *20*, 132-137.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of an absorber, 10-cm^3 in volume, and a complex system using electrical contacts in a tube for maintaining a constant gas supply pressure in the absorber. The contacts were used to start and stop a gear pump which pumped silicone oil as an "inert" medium to displace gas from a gas storage vessel. The change in volume of silicone oil utilized was read on a burette and was considered to represent the volume of gas used. The absorber initially contained 3-5 cm^3 of solvent confined in a thin-walled glass ampoule. The chamber was pressurized with gas and to initiate the experiment the ampoule was broken using a stainless steel ball.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.8%.
2. Acetone was reagent grade with water content < 0.5%.

ESTIMATED ERROR:

δP/kPa = ± 5

$\delta s / s$ = ± 10% (Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Voronkov, A.P.; Mislavskaya, V.S.; Mushii, R. Ya.; Drygina, V.V.
Zh. Prikl. Khim. 1979, *52*, 2642;
VINITI No. 458-79.

VARIABLES:

T/K = 263.15 - 373.15
P/MPa = 0.101 - 7.60

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Temperatures t/°C	T/K	Mole Fractions Acetone in Liquid $1 - x_1$	 [1]Ethene in Liquid x_1	 Acetone in Gas $1 - y_1$	 Ethene in Gas y_1	[1]Partial Pressure Ethene, p_1/atm	Total Pressure P/atm
-10	263.15	0.990	0.010	0.606	0.9494	0.9494	1
		0.976	0.024	0.0180	0.9820	2.95	3
		0.960	0.040	0.0101	0.9899	4.95	5
		0.922	0.078	0.0048	0.9952	9.95	10
		0.878	0.122	0.0032	0.9968	14.95	15
		0.844	0.156	0.0021	0.9979	19.96	20
		0.786	0.214	0.0014	0.9986	24.96	25
		0.680	0.320	0.0009	0.9991	29.97	30
10	283.15	0.995	0.005	0.3983	0.6017	0.6017	1
		0.984	0.016	0.0765	0.9235	2.77	3
		0.973	0.027	0.0385	0.9616	4.81	5
		0.953	0.047	0.0157	0.9843	9.84	10
		0.934	0.066	0.0102	0.9898	14.85	15
		0.914	0.086	0.0070	0.9930	19.86	20
		0.898	0.102	0.0053	0.9947	24.87	25
		0.870	0.130	0.0043	0.9957	29.87	30
		0.822	0.178	0.0037	0.9963	34.87	35

[1] Calculated by Compiler.
Henry's law is obeyed up to about 25 atm (2.53 MPa).
The data were from the paper deposited in VINITI, Moscow.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equipment essentially consisted of an autoclave immersed in a constant temperature bath and connected to a membrane pressure gauge.

Henry's constants for the lower pressure region and the solubilities for a pressure of 1 atm as estimated by the compiler are:

T/K	H, atm/mole fraction	x, mole fraction
263.15	125	0.00800
283.15	225	0.00444
303.15	244	0.00410
323.15	286	0.00351
353.15	300	0.00333
373.15	313	0.00319

SOURCE AND PURITY OF MATERIALS:

The sources and purities of gas and solvent were not specified.

ESTIMATED ERROR:

δT/K = ± 0.2
δp/atm = ± 0.05
δx/mole fraction = ± 0.002
(Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Voronkov, A.P.; Mislavskaya, V.S.; Mushii, R. Ya.; Drygina, V.V.
Zh. Prikl. Khim. <u>1979</u>, *52*, 2642;

VINITI No. 458-79.

VARIABLES:

T/K = 263.15 - 373.15

P/MPa = 0.101 - 7.60

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

Temperatures		Mole Fractions				[1]Partial Pressure Ethene, p_1/atm	Total Pressure P/atm
t/°C	T/K	Acetone in Liquid $1 - x_1$	[1]Ethene in Liquid x_1	Acetone in Gas $1 - y_1$	Ethene in Gas y_1		
30	303.15	0.997	0.003	0.4240	0.5760	0.576	1
		0.984	0.016	0.0744	0.9256	2.78	3
		0.978	0.022	0.0410	0.9590	4.80	5
		0.960	0.040	0.0194	0.9806	9.81	10
		0.946	0.054	0.0115	0.9885	14.83	15
		0.924	0.076	0.0096	0.9904	19.81	20
		0.896	0.104	0.0078	0.9922	24.81	25
		0.878	0.122	0.0064	0.9936	29.81	30
		0.854	0.146	0.0056	0.9944	34.80	35
		0.824	0.176	0.0048	0.9952	39.81	40
		0.794	0.206	0.0040	0.9960	44.82	45
		0.764	0.236	0.0036	0.9964	49.82	50
50	323.15	0.993	0.007	0.1518	0.8482	2.54	3
		0.985	0.015	0.0867	0.9133	4.57	5
		0.968	0.032	0.0421	0.9579	9.58	10
		0.951	0.049	0.0280	0.9720	14.58	15
		0.930	0.070	0.0212	0.9831	19.58	20
		0.914	0.086	0.0169	0.9880	24.58	25

[1] Calculated by Compiler.

Henry's law is obeyed up to about 25 atm (2.53 MPa).

The data were from the paper deposited in VINITI, Moscow.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equipment essentially consisted of an autoclave immersed in a constant temperature bath and connected to a membrane pressure gauge.

Henry's constants for the lower pressure region and the solubilities for a pressure of 1 atm as estimated by the compiler are:

T/K	H, atm/mole fraction	x, mole fraction
263.15	125	0.00800
283.15	225	0.00444
303.15	244	0.00410
323.15	286	0.00351
353.15	300	0.00333
373.15	313	0.00319

SOURCE AND PURITY OF MATERIALS:

The sources and purities of gas and solvent were not specified.

ESTIMATED ERROR:

δT /K = ± 0.2
δp/atm = ± 0.05
δx/mole fraction = ± 0.002
(Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Voronkov, A.P.; Mislavskaya, V.S.; Mushii, R. Ya.; Drygina, V.V.
Zh. Prikl. Khim. 1979, *52*, 2642;

VINITI No. 458-79.

VARIABLES:

T/K = 263.15 - 373.15

p/MPa = 0.101 - 7.60

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

Temperatures t/°C	T/K	Mole Fractions: Acetone in Liquid $1 - x_1$	[1]Ethene in Liquid x_1	Acetone in Gas $1 - y_1$	Ethene in Gas y_1	[1] Partial Pressure Ethene, p_1/atm	Total Pressure p/atm
50	323.15	0.896	0.104	0.0140	0.9860	29.58	30
		0.872	0.128	0.0120	0.9880	34.58	35
		0.858	0.142	0.0106	0.9894	39.58	40
		0.832	0.168	0.0096	0.9904	44.57	45
		0.812	0.188	0.0087	0.9913	49.57	50
		0.788	0.212	0.0080	0.9920	54.56	55
		0.764	0.236	0.0074	0.9926	59.56	60
80	353.15	0.988	0.012	0.2971	0.7029	3.51	5
		0.974	0.026	0.1339	0.8661	8.66	10
		0.956	0.044	0.0890	0.9110	13.67	15
		0.940	0.060	0.0653	0.9347	18.69	20
		0.920	0.080	0.0532	0.9468	23.67	25
		0.904	0.096	0.0440	0.9560	28.68	30
		0.886	0.114	0.0379	0.9621	33.67	35
		0.864	0.136	0.0326	0.9674	38.70	40
		0.854	0.146	0.0298	0.9702	43.66	45
		0.832	0.168	0.0270	0.9730	48.65	50
		0.812	0.188	0.0242	0.9758	53.67	55

[1]Calculated by Compiler.
Henry's law is obeyed up to about 25 atm (2.53 MPa).
The data were from the paper deposited in VINITI, Moscow.

continued...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equipment essentially consisted of an autoclave immersed in a constant temperature bath and connected to a membrane pressure gauge.

Henry's constants for the lower pressure region and the solubilities for a pressure of 1 atm as estimated by the compiler are:

T/K	H, atm/mole fraction	x, mole fraction
263.15	125	0.00800
283.15	225	0.00444
303.15	244	0.00410
323.15	286	0.00351
353.15	300	0.00333
373.15	313	0.00319

SOURCE AND PURITY OF MATERIALS:

The sources and purities of gas and solvent were not specified.

ESTIMATED ERROR:

δT/K = ± 0.2
δp/atm = ± 0.05
δx/mole fraction = ± 0.002
(Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone (acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Voronkov, A.P.; Mislavskaya, V.S.; Mushii, R. Ya.; Drygina, V.V.
Zh. Prikl. Khim. 1979, *52*, 2642;

VINITI No. 458-79.

VARIABLES:

T/K = 263.15 - 373.15

P/MPa = 0.101 - 7.60

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ...continued

Temperatures		Mole Fractions				[1]Partial Pressure	Total Pressure
t/°C	T/K	Acetone in Liquid $1 - x_1$	[1]Ethene in Liquid x_1	Acetone in Gas $1 - y_1$	Ethene in Gas y_1	Ethene, P_1/atm	P/atm
80	353.15	0.800	0.200	0.0228	0.9772	58.63	60
		0.772	0.228	0.0212	0.9788	63.62	65
		0.766	0.234	0.0197	0.9803	68.62	70
		0.748	0.252	0.0185	0.9815	73.61	75
100	373.15	0.997	0.003	0.6280	0.3720	1.86	5
		0.980	0.020	0.2634	0.7366	7.37	10
		0.962	0.038	0.1676	0.8324	12.49	15
		0.946	0.054	0.1234	0.8766	17.53	20
		0.928	0.072	0.1090	0.8910	22.28	25
		0.912	0.088	0.0822	0.9178	27.53	30
		0.894	0.106	0.0710	0.9290	32.52	35
		0.876	0.124	0.0621	0.9379	37.52	40
		0.856	0.144	0.0553	0.9447	42.51	45
		0.844	0.156	0.0500	0.9500	47.50	50
		0.832	0.168	0.0458	0.9542	52.48	55
		0.812	0.188	0.0423	0.9577	57.46	60
		0.790	0.210	0.0392	0.9608	62.45	65
		0.776	0.224	0.0366	0.9634	67.44	70

[1]Calculated by Compiler.
Henry's law is obeyed up to about 25 atm (2.53 MPa).
The data were from the paper deposited in VINITI, Moscow.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equipment essentially consisted of an autoclave immersed in a constant temperature bath and connected to a membrane pressure gauge.

Henry's constants for the lower pressure region and the solubilities for a pressure of 1 atm as estimated by the compiler are:

T/K	H, atm/mole fraction	x, mole fraction
263.15	125	0.00800
283.15	225	0.00444
303.15	244	0.00410
323.15	286	0.00351
353.15	300	0.00333
373.15	313	0.00319

SOURCE AND PURITY OF MATERIALS:

The sources and purities of gas and solvent were not specified.

ESTIMATED ERROR:

δT/K = ± 0.2
δp/atm = ± 0.05
δx/mole fraction = ± 0.002
(Authors)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Propanone, (Acetone); C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya.D.; Ivanovskii, F.P.

Zhur.Fiz.Khim. 1962, *36*, 801-808.

VARIABLES:

T/K = 228.05 - 248.15

P/MPa = 0.101 - 1.82

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	p/atm	p/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	Solubility,$^+$
248.15	1	1.0	0.0255	10.02
	3	3.0	0.0750	30.98
	5	5.1	0.1300	57.09
	10	10.1	0.2825	150.55
	12	12.2	0.3500	205.75
	15	15.2	0.4680	336.13
	18	18.2	0.6100	597.65
238.15	1	1.0	0.0320	12.61
	3	3.0	0.1000	42.46
	5	5.1	0.1650	75.51
	10	10.1	0.3825	236.88
	12	12.2	0.5125	402.11
	15	15.2	0.8100	1628.0
228.05	1	1.0	0.0410	16.35
	3	3.0	0.1275	55.87
	5	5.0	0.2230	109.66
	10	10.1	0.6050	515.50

+ $cm^3 g^{-1}$ at P = 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with magnetic stirrer. Pressure measured with Bourdon gauge. Samples of liquid analysed by stripping out ethene. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Prepared from ethanol by dehydration and purified by absorption in cuprous chloride under pressure.
2. Distilled.

ESTIMATED ERROR:

δT/K = ±0.1; δp/bar = ±0.3;

$\delta x_{C_2H_4}$ = ±2%.

(estimated by compiler.)

REFERENCES:

1. Shenderei, E.R. Zel'venskii, Ya.D.; Ivanovskii, F.P.

   Khim. Prom. 1960, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Propanoic acid (propionic acid); $C_3H_6O_2$; [79-09-4]

ORIGINAL MEASUREMENTS:

Efremova, G.D.; Sokolova, E.S.

Zh. Fiz. Khim. 1973, *47*, 1228-9;

VINITI No. 6067-73.

VARIABLES:

T/K = 323.15 - 423.15

P/MPa = 2.53 - 12.41

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Henry's Constant, H/atm (mole fraction)$^{-1}$	[1]Mole Fraction Ethene, x_1
50	323.15	133	0.00752
100	373.15	178	0.00562
150	423.15	257	0.00389

[1] Calculated by compiler for a gas partial pressure of 101.3 kPa; it is stated that the Krichevskii-Kazarnovskii equation applies at high pressures but the parameters are not given here.

The data were obtained from the portion of the paper deposited in VINITI, Moscow.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A titanium autoclave whose volume was calibrated, was used. The autoclave was equipped with a membrane pressure gauge along with a thermocouple placed near the bottom of the autoclave.

SOURCE AND PURITY OF MATERIALS:

1. Ethene critical temperature was measured as 9.30°C (reported value 9.60°C).
2. Solvent purified by fractional crystallization; resulting melting point was -21.0°C compared with reported value of -20.8°C.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.2$

$\delta x_1/x_1 = \pm 2\%$ (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Acetic acid, ethenyl ester (vinyl acetate); $C_4H_6O_2$; [108-5-4]

ORIGINAL MEASUREMENTS:

Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.
J. Appl. Chem. (USSR) 1971, *44*, 1837-40.
OR *Zhur. Prikl. Khim.* 1971, *44*, 1819-23.

VARIABLES:

T/K = 293.1 - 423.1

P/MPa = 0.20 - 7.09

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

T/K	P/MPa	Mole Fraction in Liquid		Mole Fraction in Gas	
		Solvent, x_2	[1] Solute, x_1	Solvent vapor, y_2	[1]Solute, y_1
293.1	0.20	0.989	0.011	0.063	0.937
	0.41	0.975	0.025	0.036	0.964
	0.71	0.953	0.047	0.034	0.966
	1.01	0.940	0.060	0.034	0.966
	2.02	0.760	0.240	0.034	0.966
	3.03	0.593	0.407	0.034	0.966
	4.05	0.530	0.470	0.036	0.964
	5.06	0.487	0.513	0.034	0.966
313.1	0.21	0.989	0.011	0.150	0.850
	0.44	0.975	0.025	0.075	0.925
	0.67	0.960	0.040	0.060	0.940
	1.01	0.951	0.049	0.047	0.953
	2.02	0.839	0.161	0.047	0.953
	3.04	0.657	0.343	0.047	0.953
	4.05	0.582	0.418	0.047	0.953
	5.06	0.541	0.459	0.046	0.954

[1] Calculated by compiler.
Liquid and gas molar volumes as well as partial molal volumes of dissolved ethene also given in this paper.
Normal Henry's law not even approximately obeyed above 1 MPa pressure.

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A description of the apparatus is found in ref. 1. It consists of two graduated thick-walled glass tubes, 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury can be independently charged to the bottom of each tube. The saturation tube is equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir is pressurized with nitrogen whose pressure can be regulated. Ethylene is stored in one tube, while the solvent is condensed in the equilibration tube. The ethene is transferred to the solvent tube as required. The solubility method is thus a volumetric one.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.3%.
2. Twice distilled. Normal boiling point = 345.4 K and refractive index n_D^{20} = 1.3953. Note: At high temperatures and pressures 0.0001 mole % hydroquinone inhibitor was added.

ESTIMATED ERROR:

δT/K = ± 0.05
$\delta P/P$ = ± 0.25%
$\delta x_1/x_1$ = ± 0.04 (compiler)

REFERENCES:

1. Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.; Duntov, F.I.
Zh. Prikl. Khim 1971, *44*, 683.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Acetic acid, ethenyl ester (vinyl acetate); $C_4H_6O_2$; [108-5-4]

ORIGINAL MEASUREMENTS:

Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.
J. Appl. Chem. (USSR) 1971, *44*, 1837-40.
OR *Zhur. Prikl. Khim.* 1971, *44*, 1819-23.

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VARIABLES:

T/K = 293.1 - 423.1

P/MPa = 0.20 - 7.09

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

....continued

T/K	P/MPa	Mole Fraction in Liquid		Mole Fraction in Gas	
		Solvent, x_2	[1]Solute, x_1	Solvent vapor, y_2	[1]Solute, y_1
333.1	0.22	0.989	0.011	0.165	0.835
	0.49	0.975	0.025	0.170	0.830
	0.79	0.952	0.048	0.080	0.920
	2.02	0.877	0.123	0.068	0.932
	3.04	0.698	0.302	0.068	0.932
	4.05	0.627	0.373	0.068	0.932
	5.06	0.588	0.412	0.068	0.932
	6.08	0.545	0.455	0.068	0.932
	7.09	0.516	0.484	0.069	0.931
353.1	0.25	0.989	0.011	0.220	0.780
	0.54	0.975	0.025	0.173	0.827
	0.81	0.960	0.040	0.165	0.835
	2.02	0.905	0.195	0.114	0.886
	3.04	0.730	0.270	0.095	0.905
	4.05	0.651	0.349	0.093	0.907
	5.06	0.612	0.388	0.093	0.907
	6.08	0.573	0.427	0.093	0.907

[1] Calculated by compiler.

Liquid and gas molar volumes as well as partial molal volumes of dissolved ethene also given in this paper.

Normal Henry's law not even approximately obeyed above 1 MPa pressure.

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A description of the apparatus is found in ref. 1. It consists of two graduated thick-walled glass tubes, 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury can be independently charged to the bottom of each tube. The saturation tube is equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir is pressurized with nitrogen whose pressure can be regulated. Ethylene is stored in one tube, while the solvent is condensed in the equilibration tube. The ethene is transferred to the solvent tube as required. The solubility method is thus a volumetric one.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.3%.
2. Twice distilled. Normal boiling point = 345.4 K and refractive index n_D^{20} = 1.3953. Note: At high temperatures and pressures 0.0001 mole % hydroquinone inhibitor was added.

ESTIMATED ERROR:

δT/K = ± 0.05
$\delta P/P$ = ± 0.25%
$\delta x_1/x_1$ = ± 0.04 (compiler)

REFERENCES:

1. Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.; Duntov, F.I. *Zh. Prikl. Khim.* 1971, *44*, 683.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Acetic acid, ethenyl ester (vinyl acetate); $C_4H_6O_2$; [108-5-4]

ORIGINAL MEASUREMENTS:

Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.
J. Appl. Chem. (USSR) 1971, *44*, 1837-40.
OR *Zhur. Prikl. Khim.* 1971, *44*, 1819-23.

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VARIABLES:

T/K = 293.1 - 423.1

P/MPa = 0.20 - 7.09

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES: ....continued

		Mole Fraction in Liquid		Mole Fraction in Gas	
T/K	P/MPa	Solvent, x_2	[1]Solute, x_1	Solvent vapor, y_2	[1]Solute, y_1
373.1	0.28	0.989	0.011	0.232	0.768
	0.62	0.975	0.025	0.218	0.782
	1.00	0.960	0.040	0.158	0.842
	1.23	0.941	0.059	0.140	0.860
	3.04	0.835	0.165	0.138	0.862
	4.05	0.680	0.320	0.138	0.862
	5.06	0.639	0.361	0.138	0.862
	6.08	0.600	0.400	0.138	0.862
	7.09	0.563	0.457	0.139	0.861
398.1	0.55	0.989	0.011		
	1.04	0.975	0.025	0.297	0.703
	1.42	0.960	0.040	0.283	0.718
	3.04	0.865	0.135	0.227	0.773
	4.05	0.710	0.290	0.225	0.775
	5.06	0.665	0.335	0.225	0.775
	6.08	0.630	0.370	0.225	0.775
	7.09	0.589	0.411	0.226	0.774

[1] Calculated by compiler.
Liquid and gas molar volumes as well as partial molal volumes of dissolved ethene also given in this paper.
Normal Henry's law not even approximately obeyed above 1 MPa pressure.

continued....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A description of the apparatus is found in ref. 1. It consists of two graduated thick-walled glass tubes, 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury can be independently charged to the bottom of each tube. The saturation tube is equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir is pressurized with nitrogen whose pressure can be regulated. Ethylene is stored in one tube, while the solvent is condensed in the equilibration tube. The ethene is transferred to the solvent tube as required. The solubility method is thus a volumetric one.

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.3%.
2. Twice distilled. Normal boiling point = 345.4 K and refractive index n_D^{20} = 1.3953. Note: At high temperatures and pressures 0.0001 mole % hydroquinone inhibitor was added.

ESTIMATED ERROR:

$\delta T/K = \pm 0.05$
$\delta P/P = \pm 0.25\%$
$\delta x_1/x_1 = \pm 0.04$ (compiler)

REFERENCES:

1. Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.; Duntov, F.I.
Zh. Prikl. Khim. 1971, *44*, 683.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Acetic acid, ethenyl ester (vinyl acetate); $C_4H_6O_2$; [108-5-4]	Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G. *J. Appl. Chem. (USSR)* 1971, *44*, 1837-40. OR *Zhur.Prikl.Khim.* 1971, *44*, 1819-23.

VARIABLES:	PREPARED BY:
T/K = 293.1 - 423.1 P/MPa = 0.20 - 7.09	W. Hayduk

EXPERIMENTAL VALUES:

....continued

T/K	P/MPa	Mole Fraction in Liquid		Mole Fraction in Gas	
		Solvent, x_2	[1]Solute, x_1	Solvent vapor, y_2	[1]Solute, y_1
423.1	0.82	0.989	0.011	0.410	0.590
	1.24	0.975	0.025	0.395	0.605
	1.82	0.960	0.040	0.383	0.617
	3.04	0.917	0.083	0.346	0.654
	4.05	0.765	0.235	0.344	0.656
	5.05	0.730	0.270	0.344	0.656
	6.08	0.680	0.320	0.344	0.656
	7.09	0.641	0.359	0.345	0.655

[1] Calculated by compiler.

Liquid and gas molar volumes as well as partial molal volumes of dissolved ethene also given in this paper.

Normal Henry's law not even approximately obeyed above 1 MPa pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A description of the apparatus is found in ref. 1. It consists of two graduated thick-walled glass tubes, 5 mm in diameter and 60 cm in length sealed in a temperature-controlled jacket. Mercury can be independently charged to the bottom of each tube. The saturation tube is equipped with an electromagnetic vibrator immersed in the mercury to aid in equilibration of the phases. A separate mercury reservoir is pressurized with nitrogen whose pressure can be regulated. Ethylene is stored in one tube, while the solvent is condensed in the equilibration tube. The ethene is transferred to the solvent tube as required. The solubility method is thus a volumetric one.	1. Purity 99.3%. 2. Twice distilled. Normal boiling point = 345.4 K and refractive index n_D^{20} = 1.3953. Note: At high temperatures and pressures 0.0001 mole % hydroquinone inhibitor was added.
	ESTIMATED ERROR: $\delta T/K = \pm 0.05$ $\delta P/P = \pm 0.25\%$ $\delta x_1/x_1 = \pm 0.04$ (compiler)
	REFERENCES: 1. Zernov, V.S.; Kogan, V.B.; Lyubetskii, S.G.; Duntov, F.I. *Zh. Prikl. Khim.* 1971, *44*, 683.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1,3-Dioxolan-2-one,4-methyl- (Propylene carbonate); $C_4H_6O_3$; [108-32-7]

ORIGINAL MEASUREMENTS:

Shakhova, S.F.; Zubchenko, Yu P.; Rezina, O.A.

Khim. Prom., 1973, *49*, 271.

VARIABLES:

T/K = 298.15 - 343.15

P/MPa = 0.52 - 4.22

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	P/MPa	Mole fraction of ethene in liquid, $x_{C_2H_4}$	$\mathrm{vol}^{\alpha+}/\mathrm{vol}$
298.15	0.517	0.0216	5.8
	0.719	0.0310	8.4
	0.861	0.0356	9.7
	0.983	0.0409	11.2
	2.077	0.0843	24.2
	2.695	0.1034	30.3
	3.830	0.1423	43.6
323.15	0.557	0.0196	5.25
	0.811	0.0250	6.75
	1.246	0.0384	10.5
	1.600	0.0492	13.6
	2.209	0.0667	18.8
	3.040	0.0900	26.0
	4.021	0.1124	33.3
	4.361	0.1246	37.4
343.15	0.661	0.0175	4.68
	1.021	0.0258	6.97
	1.031	0.0270	7.30
	1.401	0.0345	9.40
	2.471	0.0641	18.0
	3.441	0.0843	24.2
	4.171	0.1031	30.2
	4.221	0.1034	30.3

+ 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. Samples of liquid analysed by volumetric method. Details in ref. (1).

Henry's constants were listed as follows:

t/C	H/atm mole fraction^{-1}
25	235
50	298
70	333

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.97 mole per cent.
2. Distilled, no other details given.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.1$; $\delta P/\mathrm{MPa} = \pm 0.01$; $\delta x_{C_2H_4} = \pm 5\%$

(estimated by compiler)

REFERENCES:

1. Shakhova, S.F.; Zubchenko, Yu.P.; Kaplan, L.K.; *Khim. Prom.*, 1973, *5*, 108.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Butanone, (methyl ethylketone); C_4H_8O; [74-93-3]

ORIGINAL MEASUREMENTS:

Shenderei, E.R.; Zel'venskii, Ya, D.; Ivanovskii, F.P.

Zhur. Fiz. Khim. 1962, *36*, 801-808.

2) f

VARIABLES:

T/K = 223.05 - 248.15

P/MPa = 0.30 - 1.82

PREPARED BY:

C.L. Young.

EXPERIMENTAL VALUES:

T/K	p/atm	p/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	Solubility$^+$
248.15	3	3.0	0.0950	32.32
	5	5.1	0.1622	59.52
	10	10.1	0.3349	155.11
	12	12.2	0.4169	220.24
	15	15.2	0.5381	352.56
	18	18.2	0.6070	708.29
238.15	3	3.0	0.1180	41.02
	5	5.1	0.2000	76.08
	10	10.1	0.4477	249.62
	12	12.2	0.5685	404.49
	15	15.2	0.8300	1503.32
223.05	3	3.0	0.1620	59.52
	5	5.1	0.2787	118.56
	10	10.1	0.6830	663.42

$+$ $cm^3 g^{-1}$ at P = 101.325 kPa

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with magnetic stirrer. Pressure measured with Bourdon gauge. Samples of liquid analysed by stripping out ethene. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. Prepared from ethanol by dehydration and purified by absorption in cuprous chloride under pressure.
2. Distilled.

ESTIMATED ERROR:

δT/K = ±0.1; δp/bar = ±0.3;
$\delta x_{C_2H_4}$ = ±2%.
(estimated by compiler).

REFERENCES:

1. Shenderei, E.R.; Zel'venskii, Ya. D.; Ivanovskii, F.P.

   Khim. Prom. 1960, 370.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Solvents containing nitrogen

EVALUATOR:

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

November, 1993

CRITICAL EVALUATION:

Critical evaluation of the solubility of ethene at a partial pressure not greater than 101.3 kPa in solvents containing nitrogen.

In general solubility in compounds containing nitrogen which have been studied is lower than solubility in halogen or oxygen compounds measured under the same conditions. It is considerably lower than solubility in hydrocarbons.

1-Methyl-2-pyrrolidinone; C_5H_9NO; [872-50-4]

Solubility in 1-methyl-2-pyrrolidinone at, or below 101.3 kPa was measured by Wu *et al.*(1), Shenderei and Ivanovskii (2) and by Lenoir *et al.*(3). Measurements by Shenderei from 273.15 to 288.15 K and pressures from about 13 kPa to 101.3 kPa indicate that mole fraction solubility is, within the limits of the experimental accuracy, proportional to pressure to at least 101.3 kPa. Lenoir *et al.* measured Henry's constant at 298.15 K and low pressure by gas chromatography. The corresponding mole fraction solubility at a partial pressure of 101.3 kPa, calculated on the basis of a linear variation with change in pressure, is within about 5% of the value corrected to 101.3 kPa from direct measurements by Wu at 100 kPa. The six data points for a partial pressure of 101.3 kPa from the three sources fit the equation

$$\ln x_1 = -503.92 + 22206/(T/\mathrm{K}) + 74.519 \ln(T/\mathrm{K})$$

standard deviation in values of $x_1 = 1.65 \times 10^{-4}$

This can be accepted on a tentative basis for the temperature range 273-298 K.

Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

The solubility in nitrobenzene was measured by Choudhari and Doraiswami (4) at a total pressure of 94.23 kPa in the temperature range 286-333 K. Lenoir *et al.*(3) measured Henry's constant at low pressure by gas chromatography. The corresponding mole fraction solubility at 101.3 kPa, calculated on the assumption of a linear variation of mole fraction solubility with variation of pressure, is 0.00794. The corrected and interpolated value from Choudharai's measurements is 0.00543. Measurements of gas solubility by gas chromatography are subject to some uncertainty because of effects due to surface adsorption. Some of the values of solubilities of other gases reported in Lenoir's paper are appreciably higher than values reported by other workers. The evaluator considers that Choudhari's measurements are likely to be the more reliable although further work on the system is required. The five mole fraction solubilities from Choudhari, corrected to a partial pressure of gas of 101.3 kPa, fit the equation

$$\ln x_1 = -233.51 + 12038/(T/\mathrm{K}) + 32.982 \ln(T/\mathrm{K})$$

standard deviation in values of $x_1 = 6.6 \times 10^{-5}$

Temperature range 386-333 K.

Ammonia; NH_3; [7664-41-7]

Hannaert *et al.*(5) reported the solubility of ethene in liquid ammonia in a paper in which the solubilities of various hydrocarbons in liquid ammonia and other solvents were reported. In each case solubilities are reported as coefficients of a two constant equation giving the variation of Henry's constant with temperature. The equation can be written in the form

$$\log H = A - B/(2.3\ RT)$$

The authors identify the constant B with a heat of solution of the gas in the solvent. Mole fraction solubilities can be calculated from values of H

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents containing nitrogen	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

if it is assumed that solubilities vary linearly with partial pressure of gas. The equation for solubility of ethene in ammonia is reported to be valid for the temperature range of 208-318 K. What is unusual about the equation for ethene in ammonia is the very low value of **B** or heat of solution compared with values for other systems which were studied by the authors. The value is 0.23 kcal mol^{-1} compared with 2.72 kcal mol-1 for ethyne in ammonia and 1.215 kcal mol^{-1} for propene in ammonia. The low value for ethene corresponds to a very small variation of solubility with change in temperature and contrasts markedly with the behaviour of ethene in nitrobenzene and in 1-methyl-2-pyrrolidinone. The evaluator is of the opinion that the solubility equation for ethene in ammonia should be treated with caution until it is confirmed by other measurements.

N,*N*-Dimethylacetamide; C_4H_9NO; [127-19-5]
N,*N*-Dimethylformamide; C_3H_7NO; [68-12-2]
N-Methylformamide; C_2H_5NO; [123-39-7]
Acetonitrile; C_2H_3N; [75-05-8]

Brückl and Kim (6) measured the solubility in the above solvents at 298.2 K. There is no reason to doubt the reliability of the measurements but they have not been confirmed by other workers. In the case of the amides the mole fraction solubility at a partial pressure of 101.3 kPa increases with increase in the number of methyl groups present. Solubility in *N*-methylformamide is low compared with the solubility in nitrobenzene and in 1-methyl-2-pyrrolidinone and is close to the solubility in ammonia as reported by Hannaert (5).

Benzenamine; C_6H_7N; [62-53-3]

Lenoir *et al.*(3) measured Henry's constant for dissolution in benzenamine by a chromatographic method. The mole fraction solubility at a partial pressure of 101.3 kPa, calculated on the assumption of a linear variation of mole fraction solubility with change in pressure, is close to the value for dissolution in nitrobenzene. However the value needs confirmation by further measurements because of unreliability of the chromatographic method.

Cyclohexylamine; C6H13N; [108-91-8]

Keevil *et al.*(7) reported a value of the solubility in cyclohexylamine at 298.1 K and 101.3 kPa. The value is higher than that in other nitrogen compounds for which data is available. This can be explained by the presence of the alicyclic ring. There is no reason to doubt the reliability of the measurement but confirmation is needed.

N,*N*-Dimethylformamide; C_3H_7NO; [68-12-2] + Ethyne; C_2H_2; [74-86-2]

Shenderei (8) measured the solubility of ethene in *N*,*N*-dimethylformamide, containing various proportions of ethyne, at 218.15 K over the pressure range 13.3 - 101.3 kPa. The measurements indicate that the mole fraction solubility (moles C_2H_4/total moles of C_2H_4, C_2H_2 & DMF) does not change when the proportion of ethyne is increased from 33.8 to 249 cm^3(STP)/g DMF. This is in contrast to the solubility of carbon dioxide in *N*,*N*-dimethylformamide containing various concentrations of ethyne. In this case the mole fraction solubility decreases with increase of ethyne concentration. The evaluator considers that the data for ethene needs to be confirmed before it can be accepted as reliable.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Solvents containing nitrogen	Peter G.T. Fogg School of Applied Chemistry University of North London Holloway Road, London, N7 8DB, U.K. November, 1993

CRITICAL EVALUATION:

References

1. Wu, Z.; Zeck, S.; Langhorst, R.; Knapp, H. *Proc. Int. Conf. Coal Gas and Air, Beijing, China* 1985, *1*, 209-229.

2. Shenderei, E.R.; Ivanovskii, F.P. *Gaz Prom.* 1962, 7, 11-17; *Khim. Prom.* 1963, *10*, 91-97.

3. Lenoir, J-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data* 1971, *16*, 340-342.

4. Choudhari, R.V.; Doraiswami, L.K. *J. Chem. Eng. Data* 1972, *17*, 428-432.

5. Hannaert, H.; Haccuria, M.; Mathieu, M.P. *Ind. Chim. Belge* 1967, *32*, 156-164.

6. Brückl, N.; Kim, J.I. *Z. Phys. Chem. (Wiesbaden)* 1981, *126*, 133-150.

7. Keevil, T.A.; Taylor, D.R.; Streitwieser, A. *J. Chem. Eng. Data* 1978, *23*, 237-239.

8. Shenderei, E.R. *Khim. Prom.* 1966, *42*, 514-516.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Ammonia; NH_3; [7664-41-7]

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M. P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 208.15 - 318.15

PREPARED BY:

H.L. Clever

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EXPERIMENTAL VALUES:

Temperature Interval of Measurements T/K	Ethene Mol % Range 10^2x_1/mol %	$K\pi\nu$/atm[1] at 293.15 K	Enthalpy of Dissolution ΔH/kcal mol^{-1}	Constant A
208.15-318.15	0 - 2	275	0.23	2.61

[1] log ($K\pi\nu$/atm) = A - (ΔH/cal mol^{-1})/(2.3R(T/K))

The author's definitions are:

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}},$$

π/atm = total pressure,

ν = coefficient of fugacity.

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = (f_1/atm)/x_1 where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe three methods:

1.A. [Saturat. n°1]. A measure of the static pressure of saturation in an apparatus which gave a precision of 10 - 15 %.

1.B. [Saturat. n°2]. A measure of the static pressure of saturation in an apparatus which gave a precision of 2 - 5 %.

2. [Chromato]. A Gas liquid chromatographic method estimated to have a precision of 2 - 5 %.

3. [Anal. directe]. Direct analysis of the gaseous and liquid phases.

Method 1.B. was used in this system plus Mes. dir. Teneurs?

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Air Liquide. For narcosis, 99.9 per cent.

(2) Ammonia. Source not given. Industrial product. Contained 0.1 per cent water. Density, ρ/g cm^{-3} = 0.717 at -65°C and 0.705 at -50°C.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Miscellaneous compounds

ORIGINAL MEASUREMENTS:

Brückl, N.; Kim, J. I.

Z. Phys. Chem. (Wiesbaden)

1981, *126*, 133-150.

VARIABLES:

$T/K = 298.2$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

$T/K = 298.2$

$\ln(H/\text{atm})$	10^3 × Mole fraction of ethene in liquid[†], $10^3 x_{C_2H_4}$
	N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]
4.81	8.148
	N,N-Dimethylformamide; C_3H_7NO; [68-12-2]
5.00	6.738
	N-Methylformamide; C_2H_5NO; [123-39-7]
5.69	3.380
	Acetonitrile; C_2H_3N; [75-05-8]
5.10	6.097

[†] at a partial pressure of 1 atmosphere, calculated by compiler, assuming $x_{C_2H_4} = 1/H$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined by a volumetric method described as "the Ostwald method". No other details given.

SOURCE AND PURITY OF MATERIALS:

1. Linde Co. sample, purity 99.8 volume per cent.
2. Uvasol and analytical grade.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta H = \pm 1.25\%$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Pyrrolidinone, 1-methyl-, (N-methylpyrrolidinone); C_5H_9NO; [872-50-4]

ORIGINAL MEASUREMENTS:

Wu, Z.; Zeck, S.; Langhorst, R.; Knapp, H.

Proc. Int. Conf. Coal Gas and Air, Beijing, China, 1985, *1*, 209-229.

VARIABLES: T/K = 298.15

P/kPa = 100 (1 bar)

PREPARED BY:

W. Hayduk

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EXPERIMENTAL VALUES:

T/K	Henry's Constants K/Bar	Henry's Constants ^1H/atm(mole fraction)$^{-1}$	Ostwald Coefficient L/cm^3 gas(cm^3 solvent)$^{-1}$	^{2}Mole Fraction x_1
298.15	135.6	132.7	1.885	0.00753

[1] Calculated by compiler.

[2] Calculated by compiler for a gas partial pressure of 101.325 kPa.

Values personally received from the first author for the gas and liquid phase compositions corresponding to a pressure of 1 bar were respectively: y_1 = 0.999, and x_1 = 0.0074274 mole fraction.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Ethylene gas was stored in a glass burette equipped with an accurate manometer for measuring pressure and situated in a constant temperature air bath. A known quantity of completely degassed solvent was charged into an equilibrium cell immersed in a liquid bath. The volume of gas absorbed was measured after the gas was admitted into the cell. The solubility was determined from the quantities of gas and solvent used. The apparatus and procedure are described in detail in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity was 99.9 vol. percent.
2. Solvent was provided by Merck with a minimum purity of 99.0% (GC). After treatment with molecular sieve 4X, the water content was reduced to less than 0.01%. The purity was then analyzed to be 99.9%. Measured values: d^{25} = 1.02812, n_D^{25} = 1.4686

ESTIMATED ERROR:

δP/kPa = ± 0.05
δT/K = ± 0.01
$\delta L/L$ = ± 0.01

REFERENCES:

1. Zeck, S.

Doctoral Dissertation, Tech. Univ. Berlin, FRG, 1985.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 2-Pyrrolidinone, 1-methyl-, (N-methylpyrrolidinone); C_5H_9NO; [872-50-4]

ORIGINAL MEASUREMENTS:

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

Gaz. Prom. 1962, *7*, 11-17.

Same paper also in:

Khim. Prom. 1963,*10*, 91-97.

VARIABLES:

T/K = 273-288

P/kPa = 101.3 (1 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

		Henry's constant		
t/C	T/K	K mm Hg(mole fraction)$^{-1}$	^1H atm(mole fraction)$^{-1}$	^{1}Mole Fraction Ethene, x_1
0	273.15	74200	97.63	0.01024
5	278.15	81500	107.2	0.00933
10	283.15	88000	115.8	0.00864
15	288.15	96250	126.6	0.00790

[1] Calculated by compiler; x_1 is for a partial pressure of 101.325 kPa.

Experiments were performed at several pressures between 100 and 760 mm mercury and Henry's law was found to be obeyed.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Glass equilibrium cell fitted with a magnetic stirrer. Pressure measured with a Bourdon gauge. Samples of liquid analyzed by stripping out ethene. The solubilities were measured at several pressures below atmospheric and Henry's constant was determined. Details in ref. (1).

SOURCE AND PURITY OF MATERIALS:

Sources and purities of materials not given.

2. Properties of solvent as used by authors:

Normal boiling point = 479.15 K

Density at 20°C = 1.0220 g/cm^3

Refractive index, n_D^{20} = 1.4700

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

(Estimated by compiler)

REFERENCES:

1. Shenderei, E.R.; Zelvenskii, Ya.D.; Ivanovskii, F.P. *Gaz. Prom.* 1958, *12*, 36.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Choudhari, R.V.; Doraiswami, L.K.

J. Chem. Eng. Data 1972, *17*, 428-432.

VARIABLES:

T/K = 286.0-333.0

P/kPa = 94.23

PREPARED BY:

W. Hayduk

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EXPERIMENTAL VALUES:

T/K	Solubility at p =94.23 (0.93 atm) s/g(l)$^{-1}$	[1] Solubility at p = 101.325 kPa Mole Fraction, x_1	[1] Henry's Constant H/atm(mole fraction)$^{-1}$
286	1.97	0.00763	131.1
303	1.26	0.00496	201.6
313	0.99	0.00394	254.1
323	0.84	0.00337	296.7
333	0.76	0.00308	324.5

[1] Calculated by compiler; x_1 is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The glass absorption vessel was equipped with a stainless steel stirrer and a jacket through which constant temperature water was circulated. A volume of 400-500 cm^3 of solvent was charged into the vessel, thermal equilibrium was established and then gas was bubbled through the solvent. Samples were withdrawn at 10-15 min. intervals for analysis using a chemical analysis for the olefin content. When the concentrations remained constant, equilibrium was considered established. Precautions were taken to exclude water vapor from the air from entering the vessel. Experiments were performed at atmospheric pressure, 0.93 atm (at Poona, India). Reference 1 refers to the method of olefin analysis.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity 99.0%.
2. Nitrobenzene purity 99.0%.

The purities were tested by chromatography.

ESTIMATED ERROR:

T/K = ± 0.05

$\delta s/s$ = ± 2%

REFERENCES:

1. Thomas, C.L.; Block, H.S.; Hockstra, J. *Ind. Eng. Chem. Anal. Ed.* 1938, *10*, 153.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Cyclohexylamine, $C_6H_{13}N$; [108-91-8]	Keevil, T.A.; Taylor, D.R. Streitwieser, A. *J. Chem. Engng. Data.* 1978, *23*, 237-239.
VARIABLES:	PREPARED BY:
T/K = 298.1 p_1/kPa = 101.3	C.L. Young

EXPERIMENTAL VALUES:

Partial pressure of ethene = 1 atm = 101.3 kPa.

T/K	Mole fraction of ethane.
298.1	0.0105

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Volumetric apparatus of moderate accuracy. Solvent confined to glass bulb and known amount of gas added. Pressure measured using a mercury manometer together with a null point manometer in which the gas pressure was balanced by dry air. Details in source.

SOURCE AND PURITY OF MATERIALS:

1. No details given.
2. Degassed and dried over lithium cyclohexylamide.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta x_{C_2H_4} = \pm 1\%$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Methyl-2-pyrrolidinone,
   Nitrobenzene,
   Benzenamine (Aniline),
   Dimethylsulfoxide, or
   Hexamethylphosphoric triamide

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data

1971, *16*, 340-2.

VARIABLES:

$T/K = 298.15$

$P/kPa = 101.32$

PREPARED BY:

C. L. Young

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EXPERIMENTAL VALUES:

Henry's constant, H/atm	[1]Mole fraction ethene, x_1
1-Methyl-2-pyrrolidinone; C_5H_9NO; [872-50-4]	
126	0.00794
Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	
126	0.007947
Benzenamine (Aniline); C_6H_7N; [62-53-3]	
208	0.00481
Sulfinylbismethane (Dimethylsulfoxide); C_2H_6SO; [67-68-5]	
312	0.00321
Hexamethylphosphoric triamide; $C_6H_{18}NO_3P$; [680-31-9]	
52.9	0.0189

[1]Calculated by compiler for a partial pressure of 101.3 kPa assuming that the mole fraction ethene is equal to $1/H$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Benzonitrile,
   1,4-Dioxane,
   Nitrobenzene,
   Dimethylsulfoxide, or
   Hexamethylphosphoric triamide

ORIGINAL MEASUREMENTS:

Brückl, N.; Kim. J. I.

Z. Phys. Chem. (Wiesbaden)

1981, *126*, 133-150.

VARIABLES:

$T/K = 298.2$

$P/kPa = 101.3$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

H is Henry's constant/atm $\ln H$	[1]Mole fraction ethene, x_1 10^3x_1
Benzonitrile; C_7H_5N; [100-47-0]	
4.71	9.00
1,4-Dioxane; $C_4H_8O_2$; [123-91-1]	
4.70	9.10
Nitrobenzene; $C_6H_5NO_2$; [98-95-3]	
4.96	7.01
Sulfinylbismethane (Dimethylsulfoxide); C_2H_6OS; [67-68-5]	
5.75	3.182
Hexamethylphosphoric triamide; $C_6H_{18}NO_3P$; [680-31-9]	
4.14	15.92

[1] Calculated by compiler for a partial pressure of 101.3 kPa assuming that the mole fraction ethene is equal to $1/H$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined by a volumetric method described as "the Ostwald method". No other details given.

SOURCE AND PURITY OF MATERIALS:

1. Linde Co. sample, purity 99.8 volume per cent.
2. Uvasol or analytical grade. Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta H/\text{atm} = \pm 1.25\%$

(estimated by compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Ethyne (Acetylene); C_2H_2; [74-86-2]
3. *N,N*-Dimethylformamide (DMF) C_3H_7NO; [68-12-2]

ORIGINAL MEASUREMENTS:

Shenderei, E.R.

Khim. Prom. 1966, *42*, 514-516.

VARIABLES:

$T/K = 218.15$ (-55 °C)

$p_1/kPa = 13.3 - 101.33$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Concentration Ethyne, cm^3 (STP) (g DMF)$^{-1}$	Ethene Partial Pressure, p_1 mm Hg	[1]kPa	[2]Solubility, S cm^3 (STP)(g DMF)$^{-1}$	Solubility Coefficient $\beta = 760\ S/p_1$	[3]Mole Fraction Ethene, x_1
33.8	100	13.33	1.33	10.10	0.003937
	300	40.00	4.02	10.18	0.01181
	500	66.66	6.76	10.27	0.01968
	760	101.325	10.38	10.38	0.02992
101	100	13.33	1.60	12.16	0.003937
	300	40.00	4.85	12.29	0.01181
	500	66.66	8.15	12.39	0.01968
	760	101.325	12.51	12.51	0.02992
164	100	13.33	1.85	14.06	0.003937
	300	40.00	5.60	14.19	0.01181
	500	66.66	9.40	14.29	0.01986
	760	101.325	14.45	14.45	0.02992
249	100	13.33	2.17	16.49	0.003937
	300	40.00	6.57	16.64	0.01181
	500	66.6	11.05	16.80	0.01968
	760	101.325	16.99	16.99	0.02992

[1] Calculated by compiler.

[2] Volumetric solubility calculated on basis of cm^3 (STP) of ethene and ethyne/g DMF.

[3] Mole fraction calculated on basis of three components in solution.

Henry's law is obeyed for ethene in ethyne-DMF solutions.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method was described in reference 1 and 2. The apparatus consisted of a thick-walled glass absorption tube containing a magnet stirring bar for vertical motion, a pressure gauge, and a steel bulb for condensing the gas, connected by high pressure tubing. The gas handling system consisted of glass bulbs, a mercury manometer and a vacuum system. The volume of solvent was measured using a cathetometer and the quantity of gas by pressure differences. The low temperature was obtained using methanol in a temperature-controlled bath cooled with dry ice.

SOURCE AND PURITY OF MATERIALS:

Sources and purities not specified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$ (compiler)

REFERENCES:

1. Shenderei, E.R.; Zelvenski, Ya.D.; Ivanovskii, F.P. *Gaz. Prom.* 1958, *12*, 36.
2. Same authors, *Khim. Prom.* 1960 *5*, 370.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic compounds containing N, for pressures greater than 0.2 MPa (2 atm)	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 March, 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Organic Compounds Containing Nitrogen for Pressures greater than 0.20 MPa

Solubilities of ethene are available for only two organic solvents containing nitrogen at pressures above 0.20 MPa. These two solvents are N,N-dimethylformamide and 1-methyl-2-pyrrolidinone.

N,N-Dimethylformamide; C_3H_7NO; [68-12-2]

Ethene solubilities in N,N-dimethylformamide were reported for the temperatures 298.15 K, 323.15 K and 343.15 K and for pressures in the range of 0.79 MPa to 4.22 MPa by Shakhova et al. (1). The vapor pressure for this solvent is very low so that the total pressure was considered to be the gas partial pressure. The data which were found to be essentially consistent were used to develop an equation relating the mole fraction solubility to the gas partial pressure in MPa. It is noted that the pressure in bar ÷ 10 is equivalent to MPa.

$$\log x_p = 457.46(T/K)^{-1} + 0.9862 \log (p/\text{MPa}) - 2.7274 \qquad (1)$$

Only the last data point for a temperature of 343.15 K was omitted because it was obviously inconsistent. Otherwise, the data are well described by equation (1); the average, and maximum deviations from the equation are 1.4%, and 4.7%, respectively. It is further noted that extrapolation of equation (1) for a temperature of 298.15 K to a pressure of 0.1013 MPa yielded a solubility of 0.0067 mole fraction in good agreement with reliable solubilities measured at that pressure and also the value obtained using the Henry's law constant reported on the data sheet.

These data are classified as tentative.

1-Methyl-2-pyrrolidinone; C_5H_9NO; [872-50-4]

Ethene solubilities in 1-methyl-2-pyrrolidinone were also reported by Shakhova et al. (1) for the temperatures 298.15 K, 323.15 K and 343.15 K, and for a large range of pressures, from 0.375 MPa to 9.46 MPa. These data were found to be consistent; however, a curvature of the line representing the relation between log (x_p/mole fraction) and log(p/MPa) was observed. The following equation which contains a correction factor for the curvature was developed for all the data for this solvent:

$$\log (x_p) = 486.13\ (T/K)^{-1} + 0.9930 \log (p/\text{MPa}) - 0.012\ p - 2.755 \qquad (2)$$

The average, and maximum deviations of the values calculated using equation (2) from the data are 1.9%, and 6.5%, respectively. It is noted that equation (2) was extrapolated to a pressure of 0.1013 MPa for a temperature of 298.15 K to obtain a mole fraction solubility of 0.0077 which can be compared with the value based on the Henry's law constant recorded on the data sheet, of 0.0074 mole fraction ethene. Similarly, this extrapolated value compares very favourably with the actual experimental value as discussed in the preceding chapter of this volume. It is further noted that the vapor pressure of this solvent is also low, so that the total pressures on the data sheet were considered to be gas partial pressures in the development of equation (2).

These data are classified as tentative.

Reference

1. Shakhova, S.F.; Zubchenko, Yu, P.; Rezina, O.A. *Khim. Prom.* 1973, *40*, 271-2.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. N,N-Dimethylformamide; C_3H_7NO; [68-12-2]

ORIGINAL MEASUREMENTS:

Shakhova, S. F.; Zubchenko, Yu. P.; Rezina, O. A.

Khim. Prom. 1973, *49*, 271-2.

VARIABLES:

T/K = 298.15 - 343.15

P/MPa = 0.79 - 4.21

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	$\alpha^{\dagger}$ vol/vol	T/K	P/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	$\alpha^{\dagger}$ vol/vol
298.15	7.90	0.0512	15.7	323.5	27.16	0.1309	43.8
	10.23	0.0680	21.2		33.84	0.1608	55.7
	12.26	0.0792	25.0	343.15	12.26	0.0487	14.9
	16.11	0.1030	33.4		17.63	0.0706	22.1
	18.64	0.1220	40.4		22.90	0.0910	29.1
	19.76	0.1275	42.5		28.98	0.1207	39.9
323.15	8.00	0.0390	11.8		31.51	0.1239	41.1
	14.08	0.0674	21.0		36.17	0.1407	47.6
	15.50	0.0754	23.7		41.85	0.1610	55.8
	21.28	0.1030	33.4		42.15	0.1804	64.0

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† 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. Samples of liquid analysed by a volumetric method. Details in ref. (1).

Henry's constants were listed as follows:

t/C	H/atm mole fraction^{-1}
25	150
50	183
70	221

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.97 mole per cent.
2. Distilled, no other details given.

ESTIMATED ERROR:

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

$\delta x_{C_2H_4} = \pm 5\%$.

REFERENCES:

1. Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. *Khim. Prom.* 1973, *5*, 108.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. 1-Methyl-2-pyrrolidinone, (N-methylpyrrolidinone); C_5H_9NO; [872-50-4]

ORIGINAL MEASUREMENTS:

Shakhova, S. F.; Zubchenko, Yu. P.; Rezina, O. A.

Khim. Prom. 1973, *49*, 271-2.

VARIABLES:

$T/K = 298.15 - 343.15$

$P/MPa = 0.37 - 9.46$

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

T/K	P/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	$\alpha^\dagger$ vol/vol	T/K	P/bar	Mole fraction of ethene in liquid, $x_{C_2H_4}$	$\alpha^\dagger$ vol/vol
298.15	3.75	0.0274	6.52	323.15	18.14	0.0970	24.9
	5.78	0.0407	9.83		24.01	0.1249	33.1
	6.38	0.0473	11.5		25.53	0.1331	35.6
	8.00	0.0596	14.7		27.46	0.1506	41.1
	10.54	0.0765	19.2		38.81	0.1962	56.6
	14.89	0.1074	27.9		50.36	0.2427	74.3
	18.64	0.1383	37.2		51.98	0.2462	75.7
	25.53	0.1748	49.1		73.06	0.3103	104.3
	47.32	0.2933	96.2		83.39	0.3649	133.2
	56.44	0.3546	127.4	343.15	5.78	0.0262	6.24
	63.94	0.3919	149.4		8.71	0.0396	9.57
	64.75	0.4115	162.1		13.37	0.0581	14.3
323.15	3.85	0.0214	5.08		30.40	0.1302	34.7
	6.08	0.0342	8.21		53.80	0.2067	60.4
	6.79	0.0381	9.18		86.84	0.3190	108.6
	10.94	0.0596	14.7		94.64	0.3390	118.9

† 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. Samples of liquid analysed by a volumetric method. Details in ref. (1).

Henry's constants were listed as follows:

t/C	H/atm mole fraction^{-1}
25	135
50	174
70	208

SOURCE AND PURITY OF MATERIALS:

1. Purity 99.97 mole per cent.
2. Distilled, no other details given.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P/bar = \pm 0.1$;

$\delta x_{C_2H_4} = \pm 5\%$ (estimated by compiler)

REFERENCES:

1. Shakhova, S. F.; Zubchenko, Yu. P.; Kaplan, L. K. *Khim. Prom.* 1973, *5*, 108.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic solvents containing sulfur or phosphorus for pressures less than 0.2 MPa	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 March, 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Organic Solvents Containing Sulfur or Phosphorus for pressures less than 0.20 MPa

Seven research groups reported solubilities of ethene in organic sulfur or organic phosphorus compounds usually expressed as the Henry's constants. Particularly the data of Lenoir et al. (1) were obtained using a chromatographic method at low gas partial pressures, leading to possible errors when the results were extrapolated to 0.1013 MPa pressure. For only four of the eleven solvents were the results reported for three or more temperatures. Thus, for most of the solvents the effect of temperature on the solubility could not be determined from the results available. The sulfur and phosphorus-containing solvents were mainly the organic esters of either sulfuric or phosphoric acids. The ethene solubilities in the high boiling phosphoric acid esters were of particular interest because five of these solvents belonged to a homologous series. Thus the effect of solvent molecular weight could be qualitatively observed.

There is a data sheet describing the solubility of ethene in triphenylphosphine at pressures up to 0.595 MPa which, strictly speaking, should have appeared in a chapter all of its own.

The solubilities in individual solvents will now be considered.

Carbon disulfide; CS_2; [75-15-0]

The solubility of ethene in carbon disulfide was reported by Sahgal et al. (2) for 298.15 K and a partial pressure of 0.1013 MPa. No comparable data are available in the literature.

This result is classified as tentative.

Sulfinylbismethane (dimethyl sulfoxide); C_2H_6SO; [67-68-5]

The solubility of ethene in sulfinylbismethane at 298.15 K and for a gas partial pressure of 101.3 kPa was reported by Brückl and Kim (3) and also by Lenoir et al. (1). The two solubilities differ by less than 1%.

These values are classified as tentative.

Sulfuric acid, diethyl ester (diethyl sulfate); $C_4H_{10}O_4S$; [64-67-5]

Ethene solubilities in sulfuric acid, diethyl ester were reported for temperatures ranging from 273.15 K to 353.15 K and for a gas partial pressure of 101.3 kPa by Truchard et al. (4). These data are entirely consistent and are well represented by the following equation:

$$\log x_1 = 479.73\ (T/K)^{-1} - 3.5998 \qquad (1)$$

Equation (1) is simpler than that of the authors, and it represents the data with an average deviation of 0.7% and a maximum deviation of 1.5% for the whole temperature range.

The results of Truchard et al. (4) are classified as tentative.

Amidosulfurous acid, diethylmethyl ester (N,N-dimethylsulfonamide, methyl ester); $C_5H_{13}NO_2S$; [21954-69-8]

Ethene solubilities of Makitra et al. (5) in the sulfonamide solvent for pressures below atmospheric are available for temperatures ranging from 253.15 K to 333.15 K. Unfortunately these data appear to be quite inconsistent. Henry's law is not even approximately obeyed; for each

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic solvents containing sulfur or phosphorus for pressures less than 0.2 MPa	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 March, 1994

CRITICAL EVALUATION:

temperature the solubility results cannot be extrapolated to zero solubility corresponding to a zero partial pressure of gas. At pressures below atmospheric it would be expected that Henry's law would be obeyed. Furthermore, there is a large degree of scattering of the data. Also, the solubilities at any one pressure (at 725 mm of mercury pressure for example) do not follow a regular function of temperature.

As a result, it is considered that these solubilities are of qualitative value only.

Phosphoric acid, trimethyl ester; $C_3H_9O_4P$; [512-56-1]
Phosphoric acid, triethyl ester; $C_6H_{15}O_4P$; [78-40-0]
Phosphoric acid, tripropyl ester; $C_9H_{21}O_4P$; [513-08-06]
Phosphoric acid, tributyl ester; $C_{12}H_{27}O_4P$; [126-73-8]
Phosphoric acid, tri (2-methylpropyl) ester; $C_{12}H_{27}O_4P$; [126-71-6]

Solubilities of ethene in five esters of phosphoric acid were reported by Lenoir et al. (1) for a temperature of 325.2 K (and for three temperatures for the tripropyl ester) as Henry's law constants. There is some doubt that these Henry's constants, by a chromatographic technique at low partial pressures of gas, are representative of the true value at 0.1013 MPa pressure. However, a check on the value obtained by Lenoir et al. for the tributyl ester is available from the results of Kosyakov et al. (6) for that solvent. The latter researchers reported results for temperatures ranging from 223.15 K to 313.15 K from which they determined Henry's constants. The results of both research groups appear consistent with one another, and were used to develop an equation for the temperature effect of solubility at a pressure of 0.1013 MPa for phosphoric acid, tributyl ester as follows:

$$\log x_1 = 568.32\ (T/\mathrm{K})^{-1} - 3.4716 \qquad (2)$$

The average, and maximum deviation of the data from equation (2) for this solvent is 0.5%, and 1.2%, respectively. Equation (2) was developed for a temperature range from 223.15 K to 325.15 K and extrapolation beyond this temperature range is not recommended.

As part of the consistency check, Figure 1 was constructed to indicate the effect on the solubilities of ethene of the solvent molecular weight for the phosphoric acid esters for the constant temperature of 325.2 K. Figure 1 indicates that there is a consistent increase in ethene solubility at a temperature of 325.2 K as the molecular weight of the phosphoric acid ester is increased. Thus, Figure 1 may have some value in extending solubility data to the many different esters of phosphoric acid.

The data of Lenoir et al. (1) and of Kosyakov et al. (6) are classified as tentative.

Hexamethylphosphoric triamide; $C_6H_{18}N_3OP$; [680-31-9]

Two sources for the ethene solubility in hexamethylphosphoric acid triamide for a temperature of 298.2 K are available: Brückl and Kim (3), and Lenoir et al. (1), with values of 0.0159 mole fraction ethene, and 0.0189 mole fraction, respectively. The difference between these two comparable results of 19% is clearly beyond any normal experimental error. Given the low pressure chromatographic method used by Lenoir et al. (1), their value is rejected, and the value of Brückl and Kim (3) is classified as tentative.

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Organic solvents containing sulfur or phosphorus for pressures less than 0.2 MPa	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 March, 1994

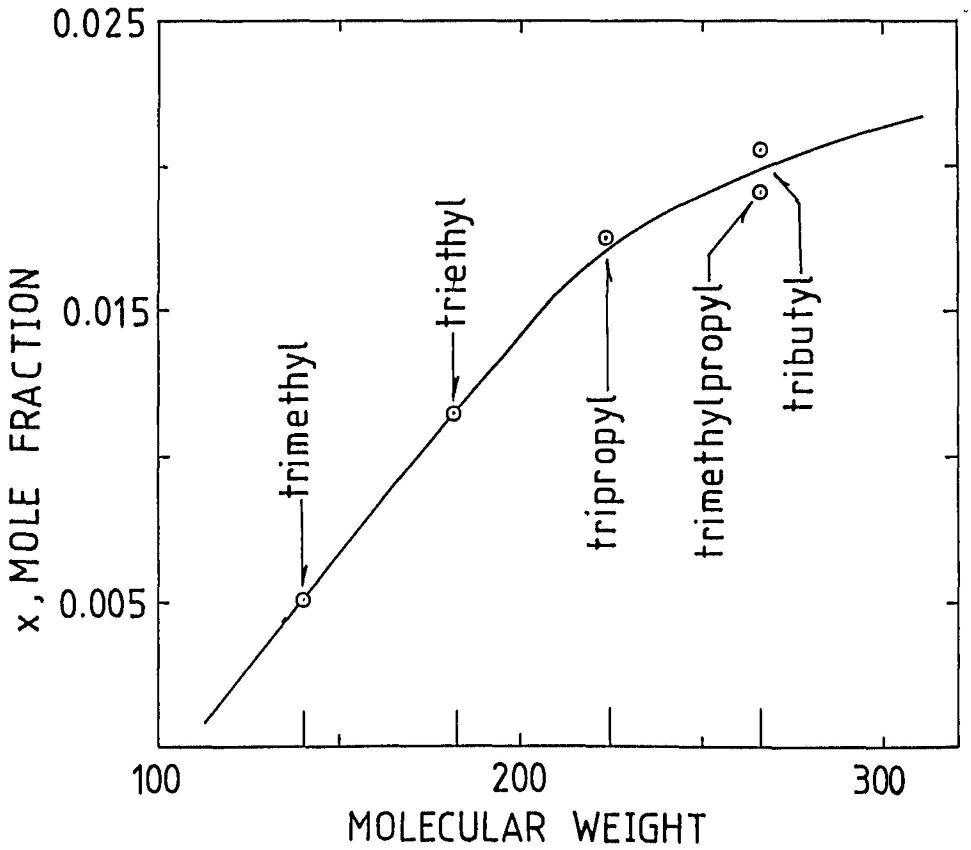
CRITICAL EVALUATION:

Triphenylphosphine; $C_{18}H_{15}P$; [603-35-0]

Ethene solubilities at the three temperatures, 363.2 K, 378.2 K, and 393.2 K, for the three pressures, 0.491 MPa, 0.546 MPa and 0.595 MPa, respectively, were reported by Herman et al. (7). There are insufficient data to check for consistency. A linear extrapolation to a pressure of 0.1013 MPa results in mole fraction solubilities of 0.0060 at 363.2 K, 0.0054 at 378.2 K and 0.0049 at 393.2 K. The extrapolated results must be considered approximate only.

The original data are classified as tentative.

Figure 1 Solubility of ethene at 325.2 K and 0.1013 MPa in esters of phosphoric acid as a function of solvent molecular weight



References

1. Lenoir, J.-Y.; Renault, P.; Renon, H. *J. Chem. Eng. Data*, 1971, *16*, 340-342.
2. Sahgal, A; La, H.M.; Hayduk, W. *Can. J. Chem. Eng.* 1978, *56*, 354-357.
3. Brückl, N.; and Kim, J.I. *Z. Phys. Chem. (Wiesbaden)*, 1981, *126*, 133-150.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Organic solvents containing sulfur or phosphorus for pressures less than 0.2 MPa

EVALUATOR:

Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, ON
Canada K1N 6N5

March, 1994

CRITICAL EVALUATION:

4. Truchard, A.M.; Harris, H.G.; Himmelblau, D.M. *J. Phys. Chem.* 1961, *65*, 575-576.

5. Makitra, R.G.; Moin, F.B.; Politanskaya, T.I. Yas'kovyak, A. *Zh. Fiz. Khim.* 1975, *49*, 2723-2724; *VINITI No.* 1877-75.

6. Kosyakov, N.E.; Yushko, V.L.; Sergienko, I.D.; Khokhlov, C.F.; Taraba, P.F. *Khim Prom.* 1972, *48*, 432-433.

7. Herman, J.M.; Gerritson, L.A.; de Loos, T.W. *J. Chem. Eng. Data,* 1981, *26*, 185-187.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Sahgal, A.; La, H.M.; Hayduk, W.

Can. J. Chem. Eng. 1978, *56*, 354-357.

VARIABLES: T/K = 298.15

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

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		Mole Fraction	Ostwald Coefficient
t/C	T/K	Ethene, x_1	L/ cm^3 gas $(cm^3 \text{ solvent})^{-1}$
25.2	298.15	0.00646	2.61

Mole fraction ethene, x_1, is for a gas partial pressure of 101.325 kPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass apparatus equipped with a gas storage burette, a spiral tube for gas absorption, a miniature internal manometer and a solution storage burette was used. Degassed solvent was injected at a constant rate into the absorption spiral by means of a syringe-pump while the gas was displaced by mercury using a mechanical elevating device for a mercury bottle, at a rate required to keep the gas pressure constant. Readings of the volume of vapor-free gas consumed and volume of solvent required to achieve saturation were obtained from which the solubility was calculated. Constant temperature fluid was circulated through a jacket enclosing the burettes and absorption spiral.

SOURCE AND PURITY OF MATERIALS:

1. Ethene was CP grade from Matheson, 99.5 mole % minimum purity.
2. Carbon disulfide was of the chromatography grade from Matheson Coleman and Bell, minimum purity 99.0 mole %.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$

$\delta T/K = \pm 0.05$

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4 ; [74-85-1]
2. Sulfuric acid, diethyl ester (diethyl sulfate); $C_4H_{10}O_4S$; [64-67-5]

ORIGINAL MEASUREMENTS:

Truchard, A.M.; Harris, H.G.;

Himmelblau, D.M.

J. Phys. Chem. 1961, *65* , 575-576.

VARIABLES: T/K = 273-353

P/kPa = 101.325

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	Henry's Constant H/atm (mole fraction)$^{-1}$	¹Mole Fraction Ethene, x_1	²Partial Molal Heat of Solution $-\Delta H$/cal (mole)$^{-1}$
0	273.15	68.71	0.01455	2430
20	293.15	92.24	0.01084	2300
25	298.15	98.73	0.01013	2270
30	303.15	105.1	0.00951	2240
40	313.15	117.3	0.00853	2180
60	333.15	144.2	0.00693	2080
80	353.15	172.8	0.00579	1995

Calculated by compiler; mole fraction ethene, x_1, is for a partial pressure of 101.325 kPa.

Partial molal heat of solution tabulated by authors and based on equation:

$$\Delta H = 2.303\ [\,\partial \log H/\partial\ (1/T)]$$

Temperature coefficient of H expressed by:

$$\log H = 3.04666 - 0.132845\ (10^3)(1/T) - 5.39706(10^4)\ (1/T)^2\ ;\ T/\text{K}$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two calibrated glass spheres, one larger than the other, immersed in a bath connected to a mercury manometer were used. Approximately 200 cm^3 of solvent was placed in the larger sphere and both were thoroughly evacuated. A supply of ethene was charged to the smaller flask to 2 atm pressure. Ethene was admitted to the flask containing the solvent and allowed to reach equilibrium by stirring. The pressures were read and material balances made to determine the solubility. Solubilities were measured for equilibrium pressures between 50 and 1300 mm of mercury pressure and Henry's law was found to apply in all cases.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not given.
2. Diethyl sulfate was Eastman practical grade purified by washing with Na_2CO_3 solution and drying with $CaCl_2$.

ESTIMATED ERROR:

$\delta H/H$ = ± 0.02

δT/K = ± 0.05

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Amidosulfurous acid, diethyl-, methyl ester, (N-N diethyl sulfonamide, methylester); $C_5H_{13}NO_2S$; [21954-69-8]

ORIGINAL MEASUREMENTS:

Makitra, R.G.; Moin, F.B.;

Politanskaya, T.I.; Yas'kovyak, A. *Zh. Fiz. Khim.* 1975, *49*, 2723-2724;

VINITI No. 1877-75.

VARIABLES:

T/K = 253.15 - 338.15

p_1/kPa = 13.3 - 96.7

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Temperature t/°C		-20	0	20	35	50	65
T/K		253.15	273.15	293.15	308.15	323.15	338.15
Partial Pressure, p mm Hg,	kPa						
100	13.3	5	4	2	2	1	-
200	26.7	7	6	5	4	3	1
300	40.4	10	8	6	6	5	2
400	53.3	12	11	7	7	6	3
500	66.7	15	13	8	8	7	4
600	80.0	20	17	10	8	8	6
725	96.7	25	19	12	11	10	7
[1]760	101.3	19.4	18.9	13.0	11.9	10.7	8.1
[2]760	101.3	25.97	20.5	12.7	12.2	10.3	5.7

The solubility is expressed as $10^4 x_1$ where x_1 is the mole fraction.

[1] The solubility at 101.3 kPa was calculated by the compiler from Henry's constants given in the paper.

[2] Solubility at 101.3 kPa as calculated by the compiler from H values listed below.

The data were obtained from the paper deposited in VINITI, Moscow.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method of measurement was not specified.
It is stated in the paper that Henry's law is obeyed. A check of the data shows that Henry's law is only very approximately obeyed.
Henry's constants, H in mm Hg/ mole fraction, as determined by the authors and as calculated by the compiler are as follows:

t/°C	(authors) $10^{-2}H$	(compiler) $10^{-2}H$
-20	3920	2927
0	4025	3714
20	5830	6000
35	6380	6222
50	7090	7407
65	9350	13,333

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity by gas chromatography was 99.5%.
2. The solvent was washed and boiling temperature was measured at 4 mm mercury pressure as 115°C. Actual purity not determined.

ESTIMATED ERROR:

$\delta x_1/x_1$ = 0.1 or 10% (Compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]

2 Esters of phosphoric acid

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

T/K = 298.2 - 343.2

P/kPa = 101.3

PREPARED BY:

C. L. Young

EXPERIMENTAL VALUES:

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T/K	Henry's constant $H_{C_2H_4}$/atm	Mole fraction at 1 atm* $x_{C_2H_4}$
Phosphoric acid, trimethyl ester; $C_3H_9O_4P$; [512-56-1]		
325.2	199	0.00503
Phosphoric acid, triethyl ester; $C_6H_{15}O_4P$; [78-40-0]		
325.2	87.0	0.0115
Phosphoric acid, tripropyl ester; $C_9H_{21}O_4P$; [513-08-6]		
298.2	41.1	0.0243
323.2	57.3	0.0175
343.2	71.1	0.0141
Phosphoric acid, tributyl ester; $C_{12}H_{27}O_4P$; [126-73-8]		
325.2	52.5	0.0190
Phosphoric acid, tri(2-methylpropyl) ester; $C_{12}H_{27}O_4P$; [126-71-6]		
325.2	48.7	0.0205

* Calculated by compiler assuming a linear function of $H_{C_2H_4}$ vs $x_{C_2H_4}$, i.e., $x_{C_2H_4}$(1 atm) = $1/H_{C_2H_4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A conventional gas-liquid chromatographic unit fitted with a thermal conductivity detector was used. The carrier gas was helium. The value of Henry's law constant was calculated from the retention time. The value applies to very low partial pressures of gas and there may be a substantial difference from that measured at 1 atm. pressure. There is also considerable uncertainty in the value of Henry's constant since surface adsorption was not allowed for although its possible existence was noted.

SOURCE AND PURITY OF MATERIALS:

(1) L'Air Liquide sample, minimum purity 99.9 mole per cent.

(2) Touzart and Matignon or Serlabo sample, purity 99 mole per cent.

ESTIMATED ERROR:

δT/K = ± 0.1; δH/atm = $\pm 6\%$ (estimated by compiler).

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Phosphoric acid, tributyl ester (tributyl phosphate); $C_{12}H_{27}O_4P$; [126-73-8]

ORIGINAL MEASUREMENTS:

Kosyakov, N.E.; Yushko, V.L.;
Sergienko, I.D.; Khokhlov, C.F.;
Taraba, P.F.

Khim. Prom. 1972, *48* , 432-433.

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VARIABLES:

T/K = 223-313

P/kPa = 101.3 (1 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	[1]T/K	[2] Henry's Constant H/atm (mole fraction)$^{-1}$	[2] Mole Fraction Ethene, x_1
40	313.15	45.2	0.0221
20	293.15	34.1	0.0293
0	273.15	24.9	0.0401
-20	253.15	16.9	0.0593
-40	233.15	10.9	0.0921
-50	223.15	8.33	0.120

[1] Calculated by compiler.

[2] Only graphical data given in paper; mole fraction solubility, x_1, read from enlarged graph corresponding to a gas partial pressure of 101.325 kPa.

Data measured at several pressures between 100 and 760 mm mercury pressure shows that Henry's law is obeyed.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A static method was used. Details are given in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene minimum purity 99.0 mole %.
2. Purity and source unspecified.

ESTIMATED ERROR:

$\delta x_1/x_1 = \pm 2\%$ (Original data)
$\delta x_1/x_1 = \pm 4\%$ (As read from graph by compiler)

REFERENCES:

1. Braude, G.E.; Shakhova, C.F. *Khim. Prom.* 1961, *3*, 177.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Triphenylphosphine; $C_{18}H_{15}P$; [603-35-0]

ORIGINAL MEASUREMENTS:

Herman, J.M.; Gerritson, L.A. de Loos, T.W.

J. Chem. Eng. Data, 1981, *26*, 185-187.

VARIABLES:

$T/K = 363.2 - 393.2$

$P/MPa = 0.491 - 0.595$

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K	P/MPa	Mole fraction of ethene in liquid, $x_{C_2H_4}$
363.2	0.491	0.029
378.2	0.546	0.029
393.2	0.595	0.029

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Cailletet tube with sample of known composition confined over mercury. Pressure on the sample was increased by small increments until bubble point reached. Equilibrium established at each step. Sample stirred with magnetically operated device. Pressure measured using Bourdon gauge.

SOURCE AND PURITY OF MATERIALS:

1. Phillips sample, purity 99.98 mole per cent.
2. Fluka sample, purity 99.5 wt per cent.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta P/MPa = \pm 0.001$

$\delta x_{C_2H_4}$; $= \pm 5\%$.

REFERENCES:

COMPONENTS:	EVALUATOR:
1. Ethene; C_2H_4; [74-85-1] 2. Biological fluids, a natural oil and a petroleum fraction for pressures less than 0.1013 MPa	Walter Hayduk Department of Chemical Engineering University of Ottawa Ottawa, ON Canada K1N 6N5 March, 1994

CRITICAL EVALUATION:

Critical Evaluation of Ethene Solubilities in Biological Fluids, Olive Oil and Petroleum for Pressures less than 0.1013 MPa

The solubility for a temperature of 298.15 K of ethene for a range of pressures below atmospheric was reported for components of dog blood including water, hemoglobin solution, blood plasma as well as in whole blood by Grollman (1). The solubilities were reported as the Bunsen and Ostwald coefficients. It can be concluded that Henry's law is obeyed for water and approximately obeyed for the other three solvents. It is also apparent that the ethene solubility is lowest in the hemoglobin solution and increases in water, in blood plasma and finally reaches the highest value in whole blood for constant gas pressures. Further, the solubilities in whole blood of three different species were compared at 310.65 K; lowest values were obtained for human blood, higher values in rabbit blood and highest values in dog blood. These results may be of qualitative value only because the results for water are too low when compared with modern values. Please see the chapter for solubilities in water in this volume.

Orcutt and Waters (2) reported ethene solubilities at 298.15 K in human blood and in aqueous solutions containing increasing quantities of chemical reagents. These reagents were acid ferricyanide, caustic and alkaline hydrosulfite reagent added sequentially, with the ethene solubility determined after each addition. The solubility decreased with each addition of the chemical solutions. It is of interest that the extrapolated value for the ethene solubility in human blood at 298.15 K expressed as the Ostwald coefficient is 0.143 cm^3 ethene/cm^3 of blood and is nearly identical to the value obtained by the previous researcher of 0.142 cm^3 ethene/cm^3 blood except in the latter case it is for dog blood. This contradicts the findings of Grollman at 310.65 K.

The solubilities of Orcutt and Waters are classified as tentative.

The single value for the solubility of ethene in olive oil at 310.2 K of Saidman et al. (3) is classified as tentative.

The solubilities of ethene in a petroleum fraction at two temperatures were reported both as the Bunsen and Ostwald coefficients by Gniewosz and Walfisz (4). Without further specifications as to properties and analysis of the petroleum fraction, this data is of little use.

References

1. Grollman, A. *J. Biol. Chem.* 1929, *82*, 317-325.

2. Orcutt, F.S.; Waters, R.M. *J. Biol. Chem.* 1937, *117*, 509-515.

3. Saidman, L.J.; Eger, E.I.; Munson, E.S.; Severinghaus, J.W. *Anesth.* 1966, *27*, 180-184.

4. Gniewosz, S.; Walfisz, A. *Z. Phys. Chem.* 1887, *1*, 70-72.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Water; H_2O; [7732-18-5]
   Dog blood, dog plasma, and
   dog hemoglobin.

ORIGINAL MEASUREMENTS:

Grollman, A.

J. Biol. Chem. 1929, *82*,

317-325.

VARIABLES: $T/\mathrm{K} = 298.15$ (25.0°C)

$p_1/\mathrm{kPa} = 73.3\text{-}133.3$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Ethene Partial Pressure p_1/mm mercury	$^1p_1$/kPa	Ostwald Coefficient, L/cm^3(gas) cm^{-3}(solvent) Water	[2]Plasma	[3]Hemoglobin	Whole Blood
550	73.33	0.112	0.114	0.104	0.141
600	79.99	0.113	0.114	0.104	0.141
650	86.66	0.113	0.114	0.105	0.141
700	93.33	0.112	0.115	0.106	0.142
750	99.99	0.113	0.115	0.105	0.142
800	106.7	0.113	0.115	0.106	0.141
850	113.3	0.113	0.116	0.106	0.143
900	112.0	0.114	0.115	0.106	0.142
950	126.7	0.113	0.116	0.107	0.143
1000	133.3	0.113	0.117	0.107	0.144
Average L	--	0.1129	0.1151	0.1056	0.1420

[1] Calculated by compiler.

[2] Plasma was obtained by centrifugation of the dog blood.

[3] The hemoglobin solution contained 8.5 g purified hemoglobin in 100 cm^3 of solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A glass bubbling-type of saturator immersed in a constant temperature bath was used. A known volume of saturated solution was transferred over mercury into a Van Slyke desorption apparatus. Gas removed in three evacuations was transferred to a sample tube where the volume was determined and a sample of the gas was analyzed. Solubilities were determined at several pressures below atmospheric and above atmospheric and expressed as Ostwald coefficients.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity was not given.
2. Heparin was used as a blood anticoagulant.

ESTIMATED ERROR:

$\delta T/\mathrm{K} = \pm 0.05$

$\delta L/L = \pm 4\%$
(compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Ethene; C_2H_4; [74-85-1] 2. Water; H_2O; [7732-18-5] Human blood, dog blood, rabbit blood, and aqueous lipoidal suspensions of dog blood.	Grollman, A. *J. Biol. Chem.* 1929, *82*, 317-325.
VARIABLES: $T/K = 310.65$ (37.5°C) $P/kPa = 101.325$	PREPARED BY: W. Hayduk

EXPERIMENTAL VALUES:

Solvent	Bunsen Coefficient β/cm^3(gas) NTP cm^{-3}(solvent)	[1]Ostwald coefficient L/cm^3(gas)cm^{-3}(solvent)	[2] Solubility, s/cm^3 gas (g water)$^{-1}$
Water, distilled	0.078	0.089	0.0785
Lipoidal suspension of dog blood	0.120	0.136	--
Human blood	0.123	0.140	0.156
Dog blood	0.141	0.160	0.167
Rabbit blood	0.128	0.146	0.148

[1] Calculated by compiler.

[2] Water content of blood samples was determined by drying overnight at 110°C and determining loss in weight.

[3] Blood lipoids were extracted from blood corpuscles with ethyl ether and petroleum ether.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A glass bubbling-type of saturator immersed in a constant temperature bath was used. The gas was presaturated with water vapor. A known volume of saturated solution was transferred over mercury into a Van Slyke desorption apparatus. Gas removed in three evacuations was transferred to a sample tube where the volume was determined and a sample of the gas was analyzed. The solubilities were expressed as the Bunsen coefficients.	1. Ethene source and purity not given. 2. Heparin was used as a blood anticoagulant in all cases.
	ESTIMATED ERROR: $\delta\beta/\beta = \pm 0.04$ (compiler) $\delta T/K = \pm 0.05$
	REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Human blood.
3. Various aqueous solutions.

ORIGINAL MEASUREMENTS:

Orcutt, F.S.; Waters, R.M.

J. Biol. Chem. 1937, *117*, 509-515.

VARIABLES: $T/K = 298.15$

$P/kPa = 101.325$

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

Solution, defined below	Ostwald coefficient L/ cm^3(gas) cm^{-3}(solvent solution)
I	0.118
II	0.110
III	0.093

I: Solution I contains 1 cm^3 blood added to 2.5 cm^3 aqueous acid ferricyanide reagent, total 3.5 cm^3.

II: Solution II contains Solution I to which is added 1 cm^3 1 N caustic, total 4.5 cm^3.

III: Solution III contains Solution II to which is added 1 cm^3 alkaline hydrosulfite reagent, total 5.5 cm^3.

The value of the Ostwald coefficient in dilute aqueous salt solutions containing blood exceeds that in water suggesting that the Ostwald coefficient in blood is greater than that in water, $L = 0.108$ cm^3 gas/cm^3 water. The Ostwald coefficient was estimated by the compiler for "pure" blood using reference 1 and was found to be $L = 0.143$ cm^3 ethene/cm^3 blood.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The Van Slyke-Neill manometric method which is based on the desorption of gases from blood in a partial vacuum was used. A small volume of solvent is saturated with gas by alternately bubbling the gas through the solvent and shaking the saturator at constant temperature and atmospheric pressure. A small, carefully measured volume of saturated solution is drawn into a 50 cm^3 burette by lowering the mercury level in it. A partial vacuum is produced releasing most of the gas. The pressure, volume and temperature are measured. Corrections are made for the solvent vapor pressure (assumed to be as for water) and for the residual gas solubility in the solvent at the low pressure. Details in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene source and purity not specified.
2. Human, blood, not otherwise specified.
3. Aqueous solutions as given above, not otherwise specified.

ESTIMATED ERROR:

$\delta L/L = \pm 0.10$
(compiler)

REFERENCES:

1. Orcutt, F.S.; Seevers, M.H. *J. Biol. Chem.* 1937, *117*, 501.

COMPONENTS:

1. Ethene, (Ethylene); C_2H_4; [74-85-1]
2. Olive oil.

ORIGINAL MEASUREMENTS:

Saidman, L.J.; Eger, E.I.; Munson, E.S.; Severinghaus, J.W.

Anesthesiology, 1966, *27*, 180-184.

VARIABLES:

$T/\text{K} = 310.2$

PREPARED BY:

C.L. Young.

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EXPERIMENTAL VALUES:

$t/°\text{C}$	T/K	No of Samples	Ostwald coefficient Mean	Ostwald coefficient Standard deviation
37	310.2	6	1.260	0.028

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Modified Scholander apparatus used. Known amount of water equilibrated with a known volume of gas and change in volume used to estimated Ostwald coefficient. Details of apparatus in source and ref. (1).

SOURCE AND PURITY OF MATERIALS:

1. No details given.
2. Degassed.

ESTIMATED ERROR:

$\delta T/\text{K} = \pm 0.1$. (estimated by compiler)

REFERENCES:

1. Douglas, E. *J. Phys. Chem.* 1964, *68*, 169.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Petroleum.

ORIGINAL MEASUREMENTS:

Gniewosz, S.; Walfisz, A.

Z. Phys. Chem. 1887, *1*, 70 - 72.

VARIABLES:

T/K = 283.15, 293.15
p/kPa = 101 ("atmospheric")

PREPARED BY:

M. E. Derrick
H. L. Clever

EXPERIMENTAL VALUES:

Temperature			
$t/^\circ C$	T/K	Bunsen Coefficient $\alpha/cm^3(STP)cm^{-3}atm^{-1}$	Ostwald Coefficient $L/cm^3\ cm^{-3}$
10	283.15	0.165	
		0.162	
		0.166	
		0.164 Av.	0.170
20	293.15	0.144	
		0.141	
		0.142	
		0.142 Av.	0.152

The Ostwald coefficients were calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of an absorption flask connected to a gas buret by a flexible lead capillary. The system was thermostated in a large water bath.

The volume of gas absorbed in a known volume of degassed petroleum was measured direcly using the gas buret.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. No information.

(2) Petroleum. Russian petroleum. Cleaned by boiling in a large copper flask.

ESTIMATED ERROR:

$\delta\alpha/\alpha = \pm 0.05$ (compiler)

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Hydrocarbon fuels, crude oils and waxes for pressures greater than 0.20 MPa

EVALUATOR:

Walter Hayduk
Department of Chemical Engineering
University of Ottawa
Ottawa, ON
Canada K1N 6N5

March, 1994

CRITICAL EVALUATION:

Critical Evaluation for Ethene Solubilities in Hydrocarbon Fuels, Russian Crude Oils and Waxes for pressures greater than 0.20 MPa

Solubilities of ethene in gasoline and kerosenes were reported by Hannaert et al. (1) for temperatures ranging from 233.15 K to 293.15 K expressed as an exponential function of the equilibrium ratio $K = y_1/x_1$ in which y_1, and x_1 are mole fractions in the gas, and liquid phase, respectively. It was possible to calculate mole fractions because the boiling fractions and densities of these hydrocarbons were measured and were associated with certain average molecular weights. In consequence, the results must be of lower accuracy because the true composition was actually unknown. The authors claimed accuracies ranging from 2% to 15%.

Hannaert et al. (1) also reported solubilities of ethene in two types of Carbowax for a range of temperatures from 273.15 K to 353.15 K. As for gasoline and kerosenes, a similar exponential function was used to express the solubility results. Here also, the molecular weights of the Carbowax had been previously determined so that mole fraction solubilities could be determined.

Both results of Hannaert et al. (1) are classified as tentative.

Chou and Chao (2) reported solubilities of ethene in Fischer-Tropsch SASOL wax for pressures ranging from 1.016 MPa to 5.163 MPa and for temperatures 473.2 K and 533.1 K. The results are consistent and obey Henry's law.

These data are classified as tentative.

Safronova and Zhuze (3,4) reported ethene solubilities in three Russian crude oils for three temperatures, 293 K, 323 K and 373 K for pressures to 20 MPa, in the form of modified Bunsen coefficients. In the first paper, published in 1958, some numerical results were reported and in the second paper, published in 1962, only graphical results were reported, for the same crude oils. Densities, viscosities and some analyses of the oils were also given. Even for identical conditions deviations between results were up to 9% from the two sources. Thus, the accuracy is probably of this order.

These data are classified as tentative.

References

1. Hannaert, H.; Haccuria, M.; Mathieu, M.P. *Ind. Chim. Belge* 1967, *32*, 156-164.
2. Chou, J.S.; Chao, K-C. Ind. Eng. Chem. Res. 1992, 31, 621-623.
3. Safronova, T.P.; Zhuze, T.P. *Khim. Tekn. Topl. Mas.* 1958, *3(2)*, 41-46., or *Chem. Abstr.* 1958, *52*, 8518d.
4. Safronova, T.P.; Zhuze, T.P. *Neft. Khoz.* 1962, *40*, 34-47.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Kerosenes; Gasoline.

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M. P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 233.15 - 293.15

PREPARED BY:

E. L. Boozer
H. L. Clever

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EXPERIMENTAL VALUES:

Temperature Interval of Measurements T/K	Ethene Mol % Range $10^2 x_1$/mol %	$K\pi\nu$/atm[1] at 293.15 K	Enthalpy of Dissolution ΔH/kcal mol^{-1}	Constant A
Kerosene A-1				
233.15-293.15	1 - 2	44	2.65	3.62
Kerosene A-2				
233.15-293.15	1 - 2	44	2.41	4.42
Kerosene A-3				
243.15-293.15	2 - 5	48	2.74	3.73
Gasoline				
243.15-293.15	1 - 3	43	2.42	3.435

[1] $\log (K\pi\nu/\text{atm}) = A - (\Delta H/\text{cal mol}^{-1})/(2.3R(T/K))$

The author's definitions are:

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}},$$

π/atm = total pressure,

ν = coefficient of fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe three methods:

1.A. [Saturat. n°1]. A measure of the static pressure of saturation in an apparatus which gave a precision of 10 - 15 %.

1.B. [Saturat. n°2]. A measure of the static pressure of saturation in an apparatus which gave a precision of 2 - 5 %.

2. [Chromato]. A Gas liquid chromatographic method estimated to have a precision of 2 - 5 %.

3. [Anal. directe]. Direct analysis of the gaseous and liquid phases.

Method 1.B. was used for all of the kerosene systems except kerosene A-6/A-5 between 243 and 293 K for which method 1.A. was used.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Air Liquide. For narcosis, 99.9 per cent.

(2) Kerosenes and gasoline.

	Distillation Range, t/°C	Density ρ^{20}/g cm^{-3}	mol wt
A-1	150-280	0.7805	170
A-2	150-185	0.7700	145
A-3	207-255	0.784	192
Gasoline	94-168	0.7521	122

ESTIMATED ERROR:

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}$/atm = $(f_1/\text{atm})/x_1$ where f_1 is the fugacity.

COMPONENTS:

(1) Ethene or ethylene; C_2H_4; [74-85-1]

(2) Carbowaxes; Carbowax 400, Carbowax 350.

ORIGINAL MEASUREMENTS:

Hannaert, H.; Haccuria, M.; Mathieu, M. P.

Ind. Chim. Belge 1967, *32*, 156-164.

VARIABLES:

T/K = 273.15 - 353.15

PREPARED BY:

H.L. Clever

EXPERIMENTAL VALUES:

Temperature Interval of Measurements T/K	Ethene Mol % Range 10^2x_1/mol %	$K\pi\nu$/atm[1] at 293.15 K	Enthalpy of Dissolution ΔH/kcal mol^{-1}	Constant A
Carbowax 400				
273.15-353.15	---	83	1.69	3.185
Carbowax 350				
293.15-313.15	---	81.5	2.66	3.90

[1] $\log (K\pi\nu/\text{atm}) = A - (\Delta H/\text{cal mol}^{-1})/2.3R(T/K))$

The author's definitions are:

$$K = y_1/x_1 = \frac{\text{mole fraction gas in gas phase}}{\text{mole fraction gas in liquid phase}},$$

$$\pi/\text{atm} = \text{total pressure},$$

$$\nu = \text{coefficient of fugacity}.$$

The function, $K\pi\nu$/atm, is equivalent to a Henry's constant in the form $H_{1,2}/\text{atm} = (f_1/\text{atm})/x_1$ where f_1 is the fugacity.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The authors describe three methods:

1.A. [Saturat. n°1]. A measure of the static pressure of saturation in an apparatus which gave a precision of 10 - 15 %.

1.B. [Saturat. n°2]. A measure of the static pressure of saturation in an apparatus which gave a precision of 2 - 5 %.

2. [Chromato]. A Gas liquid chromatographic method estimated to have a precision of 2 - 5 %.

3. [Anal. directe]. Direct analysis of the gaseous and liquid phases.

Method 2 was used for these systems.

SOURCE AND PURITY OF MATERIALS:

(1) Ethene. Air Liquide. For narcosis, 99.9 per cent.

(2) Carbowax. Union Carbide. Polyethylene glycols. Carbowax 400 molecular weight 400 ± 20. Carbowax 350 molecular weight 350 ± 15.

ESTIMATED ERROR:

REFERENCES:

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Fischer-Tropsch SASOL wax

ORIGINAL MEASUREMENTS:

Chou, J.S.; Chao, K-C.
Ind. Eng. Chem. Res., 1992,
31, 621-623.

VARIABLES:

$T/K = 473\text{-}533$; $p/MPa = 1\text{-}5$;

PREPARED BY:

C.L. Young

EXPERIMENTAL VALUES:

T/K ($t/^{\circ}C$)	p/atm	p/MPa	Solubility/mol kg^{-1}
473.2 (200.0)	10.06	1.016	0.234
	20.12	2.039	0.491
	29.99	3.039	0.746
	39.97	4.050	1.01
	49.90	5.056	1.26
533.1 (259.9)	10.04	1.017	0.200
	20.12	2.039	0.416
	30.90	3.131	0.633
	40.04	4.057	0.851
	50.95	5.163	1.07

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Single pass flow method. Gas passed through presaturator then equilibrium cell. At equilibrium liquid samples withdrawn, pressure released, solidified hydrocarbon collected in glass trap and weighed. Gas estimated volumerically. Temperature measured with chromel-alumel thermocouple and pressure with Bourdon gauge.

SOURCE AND PURITY OF MATERIALS:

1. Matheson sample, purity at least 99.5 mole %.
2. SASOL wax, av carbon no. 43, av. mol wt 605, 74% paraffins, 14% mono-olefins, 12% oxygenates, % branching 0.05, carbon no range 20-250.

ESTIMATED ERROR:

$\delta T/K = \pm 0.1$; $\delta p/MPa = \pm 0.05$
δSolubility $= \pm 1.5\%$

REFERENCES:

1. Huang, S.H.; Lin, H.M.; Tsai, F.N.; Chao, K-C.; *Ind. Eng. Chem. Res.*, 1988, *27*, 162.

COMPONENTS:

1. Ethene; C_2H_4; [74-85-1]
2. Three crude oil solvents; some properties given below:

ORIGINAL MEASUREMENTS:

Safronova, T.P.; Zhuze, T.P.

Neft. Khoz. 1962, *40*, 43-47.

VARIABLES:

T/K = 293.15 - 373.15

P/MPa = to 5.07 (50 atm)

PREPARED BY:

W. Hayduk

EXPERIMENTAL VALUES:

t/C	T/K	[1]Solubility Coefficient, K_B/cm^3 ethene at STP (cm^3 solvent.atm)$^{-1}$ Solvent I	Solvent II	Solvent III	[1] Maximum Applicable Pressure P/atm (MPa)
20	293.15	3.22	2.11	1.67	25 (2.53)
50	323.15	1.15	1.15	1.15	50 (5.07)
100	373.15	1.00	0.73	0.73	50 (5.07)

[1]Data for the solubilities were shown only graphically as a function of pressure. Values for the lower pressure region for which the relation was linear, were read from enlarged graphs by the compiler. Additional data were shown to at least 10.1 MPa.

Some properties of the solvents are shown below:

Solvent	Density, ρ, g cm^{-3}	Fraction Solvent Vaporized, % To 473K	From 473 to 573K	Average Composition of Vapor, % To 473K A	B	C	From 473 to 573 A	B	C
I	0.8530	25	19.5	65	24	11	52	21	27
II	0.8494	18	23.5	27	64.4	8.6	42	41	17
III	0.8713	20	20	47	41	12	43	35	22

Solvents: I = Romashkinskaya; II = Surakhanskaya; III = Nebitdagskaya

Fractions: A = Paraffin; B = Naphthenic; C = Aromatic

Please see next page for (apparently) same data published in a different form.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus and procedure are described in reference 1.

SOURCE AND PURITY OF MATERIALS:

1. Ethene purity and source not specified.
2. Solvents. The names of the oils must designate their source.

ESTIMATED ERROR:

$\delta K_B = \pm 6\%$ (compiler)

REFERENCES:

1. Safronova, T.P.; Zhuze, T.P. *Khim. Tekh. Topl. Mas.* 1958, *3*, 41-46.

COMPONENTS:

(1) Ethene; C_2H_4; [74-85-1]

(2) Petroleum, crude oils.

ORIGINAL MEASUREMENTS:

Safronova, T. P.; Zhuze, T. P.

Khim. i Tekhnol. Topliva i Masel 1958, *3 (2)*, 41-46.

Chem. Abstr. 1958, *52*, 8518d.

VARIABLES:

T/K = 293 - 373
p/MPa = up to 20.3

760

PREPARED BY:

H. L. Clever

EXPERIMENTAL VALUES:

Temperature t/°C	T/K	Pressure p/atm	Solubility Coefficient /cm³ cm⁻³ atm⁻¹
1. Nebit-Dag (Akchagylian layer) crude oil, Specific gravidy, d_4^{20} = 0.8713, kinematic viscosity = 8.70 centistoke.			
100	373	25	0.616
		50	0.681
		100	0.792
2. Romashkino oilfield crude oil, Specific gravity, d_4^{20} = 0.8530, kinematic viscosity = 6.54 centistokes.			
100	373	25	0.760
		50	0.919
		100	1.049
3. Surakhany oil field crude oil, Specific gravity d_4^{20} = 0.8494, kinematic viscosity = 5.19 centistokes.			
100	373	25	0.724
		50	0.709
		100	0.791
		200	0.911

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A detailed diagram of the high pressure apparatus was given in the paper.

Many of the data are presented in figures of Solubility/cm³ cm⁻³ *vs.* p/atm. A summary of the graphical data follows:

System	Temperatures t/°C	Maximum Pressure p./atm
1	20, 50, 100	200
2	20, 50, 100	160
3	20, 50, 100	180

SOURCE AND PURITY OF MATERIALS:

(1) Ethene.

(2) Petroleum crude oils. Three crude oils. Descriptions given above. Additional information on composition in the paper.

ESTIMATED ERROR:

The compiler estimates the data have an uncertainty of 3 to 5 percent.

REFERENCES:

SYSTEM INDEX

Page numbers preceded by E refer to evaluation texts whereas page numbers not preceded by E refer to compiled tables. Compounds are named as in Chemical Abstracts indexes (toluene appears under Benzene, methyl-). The word "aqueous" or "ternary" in brackets after the solvent name designates that the solvent is in solution with water, or is one component of a multicomponent non-aqueous solvent solution, repectively.

REGISTRY NUMBER INDEX

Page numbers preceded by E refer to evaluation texts whereas page numbers not preceded by E refer to compiled tables.

AUTHOR INDEX

Page numbers preceded by E refer to evaluation texts whereas page numbers not preceded by E refer to compiled tables.

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