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IUPAC-NIST Solubility Data Series 67. Halogenated Ethanes and Ethenes with Water

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Ari L. Horvath, Forrest W. Getzen, and Z. Maczynska

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IUPAC-NIST Solubility Data Series
67. Halogenated Ethanes and Ethenes with Water

Ari L. Horvath
Imperial Chemical Industries PLC, Runcorn, United Kingdom

Forrest W. Getzen[a)]
North Carolina State University, Raleigh, North Carolina

Z. Maczynska
Institute of Physical Chemistry, Warsaw, Poland

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This volume covers the solubilities of halogenated ethanes and ethenes with water, heavy water, seawater, and aqueous electrolyte solutions. All data were critically examined for their reliability and best value estimates were selected on the basis of such evaluations. Referenced works are presented in the standard IUPAC-NIST Solubility Data Series format. Reported and best value data are presented in tabular form and, where justified, data correlation equations and graphical illustrations are provided. Throughout the volume, SI conventions have been employed as the customary units. The importance of these data arises from the fact that halogenated ethanes and ethenes have commercial uses as industrial chemicals, propellants, solvents, and the like. In such applications, often from spillage, leakage, or mishandling, they contact water and are exposed to the atmosphere. The data are essential for concentration estimates for the halogenated ethanes and ethenes in drinking and ground water, foodstuffs, human tissue, marine organisms, and the atmosphere. The halogenated aliphatics are of particular interest to health scientists, engineers, environmentalists, and atmospheric chemists in that they represent a class of chemical materials which has many significant industrial applications. However, at the same time, these substances have been shown, in some cases, to be carcinogenic and also to be especially damaging to the earth's atmospheric composition through their chemical reactivity which results in atmospheric ozone depletion. The high ozone depletion potentials of this class of chemical substances emphasizes the importance of having available complete, accurate, and reliable data for mutual solubilities with water. The availability of such data is essential for estimates of halogenated hydrocarbon levels in both natural waters and aqueous industrial liquids which result from industrial fabrication, industrial waste removal processes, and the like. The data also provide significant solubility values for studies concerning the health of human and other biological systems.
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Key words: aqueous solutions; halogenated ethanes; halogenated ethenes; solubility.

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[a)] Electronic mail: getzen@chemdept.chem.ncsu.edu

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1. Preface

This volume, which continues with systems similar to those of the substituted methanes given in volume 60 of this series, contains a comprehensive collection and critical evaluation of solubility data published prior to 1993 for halogenated ethanes and ethenes with water, heavy water, seawater, and aqueous electrolyte solutions. The systems are ordered on the basis of chemical formula according to the Hill system.

A critical evaluation of the solubility data is not satisfactory without a comprehensive literature search followed by compilation of all the available information reported in journals, patents, pamphlets, brochures, books, etc. The difficulties and problems in retrieval of all solubility data are a well recognized fact. Some of the difficulties which arose during the retrieval of the original publications for this volume were:

(i) The articles, reports, etc., were not cited in the Chemical Abstracts;
(ii) The British Library did not hold the publications;
(iii) The Slavonic Section of the British Library was unable to obtain some publications from abroad;
(iv) Manufacturers' reports, leaflets, brochures, etc., were not available from industrial source;
(v) University reports from experimental stations were not available from university libraries.

In summary, there were several cases where the original sources were not obtainable and the information had to be taken from secondary sources.

The referenced literature sources can be classified into the following groups:

(a) Bibliographies,[1,2]
(b) Secondary sources (books, reviews),[1–15]
(c) Databases (computer softwares),[1]
(d) Primary sources (journals, reports, etc.).

A list of the various sources of solubility data following the above classification is summarized in Table 1.

Once a copy of the original document—usually a photocopy—was obtained, the first step was to read it carefully. Often the original article was in a foreign language which required a translation. If the description was not focused on the solubility aspect, then often some relevant details, e.g., source and purity of the solute and solvent, or both, were not included in the text. In many cases, the method, apparatus, and procedure were simply referred to other articles. Furthermore, when the experimental errors were not stated, the compiler sometimes introduced a subjective judgement for the accuracy of the measured solubility and temperature. The estimated accuracy of the measured quantities is quite subjective and the readers must take this fact into consideration.

The summaries of the procedures and abstracts were based on the available description of the method, apparatus, and procedures. Often a short statement ''Details are not available,'' had to be used when the main contents of the articles focused not on solubility measurements but some other aspects of chemistry.

The conversion of the published solubility data into conventional units often presented difficulties, particularly when the dimensions were not expressed clearly. For example, the Henry's law constants, separation coefficients, distribution ratio, partition coefficients, etc., were not specified explicitly. Some of the more relevant conversion formulas are given in Table 2.

To convert solubility data from one unit to another, often the density and vapor pressure of the pure components and/or of the mixture were needed. The physical properties of the pure compounds were taken from the DIPPR[1] and TRCVP[2] databases. To find or derive the physical properties of mixtures required a more elaborate effort. Experimental data, e.g., density and vapor pressure for aqueous solutions of halogenated hydrocarbons are extremely rare in the literature. Consequently, approximations were obtained using calculations recommended in standard handbooks, e.g., Reid *et al.*[3] An illustration of the difficulty of obtaining accurate conversions is shown by the following typical case.

TABLE 1. Sources of solubility data

(A) Bibliographies

- [1]J. Wisniak and A. Tamir, *Liquid-Liquid Equilibrium and Extraction. A Literature Source Book* (Elsevier, Amsterdam, 1980), 1252 pp.
- [2]J. Wisniak and M. Herskowitz, *Solubility of Gases and Solids. A Literature Source Book*, Parts A and B (Elsevier, Amsterdam, 1984), 2070 pp.

(B) Secondary Sources

- [1]G. W. Ware, *Review of Environmental Contamination and Toxicology* (Springer, New York, 1990), Vol. 116, 200 pp.
- [2]R. K. Freier, *Aqueous Solutions* (Walter de Gruyter, Berlin, 1976), Vol. 1, 477 pp.
- [3]*Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik*, Gleichgewichte der Absorption von Gasen in Flüssigkeiten, Vol. 4a/c1 (Springer, Berlin, 1976), 479 pp.
- [4]*Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik*, 6th ed., Vol. 1, Eigenschaften der Materie in Ihren Aggregationstäden, Part 2b, Lösungsgleichgewichte I (Springer, Berlin, 1962).
- [5]*Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik*, 6th ed., Vol. 2, Eigenschaften der Materie in Ihren Aggregatzustäden, Part 2c, Lösungsgleichgewichte II (Springer, Berlin 1964).
- [6]A. L. Horvath, *Halogenated Hydrocarbons. Solubility-Miscibility with Water* (Marcel Dekker, New York, 1982), 889 pp, Vol. 7; *International Critical Tables of Numerical Data*, edited by E. W. Washburn (McGraw-Hill, New York, 1928), Vol. 3.
- [7]*International Critical Tables of Numerical Data*, edited by E. W. Washburn (McGraw-Hill, New York, 1928), Vol. 3.
- [8]*Beilsteins Handbuch der Organischen Chemie* (Beilstein Institut für Literatur der Organischen Chemie, Springer, Berlin, 1918), Vol. 1.
- [9]*Kirk-Othmer Encyclopedia of Chemical Technology*, 1st, 2nd, 3rd, and 4th eds. (Wiley, New York).
- [10]A. Seidell, *Solubility of Organic Compounds*, 3rd ed. (Van Nostrand, New York, 1963), 926 pp.
- [11]W. F. Linke, *Solubilities of Inorganic and Metal-Organic Compounds*, 4th ed. (Van Nostrand, Princeton, NJ, Vol. 1, 1958), Vol. 2 (1965).
- [12]H. Stephen and T. Stephen, *Solubilities of Inorganic and Organic Compounds* (Pergamon, Oxford 1963), Vols. 1 and 2.
- [13]J. A. Riddich and W. B. Bunger, *Organic Solvents*, 3rd ed. (Wiley, New York, 1970), Vol. 2, 603 pp.
- [14]J. Gmeling and U. Onken, *Vapor-Liquid Equilibrium Data Collection*, Aqueous-Organic Systems, Vol. 1 (1977).
- [15]Washington, DC, R. R. Dreisbach, *Physical Properties of Chemical Compounds* (Am. Chem. Soc. Adv. in Chem. Ser. 15 1955), 536 pp.; Ser. 22 (1959), 491 pp.; 29 (1961), 489 pp.

(C) Databases

- [1]*AQUASOL Database of Aqueous Solubility*, 5th ed., edited by S. H. Yalkowsky (University of Arizona Press, Tucson, Arizona, 1991).

(D) Primary Sources

- (1) Journals
- (2) Reports
- (3) Brochures, leaflets
- (4) Patents
- (5) Private communications

TABLE 2. Conversion formulas for solubility units

(a) Henry's law constant (H):

$$\text{Mass }\% = \frac{\dfrac{P_{\text{vap}}(\text{atm})M_{\text{solute}}}{82.06T(\text{K})}}{\dfrac{H(\text{dimensionless})}{d_{\text{solvent}}}}\times 100,$$

$$\text{Mass }\% = \frac{\dfrac{P_{\text{vap}}(\text{atm})M_{\text{solute}}}{H(\text{m}^3\ \text{atm/mol})}}{d_{\text{solvent}}}\times 10^{-4},$$

$$H(\text{dimensionless}) = \frac{C_{\text{air}}}{C_{\text{solvent}}} = \frac{16.04P_{\text{vap}}(\text{atm})M_{\text{solute}}}{T(K)S_{\text{solute}}(\text{mg/dm}^3)}.$$

(b) Air/water partition coefficient (K_{AW}):

$$\text{Mass }\% = \frac{100K_{\text{AW}}P_{\text{vap}}}{82.054T(\text{K})d_{\text{solvent}}},$$

(c) Distribution ratio (p/c):

$$(p/c) = \frac{\text{solute vapor pressure}}{\text{solute concentration}}\ \frac{(\text{mm Hg})}{(\text{mmole/dm}^3)},$$

(d) Partition coefficient (K):

$$K = \frac{1}{\text{Ostwald coefficient}} = \frac{1}{L},$$

(e) Distribution coefficient (K_i):

$$K_i = \text{Ostwald coefficient} = L = \frac{y_i}{x_i}.$$

The solubility of carbon tetrachloride (CCl_4) in water (H_2O) is 0.10 $cm^3/100\ cm^3$ water at 25 °C. The solubility in mass percent ($g\ CCl_4/100$ g soln.) is required. The density of pure carbon tetrachloride is 1.5834 $g\ CCl_4/cm^3$ at 25 °C (DIPPR database). The solution density is required to convert the pure water density using the mass of the aqueous solution of carbon tetrachloride at 25 °C. However, the density of the aqueous solution of carbon tetrachloride has not been reported in the literature. The reason is quite simple; the difference between the density of pure water and that of the aqueous solution of carbon tetrachloride at 25 °C is marginal. As a consequence, the errors obtained upon the determination of solubility are considerably greater than the possible difference between the solubility in pure water or in its aqueous solutions at the same temperature. It follows, in this case, one must use the approximation

$$g\ \ CCl_4/100\ \ g\ \ H_2O \approx g\ \ CCl_4/100\ \ g\ \ \text{soln.}$$

On the other hand, for solubility values larger than, say, 2–3 mass percent, the differences become significant, as the following example illustrates. The solubility in water of dichloromethane (CH_2Cl_2) is 2.363 g/100 g water at 0 °C. The solubility in $g\ CH_2Cl_2/100$ g soln. at the same temperature is required. If 100 g water dissolves 2.363 g CH_2Cl_2, then the total mass of the solution becomes 102.363 g. This means that 100 g aqueous solution will dissolve less CH_2Cl_2 than 100 g pure water, that is

$$\frac{2.363\ \ g\ \ CH_2Cl_2}{102.363\ \ g\ \ \text{soln.}}100 = 2.3084(g\ \ CH_2Cl_2/100g\ \ \text{soln.}).$$

The result is 2.3084 $g\ CH_2Cl_2/100$ g soln. at 0 °C. Consequently, there is a 2.31% reduction in the solubility relative to 100 g pure water. This is in comparison to the reduction of only 0.10% in the case of the solubility of CCl_4 in 100 g water or 100 g aqueous solution at 25 °C.

All critical evaluations of the solubility data are presented on the evaluation sheets. The information available on the relevant compilation sheets served as the fundamental source for the critical evaluations. The following main aspects of the solubility data have been considered:

(i) purity of the components (solute and solvents),
(ii) date of the experiment,
(iii) accuracy of the method,
(iv) reproducibility of the experiment,
(v) experience of the investigator(s), previous publications, and
(vi) consistency of the data, trends in series.

Once these aspects of the works had been examined, efforts were made to weight the reliability of the reported data. As much as possible, the differences in the quality of the data have been taken into account.

The available solubility data for binary systems may be very scarce, medial, or abundant, depending on the commercial application of the systems. Whenever data from different sources exist, they often disagree. For evaluation of the agreement or disagreement among the data, graphical presentations usually provide the clearest picture. The figures normally contain the original data from all references for a given system. A plot representing the solubility data (expressed in mole fraction or mass percent) can reveal whether or not a trend exists among the data in addition to highlighting any discrepancies of the experimental solubility measurements.

The final data can be classified as:

(i) obscure or dubious—rejected data,
(ii) tentative—not recommended data,
(iii) recommended—good agreement among the published results.

A graphical presentation of the solubility data may be performed on linear, semilogarithmic, etc., scales. The unit of solubility may be given as specific or molar scales. For practical reasons, the mass percent unit is often used, whereas the mole fraction is another common unit of solubility. In this volume most figures are plotted using one of two different scales. For the solubilities in water, linear graphs are used and for the solubilities of water in halogenated hydrocarbons, the so called Cox chart is applied. In the Cox charts, the solubility of water is given as $\log_{10} x_2$ vs $1/T$. A straight line on a Cox plot can be very useful for revealing consistent data covering a limited temperature range. However, the straight line does not apply for solubility data over a very wide temperature interval, e.g., from the triple point to the critical point. Therefore, in some cases (e.g., some of the polyhalogenated ethanes with water solubilities), the normal polynomial equations were used for smoothing the solubility data.

To fit experimental data into the various equations, the individual data points are often weighted. The smoothed data may be influenced somewhat by such procedures of weighting individual data points. Data analysis is a process of mathematical and/or graphical treatment of experimental data through the use of statistical or parametric procedures. Whenever the raw data are fragmentary, the aim is to generate an extended range of internally consistent values by synthesis. In any case, the temperature dependence of solubility must be examined and any unusual irregularities must be investigated carefully.

The temperature dependence of the solubility of halogenated hydrocarbons in water has been correlated using normal polynomial equations over limited temperature intervals. These equations should be used only in the temperature range indicated. The equations play two major roles: to provide data users with interpolated data with good accuracy and to provide data users with acceptable data for use in computer programs, if desired. The deviation of the various experimental values from the fitted data are given as standard or average deviations.

If the experimental data cover a reasonable temperature interval, then the data and the smoothing equation are often illustrated in a figure. The graphical presentation of the reported and fitted data clearly indicates the risks involved when one attempts to extrapolate the raw experimental data. In some cases, an extrapolation is quite safe for the desired temperature (see for example, the solubility of water in halogenated hydrocarbons in moderate temperature intervals); whereas, in other cases, the risk is very high and it is not recommended. The shape of the solubility curves suggests the extrapolation and interpolation possibilities.

Whether the mutual solubility between two liquids is partial or complete depends on the similarities or differences between the molecules of the two chemical compounds. The halogenated hydrocarbon and water systems are only partially miscible without exception. Furthermore, the miscibility or immiscibility of water with other liquids is also very dependent upon temperature. At ambient temperature and atmospheric pressure, the miscibility is very limited between water and halogenated hydrocarbons. For most systems, the mutual solubility is less than 2 mass percent.

In a liquid–liquid system the variation of solubility with temperature depends on the sign of the heat of mixing or solution. The minimum dissolution temperature occurs for most halogenated hydrocarbon–water systems between 270 and 310 K. The interactions between the solute and solvent molecules provide the explanation for the phenomena. The temperature dependence of solubility is a result of temperature dependent structural modifications of water. A different energy is required for cavity formation and for the changes in rigidity of the lattice as temperature is changed.

The appearance of these minima resembles the dependence of the critical micelle concentration upon temperature. Here, the iceberg formation of water molecules around the monodisperse solute enhances the critical micelle concentration, the logarithm of which would be decreased linearly with $1/T$ provided the solution behaves regularly, and the

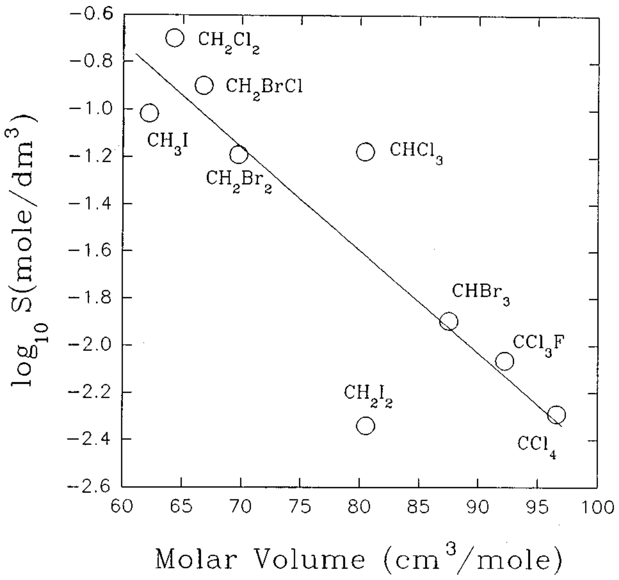

FIG. 1. Logarithm of saturated molarity vs solute molar volume at 25 °C for halogenated methanes in water.

iceberg formation increases with a temperature reduction.

It is well recognized that the rare gases and hydrocarbon gases form iceberg-like structures when dissolved in cold water, followed by an iceberg melting as the temperature is raised. The solubility of most gases in water shows a minimum when plotted against temperature. The shape of the solubility curves for molecules with alkyl groups is explained by considering that the ice-like structure of water is also formed around the nonpolar alkyl group of molecules in water. This structure tends to break down as the temperature of the solution is increased.

The minimum solubility temperature can be calculated from a calorimetric measurement of the enthalpy of solution at infinite dilution ($\Delta_{\text{soln}}H^{\infty}$). This value is very large and varies from negative to positive values within a small temperature range. Consequently, very large errors may be caused by an erroneous interpretation. In addition to the enthalpy of solution, the change in the heat capacity at infinite dilute aqueous solution ($\Delta_{\text{soln}}C_p^{\infty}$) is required for the calculation of the minimum solubility temperature (T_{min});

$$T_{\text{min}}=298.15\ \text{K}-\frac{\Delta_{\text{soln}}H^{\infty}(298.15\ \text{K})}{\Delta_{\text{soln}}C_p^{\infty}}.$$

A more detailed description of the minimum solubility phenomenon is given by Horvath,[4] Shinoda,[5] Nishino and Nakamura,[6] and Privalov and Gill.[7]

The relations between the solubility and some of the physical properties of the solute or solvent have been investigated from early times in solution studies. The various experiments showed that in very diluted solutions the influence of the solute molecules does not extend to all solvent molecules in the solution. Consequently, the large fraction of solvent molecules, which are not affected by solute molecules, must exist more or less in the same state of aggregation as in the pure state. A change of solvent molar volume in dilute solutions is very small. However, in more concentrated solutions the effects of the presence of the solute molecules on the solvent molecules are not negligible. The amount of molar volume change of the solvent depends on the nature of the solutes. The dissolution process is related to the disintegration of the solute in the solvent, as compared to its pure state molecular order, as a result of the mutual action of attraction of the solute and solvent.

In general, solubility depends on many parameters and is of a very complex nature. There is no simple relation established between solubility and the other properties of the pure components (solute and solvent). Despite the lack of a simple relationship, the solubility of halogenated benzenes in water at 25 °C has been correlated with a reasonable success using the molar volume of the solutes.[8] Similarly, the solubility of halogenated methanes in water shows a linear relationship.[9] The correlation is based on the assumption that the molar volumes in saturated solutions are not greatly different from those in the pure state. The simple linear relation at 25 °C is illustrated graphically in Fig. 1. This is a very useful and practical way to show the consistency of the solubility data. Any significant deviation from such a linear relationship suggests some inconsistency and introduces doubt concerning the reliability of the data.

Correlation equation:

$$\log(S/\text{mole/dm}^3)=1.8995-4.3707\times10^{-2}(V_m/\text{cm}^3\,\text{mole}^{-1}).$$

1.1. References for the Preface

[1] DIPPR, Design Institute for Physical Property Data, Am. Inst. Chem. Eng., New York, Software package for IBM PC (1985).
[2] TRCVP, Thermodynamic Research Center, Texas A & M University System, College Station, TX (1989).
[3] R. C. Reid, J. M. Prausnitz, and B. E. Poling, *The Properties of Gases and Liquids*, 4th ed. (McGraw-Hill, New York, 1987), 742 pp.
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2. Introduction to the Solubility Data Series Solubility of Liquids in Liquids

2.1. The 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 different sources agree sufficiently, recommended values are proposed. The evaluation sheets, recommended values, and compiled data sheets are published on consecutive pages.

This series is concerned primarily with liquid–liquid systems, but a limited number or related solid–liquid, fluid–fluid, and multicomponent (organic-water-salt) systems are included where it is considered logical and appropriate. Solubilities at elevated and low temperatures and at elevated pressures have also been included, as it is considered inappropriate to establish artificial limits on the data presented if they are considered relevant or useful.

For some systems, the two components may be miscible in all proportions at certain temperatures and pressures. Data on reported miscibility gaps and upper and lower critical solution temperatures are included where appropriate and when available.

2.2. Compilations and Evaluations

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

2.2.1. Compilations

The format used for the compilations is, for the most part, self-explanatory. 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) nonsaturating components in alphanumerical order;
(c) solvents in alphanumerical order.

The saturating components are arranged in order according to the IUPAC 18-column periodic table with two additional rows:

Columns 1 and 2: H, alkali elements, ammonium, alkaline earth elements

Columns 3 to 12: transition elements

Columns 13 to 17: boron, carbon, nitrogen groups; chalcogenides, halogens

Column 18: noble gases

Row 1: Ce to Lu

Row 2: Th to the end of the known elements, in order of atomic number.

Organic compounds within each Hill formula are ordered in the following succession:

(a) by degree of unsaturation
(b) by order of increasing chain length in the parent hydrocarbon
(c) by order of increasing chain length of hydrocarbon branches
(d) numerically by position of unsaturation
(e) numerically by position by substitution
(f) alphabetically by IUPAC name.

Example:

C_5H_8	cyclopentane
	2-methyl-1,3-butadiene
	1,4-pentadiene
	1-pentyne
C_5H_{10}	cyclopentane
	3-methyl-l-butene
	2-methyl-2-butene
	1-pentene
	2-pentene
C_5H_{12}	2,2-dimethylpropane
	2-methylbutane
	pentane
$C_5H_{12}O$	2,2-dimethyl-l-propanol
	2-methyl-l-butanol
	2-methyl-2-butanol
	3-methyl-l-butanol
	3-methyl-2-butanol
	1-pentanol
	2-pentanol
	3-pentanol
$C_6H_{12}O$	cyclohexanol
	4-methyl-l-penten-3-ol
	1-hexen-3-ol
	4-hexen-3-ol

Deuterated (^2H) compounds follow immediately the corresponding H compounds.

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 indicated 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 percent for weight percent; mol dm^{-3} for molar; etc. In most cases, both mass and molar values are given. Usually, only one type of value (e.g., mass percent) is found in the original paper, and the compiler has added the other type of value (e.g., mole percent) from computer calculations based on 1989 atomic weights.[2] 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. In addition, compiler-calculated values of mole or mass fractions are included if the original data do not use these units. If densities are reported in the original paper, conversions from concentrations to mole fractions are included, but otherwise this is done in the evaluation, with the values and sources of the densities being quoted and referenced.

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 graphs have been included, either to illustrate presented data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

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.

Source and Purity of Materials

For each component, referred to as (1), (2), etc., the following information (in this order and an abbreviated form) is provided if available in the original paper: source and specified method of preparation; properties; degree of purity.

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.[4]

Comments and/or Additional Data

Many compilations include this section which provides short comments relevant to the general nature of the work or additional experimental and thermodynamic data 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.

2.2.2. 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

The name and affiliation of the evaluator(s) and 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 solubility of comparatively few systems is known with sufficient accuracy to enable a set of recommended values to be presented. Although many systems have been studied by at least two workers, the range of 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, although both sets of results were obtained by reliable methods. In such cases, as a definitive 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.

(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 estimated 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 converted accurately.

2.3. Quantities and Units Used in Compilation and Evaluation of Solubility Data

2.3.1. Mixtures, Solutions and Solubilities

A *mixture*[5,6] describes a gaseous, liquid or solid phase containing more than one substance, where the substances are all treated in the same way.

A *solution*[5,6] 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 fraction 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.[7]

''Saturated'' implies equilibrium with respect to the processes of dissolution and demixing; 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.) Care must be taken to distinguish true metastability form supersaturation, where equilibrium does not exist.

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.

2.3.2. Physicochemical Quantities and Units

Solubilities of solids 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 few quantities follow the ISO standards[8] or the German standard;[9] see a review by Cvitas[10] for details.

A note on nomenclature

The nomenclature of the IUPAC *Green Book*[3] calls the solute component B and the solvent 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) (condensed phases), y_1 (gases):

$$x_1 = n_1 \bigg/ \sum_{s=1}^{c} n_s \tag{1}$$

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 percent* 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 nonelectrolytes j, of which some may be solvent components, a generalization of the definition in Ref. 11 gives

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

TABLE 1. Interconversions between quantities used as measures of solubilities c-component systems containing c-1 solutes i and single solvent c (ρ—density of solution; M_i—molar masses of i. For relations for two-component systems, set summations to 0.)

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

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

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

$$\sum_{i=1}^{s}(x_{i+}+x_{i-})+\sum_{i=s+1}^{c}x_i'=1. \tag{4}$$

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

$$x_1=\frac{\nu_{2+}x_1'}{\nu_{2+}-(\nu_2-1)x_{2+}},\quad x_2=\frac{x_{2+}}{\nu_{2+}-(\nu_2-1)x_{2+}}. \tag{5}$$

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 $w(1)$:

$$w_1=g_1\bigg/\sum_{s=1}^{c}g_s \tag{6}$$

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

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

$$m_1=n_1/n_2M_2 \tag{7}$$

SI base units: mol kg^{-1}. Here, M_2 is the molar mass of the solvent.

5. *Aquamolality, Solvomolality* of substance 1 in a mixed solvent with components, 2, 3,[12] $m_1^{(3)}$:

$$m_1^{(3)}=m_1\overline{M}/M_3 \tag{8}$$

SI base units: mol kg^{-1}. Here, the average molar mass of the solvent is

$$\overline{M}=x_2'M_2+(1-x_2')M_3 \tag{9}$$

and x_2' is the solvent mole fraction of component 2. This term is used most frequently in discussing comparative solubilities in water (component 2) and heavy water (component 3) and in their mixtures.

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

$$c_1=[\text{formula of solute}]=n_1/V \tag{10}$$

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.

7. *Mass concentration* of solute 1 in a solution of volume V, SI ρ_1: base units: kg m^{-3}.

$$\rho_1=g_1/V. \tag{11}$$

8. *Mole ratio*, $r_{\mathrm{A,B}}$ (dimensionless)[10]

$$r_{\mathrm{A,B}}=n_1/n_2. \tag{12}$$

Mass ratio, symbol $\zeta_{\mathrm{A,B}}$, may be defined analogously.[10]

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 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.

9. *Density*, ρ:

$$\rho=g/V \tag{13}$$

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

10. *Relative density*, $d = \rho/\rho°$: 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

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 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.

2.4. References for the Introduction

[1] E. A. Hill, J. Am. Chem. Soc. **22**, 478 (1990).

[2] IUPAC Commission on Atomic Weights and Isotopic Abundances, Pure Appl. Chem. **63**, 975 (1980).

[3] I. Mills *et al.*, eds., *Quantities, Units and Symbols in Physical Chemistry* (The Green Book). (Blackwell Scientific Publications, Oxford, UK, 1993).

[4] H. H. Ku, p. 73; C. Eisenhart, p. 69; in H. H. Ku, ed., Precision Measurement and Calibration, *NBS Special Publication 300*, Vol. 1 (Washington, 1969).

[5] J. Regaudy and S. P. Klesney, *Nomenclature of Organic Chemistry* (IUPAC) (The Blue Book) (Pergamon, Oxford, 1979).

[6] V. Gold *et al.*, eds., *Compendium of Chemical Technology* (The Gold Book) (Blackwell Scientific Publications, Oxford, UK, 1987).

[7] H. Freiser and G. H. Nancollas, eds., *Compendium of Analytical Nomenclature* (The Orange Book) (The Blackwell Scientific Publications, Oxford, UK, 1987), Sect. 9.1.8.

[8] ISO Standards Handbook, *Quantities and Units* (International Standards Organization, Geneva, 1993).

[9] German Standard, DIN 1310, *Zusammungsetzung von Mischphasen* (Beuth Verlag, Berlin, 1984).

[10] T. Cvitaŝ, Chem. Int. **17**, 123 (1995).

[11] R. A. Robinson and R. H. Stokes, *Electroyte Solutions* (Butterworths, London, 1959), 2nd ed.

[12] J. W. Lorimer, R. Cohen-Adad, and J. W. Lorimer, *Alkali Metal and Ammonium Chlorides in Water and Heavy Water (Binary Systems)*, IUPAC Solubility Data Series, Vol. 47 (Pergamon, Oxford, UK, 1991), p. 495.

Section 2 was written by:

A. F. M. Barton
Perth, WA, Australia

F. W. Getzen
Raleigh, NC, USA

G. T. Hefter
Perth, WA, Australia

D. G. Shaw
Fairbanks, AK, USA

December, 1995

3. Halogenated Ethanes and Ethenes in Water

Components:
(1) Water [7732-18-5]
(2) 1,2-Dibromo-1,1,2,2-tetrafluoroethane; $C_2Br_2F_4$; [124-73-2]

Original Measurements:
I. A. Semerikova, N. I. Mironova, and A. M. Sukhotin, Sov. Chem. Ind. **8**, 780 (1976).

Variables:
T/K=298

Prepared By:
A. L. Horvath

4. 1,2-Dibromo-1,1,2,2-Tetrafluoroethane with Water

Experimental Data

t/°C	$100w_1$	10^5x_1 (compiler)	$100w_1M_1^{-1}$/mol g^{-1} (compiler)
25	3.0×10^{-4}	4.33	1.7×10^{-5}

Auxiliary Information

Method/Apparatus/Procedure:
The concentration of water in 1,2-dibromo-1,1,2,2-tetrafluoroethane was determined by coulometric titration. More details are given by Nichugovskii.[1]

Source and Purity of Materials:
(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:
Solubility: not specified.
Temperature: ±2 K (compiler).

References:

[1] G. F. Nichugovskii, Zh. Prikl. Khim. **43**, 258 (1970).

Components:
(1) 1,1,2-trichloro-1,2,2-trifluoroethane $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

5. 1,1,2-Trichloro-1,2,2-Trifluoroethane with Water

Critical Evaluation

The 1,1,2-trichloro-1,2,2-trifluoroethane (1) and water (2) binary system is discussed in two parts; part 1 is 1,1,2-trichloro-1,2,2-trifluoroethane (1) in water and part 2 is water (2) in 1,1,2-trichloro-1,2,2-trifluoro-ethane (1).

Part 1. The solubility of 1,1,2-trichloro-1,2,2-trifluoroethane (1) in water (2) has been reported by six work groups as recorded in the Compilation Sheets immediately following this Critical Evaluation. The data at 298.15 K are in good agreement except that of du Pont,[1] which are markedly higher than other results. It may be assumed that the data in du Pont bulletins (Refs. 1 and 2) were produced in the same laboratories with similar methods during 1966, but with a significant discrepancy (factor of 2). Consequently, the higher value is rejected. The remaining three values at 298.15[2–4] show a good agreement.

The solubility data of Hellström *et al.*[5] between 303 and 366 K show a continuous rise with temperature up to 330 K, but above this temperature the data decrease and are therefore rejected. The data of Howe *et al.*[6] between 283 and 303 K are considerably lower than the likely solubility and are also rejected. The recommended solubility values for 1,1,2-trichloro-1,2,2-trifluoroethane in water at 298.15 K are given in Table 1.

TABLE 1. 1. Recommended solubility of 1,1,2-trichloro-1,2,2-trifluoroethane (1) in water (2)

Temperature		Solubility	
°C	K	$100w_1$	10^5x_1
25	298.15	0.017	1.63

Part 2. The solubility of water (2) in 1,1,2-trichloro-1,2,2-trifluoroethane (1) was reported in three references.[1–3] It may be assumed that the data reported in the du Pont bulletins were produced in the same laboratories with similar methods and accuracy at 298.15 and 294.15 K, respectively. No significant deviation exists between the two data points. The higher solubility at 298.15 K is consistent with the expected increase of solubility with temperature. The two measurements at 294.15 K of du Pont[2] and Bacquias[3] compare favorably and are classified as Tentative in Table 2.

TABLE 2. Tentative solubility of water (2) in 1,1,2-trichloro-1,2,2-trifluoroethane (1)

Temperature		Solubility	
°C	K	$100w_2$	10^4x_2
21	294.15	0.009	9.35

References:

[1] du Pont de Nemours & Company, ''Solubility Relationships between Fluorocarbons and Water,'' Tech. Bull. *B-43*, Wilmington, Del. (1966), 17 pp.

[2] du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon Compounds,'' Tech. Bull. *B-7*, Wilmington, Del. (1966), 16 pp.

[3] G. Bacquias, Galvano **40**, 677 (1971); **40**, 767 (1971).

[4] A. G. Rauws, M. Olling, and A. E. Wibowo, J. Pharm. Pharmac. **25**, 718 (1973).

[5] G. W. Hellström, H. R. Jacobs, and R. F. Boehm, Report DGL-1549-6, University of Utah, Salt Lake City, Utah (December, 1976), 74 pp.

[6] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September, 1987), (AD-A188 571), 86 pp.

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon'' *Compounds*, Tech. Bull. B-7, Wilmington, Del., (1966), 16 pp.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100w_1$	10^5x_1 (compiler)	$100w_2$	10^3x_2 (compiler)
25	1.7×10^{-2}	1.63	1.1×10^{-2}	1.14

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The original report is not obtainable; therefore, the solubility data were taken from a secondary source.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] P. A. Sanders, *Handbook of Aerosol Technology*, 2nd ed. (Van Nostrand Reinhold Co., New York, 1979), p. 184.

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

''Solubility Relationships between Fluorocarbons and Water, Tech. Bull. B-43, du Pont de Nemours & Company, Wilmington, Del. (1966), 17 pp.

Variables:

T/K=294–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100w_1$	10^5x_1 (compiler)	$100w_2$	10^4x_2 (compiler)
21	—	—	9.0×10^{-3}	9.35
25	3.5×10^{-2}	3.36	—	—

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. Bacquias, Galvano **40**, 677 (1971); **40**, 767 (1971).

Variables:

T/K=294

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100w_1$	10^5x_1 (compiler)	$100w_2$	10^4x_2 (compiler)
21.1	1.7×10^{-2}	1.63	9.0×10^{-3}	9.35

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler)

Estimated Errors:

Solubility: Not specified.
Temperature: ±0.2 K (compiler).

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. G. Rauws, M. Olling, and A. E. Wibowo, J. Pharm. Pharmac. **25**, 718 (1973).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100w_1$	10^5x_1 (compiler)	$100w_1M_1^{-1}$/mol g^{-1} (compiler)
25	1.7×10^{-2}	1.63	9.07×10^{-5}

Auxiliary Information

Method/Apparatus/Procedure:

A calibrated bottle was filled with nitrogen, a measured quantity of water and the organic vapor. After mixing and equilibration, the concentration of the vapor and the liquid phases were determined by injection of the head space samples into a gas chromatograph. The 1,1,2-trichloro1,2,2-trifluoroethane was detected by means of a tritium foil electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler)

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler)

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. W. Hellström, H. R. Jacobs, and R. F. Boehm, Report **DGL-1549-6**, University of Utah, Salt Lake City, Utah (December, 1976), 74 pp.

Variables:

T/K=303–370 and P/atm=0.5–1.1

Prepared By:

A. L. Horvath

Experimental Data

t/°C	p_1 /atm	S/ppm atm^{-1}	$100w_1$ (compiler)	10^5x_1 (compiler)
30.0	0.536	217.8	2.178×10^{-2}	2.094
34.2	0.629	248.5	2.485×10^{-2}	2.390
57.5	1.374	291.1	2.911×10^{-2}	2.800
73.0	1.31	202.2	2.022×10^{-2}	1.944
90.0	0.347	38.0	3.80×10^{-3}	0.3654
93.2	1.09	106.8	1.068×10^{-2}	1.027

Auxiliary Information

Method/Apparatus/Procedure:

The saturation of 1,1,2-trichloro-1,2,2-trifluoroethane with water took place in a steel vessel during 10 h. The mixture was stirred and left to stand for 7 h before the gas chromatographic analysis. The chromatograph was equipped with an electron capture detector. The determination of the solubility at a given condition was repeated five or six times.[1]

Source and Purity of Materials:

(1) du Pont samples, purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±4.7% std. dev.
Temperature: ±0.5 K.

References:

[1] G. W. Hellström, M. Sc. thesis, University of Utah, Salt Lake City, Utah, Dec. 1976.

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^6w_1	$100w_1$ (compiler)	10^6x_1 (compiler)
10	38	3.8×10^{-3}	3.65
20	27	2.7×10^{-3}	2.60
30	14	1.4×10^{-3}	1.35

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. Measured volumes of 1,1,2-trichloro-1,2,2-trifluoroethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a free induction decay (FID) detector. The gas chromatography (GC) responses were compared with calibration response plots to establish concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% purity; used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	G. W. Hellström, H. R. Jacobs, and R. F. Boehm, Report DGE-1549-6, University of Utah, Salt Lake City, Utah (December 1976), 74 pp.
Variables:	**Prepared By:**
T/K=296–368 and P/atm=0.4–1.3	A. L. Horvath

6. 1,1,2-Trichloro-1,2,2-Trifluoroethane with Sodium Chloride and Water

Experimental Data

Solubility of $C_2Cl_3F_3$ in 2.5 mass % NaCl solution

t/°C	p_1 /atm	S/ppm atm^{-1}	$100w_1$ (compiler)	10^5x_1 (compiler)
23.0	0.403	145.5	1.437×10^{-2}	1.406
24.4	0.430	179.8	1.778×10^{-2}	1.740
59.5	1.100	170.0	1.706×10^{-2}	1.669
66.0	1.34	187.8	1.895×10^{-2}	1.854
93.5	1.04	99.7	1.019×10^{-2}	0.997
95.2	0.517	47.0	4.84×10^{-3}	0.474

Auxiliary Information

Method/Apparatus/Procedure:

The saturation of 1,1,2-trichloro-1,2,2-trifluoroethane in the aqueous salt solution was performed in a steel vessel during 10 h. The mixture was stirred and left to stand for 7 h before the gas chromatographic analysis. The chromatograph was equipped with an electron capture detector. The determination of the solubility at a given condition was repeated five or six times. Further details are available.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:

Solubility: ±3.7% std. dev.
Temperature: ±0.5 K.

References:

[1] G. W. Hellström, M. Sc. thesis, University of Utah, Salt Lake City, Utah, Dec. 1976.

Components:	**Original Measurements:**
(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	G. W. Hellström, H. R. Jacobs, and R. F. Boehm, Report DGF-1549-6, University of Utah, Salt Lake City, Utah (December 1976), 74 pp.
Variables:	**Prepared By:**
T/K=297–366 and P/atm=0.4–1.2	A. L. Horvath

Experimental Data

Solubility of $C_2Cl_3F_3$ in 10 mass % NaCl solution

t/°C	p_1 /atm	S/ppm atm^{-1}	$100w_1$ (compiler)	10^6x_1 (compiler)
24.3	0.429	111.3	1.041×10^{-2}	10.75
63.8	1.22	98.4	9.35×10^{-3}	9.658
67.1	1.18	96.9	9.26×10^{-3}	9.565
91.5	1.20	55.1	5.33×10^{-3}	5.506
94.2	0.776	39.4	3.83×10^{-3}	3.956

Auxiliary Information

Method/Apparatus/Procedure:

The saturation of 1,1,2-trichloro-1,2,2-trifluoroethane in aqueous salt solution was performed in a steel vessel during 10 h. The mixture was stirred and left to stand for 7 h before the gas chromatographic analysis. The chromatograph was equipped with an electron capture detector. The determination of the solubility at a given condition was repeated five to six times. Further details are available.[1]

Source and Purity of Materials:

(1) Samples from du Pont, purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:

Solubility: ±3.6% std. dev.
Temperature: ±0.5 K.

References:

[1] G. W. Hellström, M. Sc. thesis, University of Utah, Salt Lake City, Utah, Dec. 1976.

Components:

(1) 1,1,2-trichloro-1,2,2-trifluoroethane; $C_2Cl_3F_3$; [76-13-1]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

G. W. Hellström, H. R. Jacobs, and R. F. Boehm, University of Utah, Report DGE-1549-6, Salt Lake City, Utah (December 1976), 74 pp.

Variables:

T/K=306–356 and P/mm Hg=0.3–1.6

Prepared By:

A. L. Horvath

Experimental Data

Solubility of $C_2Cl_3F_3$ in 25 mass % NaCl solution

t/°C	p_1 /atm	S/ppm atm^{-1}	$100w_1$ (compiler)	10^6x_1 (compiler)
32.5	0.320	24.8	2.40×10^{-3}	2.790
59.0	1.400	60.7	5.20×10^{-3}	6.045
83.0	1.59	44.9	3.89×10^{-3}	4.522

Auxiliary Information

Method/Apparatus/Procedure:

The saturation of 1,1,2-trichloro-1,2,2-trifluoroethane in aqueous salt solution was performed in a steel vessel during 10 h. The mixture was stirred and left to stand for 7 h before the gas chromatographic analysis. The chromatograph was equipped with an electron capture detector. The determination of the solubility at a given condition was repeated five or six times. Further details are available.[1]

Source and Purity of Materials:

(1) Samples from du Pont, purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:

Solubility: ±11.4% std. dev.
Temperature: ±0.5 K.

References:

[1] G. W. Hellström, M. Sc. thesis, University of Utah, Salt Lake City, Utah, Dec. 1976.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

7. Tetrachloroethene with Water

Critical Evaluation

The tetrachloroethene (1) and water (2) binary system is discussed in two parts; part 1 is tetrachloroethene (1) in water (2) and part 2 is water (2) in tetrachloroethene (1).

Part 1. The solubility of tetrachloroethene (1) in water (2) has been studied by at least 24 groups of workers as recorded in the Compilation Sheets immediately following this Critical Evaluation.

The experimental data of most investigators in the temperature interval between 273 and 373 K are in very poor agreement and in the absence of other independent studies, it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be established.

The data of Antropov *et al.*,[1] Prosyanov *et al.*,[2] Lincoff and Gossett,[3] Yoshioka *et al.*,[4] and Howe *et al.*[5] are markedly lower than other results and are therefore rejected. The solubility values of Freed *et al.*,[6] Veith *et al.*,[7] Banerjee *et al.*,[8] and Mackay *et al.*[9] appear significantly higher than the likely solubility and are also rejected.

The remaining data of Wright and Schaffer,[10] McGovern,[11] Chitwood,[12] O'Connell,[13] Simonov *et al.*,[14] McConnell *et al.*,[15] Pearson *et al.*,[16] Archer and Stevens,[17] Moiseeva *et al.*,[18] Sato and Nakijima,[19] Coca and Diaz,[20] Leighton and Calo,[21] Munz,[22] Gossett,[23] and Warner *et al.*[24] covering the temperature interval from 273 to 343 K are shown in Fig. 1. From the description of the experimental measurements and the reliability of the results reported, it is reasonable to include all the data points, with the except those mentioned above (Refs. 1–9) from further analysis. Therefore, all the tetrachloroethene in water solubility data (Refs. 20–24), except Refs. 1–9, were combined to obtain the following mass percent (1) equation:

$$\text{Solubility } [100w_1]=0.26479-1.5487\times10^{-3}(T/\text{K})+2.4477\times10^{-6}(T/\text{K})^2,$$

which gives a standard deviation of 4.37×10^{-3}.

The curve obtained from the smoothing equation shows a distinct minimum at 316.4 K as seen in Fig. 2. The existence of the minimum solubility is discussed in the Preface.

The approximate solubilities between 273 and 373 K have been calculated from the above equation and presented in Table 1 as doubtful values.

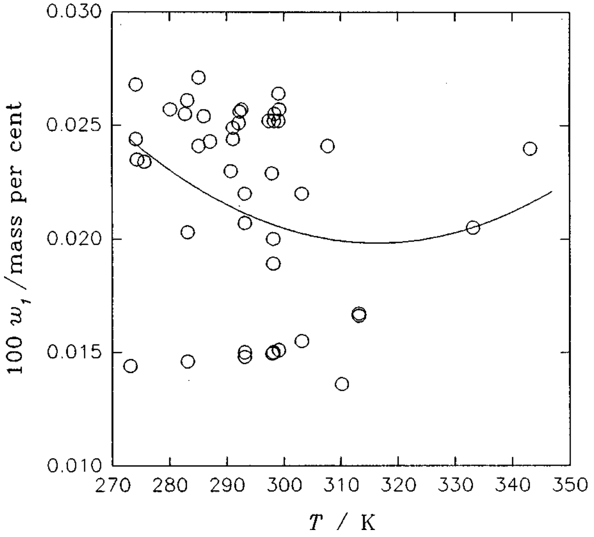

FIG. 2. Solubility of tetrachloroethene (1) in water (2).

TABLE 1. Approximate solubility of tetrachloroethene (1) in water (2)

Temperature		Solubility	
°C	K	$100w_1$	10^5x_1
0	273.15	0.0244	2.65
5	278.15	0.0234	2.54
10	283.15	0.0225	2.44
15	288.15	0.0218	2.37
20	293.15	0.0211	2.29
25	298.15	0.0206	2.24
30	303.15	0.0202	2.19
35	308.15	0.0200	2.17
40	313.15	0.0198	2.15
45	318.15	0.0198	2.15
50	323.15	0.0199	2.16
55	328.15	0.0202	2.19
60	333.15	0.0205	2.23
65	338.15	0.0210	2.28
70	343.15	0.0216	2.35

Part 2. The solubility of water (2) in tetrachloroethene (1) in the temperature interval of 283–323 K has been reported by nine groups of workers.

The solubility data of Bell[25] are markedly lower than other results and, therefore, have been rejected. The remaining data from the eight studies of McGovern,[11] Simonov *et al.*,[14] Simonov *et al.*,[26] Antropov *et al.*,[1] Simonov *et al.*,[27] Archer and Stevens,[17] Coca and Diaz,[20] and Ohtuka and Kazama[28] were compiled or used for the smoothing equation between 283 and 323 K, see Fig. 3:

$$\log_{10} x_2 = 2.7279 - 1730.74/(T/\mathrm{K}). \tag{2}$$

The above equation yielded a standard deviation of 5.70×10^{-2}. The recommended solubilities at 5 K intervals for water in tetrachloroethylene are presented in Table 2.

TABLE 2. Recommended solubility of water (2) in tetrachloroethene (1)

Temperature		Solubility	
°C	K	$100w_2$	10^4x_2
10	283.15	0.00448	4.125
15	288.15	0.00572	5.266
20	293.15	0.00725	6.668
25	298.15	0.00911	8.375
30	303.15	0.01135	10.440
35	308.15	0.01405	12.922
40	313.15	0.01729	15.889
45	318.15	0.02112	19.404
50	323.15	0.02564	23.556

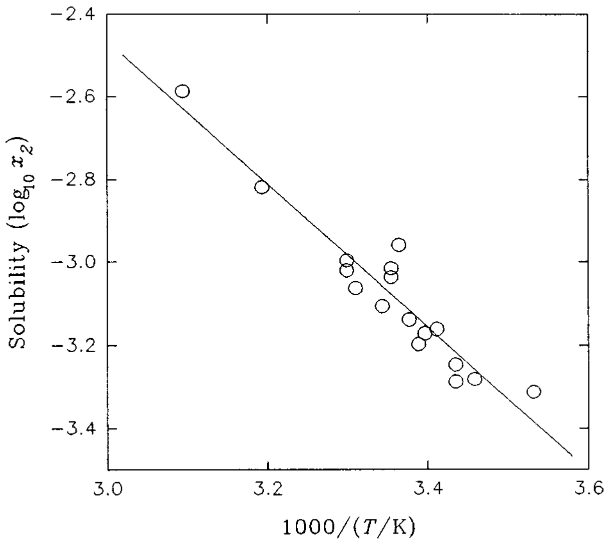

FIG. 3. Solubility of water (2) in tetrachloroethene (1).

References:

[1] L. I. Antropov, V. E. Populyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, (1972). (VINITI No. 3739-71).

[2] N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 183 (1973).

[3] A. H. Lincoff and J. M. Gossett, in *Gas Transfer at Water Surfaces*, edited by W. Brutsaert and G. H. Jirka (Reidel, Dordrecht, 1984), pp. 17–25.

[4] Y. Yoshioka, Y. Ose, and T. Sato, Ecotoxicol. Environ. Saf. **12**, 15 (1986).

[5] G. B. Howe, M. E. Mullins, and T. N. Rogers, Report ESL-TR-86-66, *Vol. 1*, AFESC Tyndall Air Force Base, Florida (September 1987), 86 pp. (AD-A188 571).

[6] V. H. Freed, C. T. Chiou, D. Schmedding, and R. Kohnert, Environ. Health Perspect. **30**, 75 (1979).

[7] G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, Philadelphia, 1980, ASTM Publ. 767, pp. 116–29.

[8] S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

[9] D. Mackay *et al.* "Volatilization of Organic Pollutants from Water," U.S. EPA Report 600/3-82-019, Athens, Georgia (1982) (PB 82-230939).

[10] W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

[11] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

[12] B. G. Chitwood, J. Am. Chem. Soc. **7**, 91 (1952).

[13] W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

[14] V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48,** 1573 (1974).

[15] G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).

[16] C. R. Pearson and G. McConnell, Proc. R. Soc. London Ser. B. **189**, 305 (1975).

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[18] L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

[19] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

[20] J. Coca and R. M. Diaz, J. Chem. Eng. Data **25**, 80 (1980).

[21] D. T. Leighton, and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

[22] C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

[23] J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

[24] H. P. Warner, J. M. Cohen, and J. C. Ireland, "Determination of Henry's Law Constants of Selected Priority Pollutants," U.S. EPA Technical Report PB87-212684, Cincinatti, OH (July 1987).

[25] R. P. Bell, J. Chem. Soc. 2905 (1932).

[26] V. D. Simonov, V. E. Pogulyai, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **44**, 1755 (1970).

[27] V. D. Simonov *et al.*, Dokl. Neftekim. Sekt., Bashkir. Respub. Pravl. Vses. Khim. Obshchest. 346 (1971).

[28] K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	5.30×10^3	1.89×10^{-2}	2.05

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of tetrachloroethene with a large volume of water and measuring the volume of the undissolved tetrachloroethene.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and then redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]

Original Measurements:

R. P. Bell, J. Chem. Soc. 2905 (1932).

Variables:

T/K=288–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1 V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
15	6.50×10^{-2}	3.98×10^{-3}	3.66
20	8.45×10^{-2}	5.21×10^{-3}	4.79
25	1.08×10^{-1}	6.69×10^{-3}	6.15

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of water and tetrachloroethene of about 1 to 5 volume ratio was placed in a sample vessel and rotated in a thermostat for 12 h. After the equilibrium attained, samples were taken and filtered through cottonwool. The determination of the water content was based upon the reaction with α-naphthoxydichlorophosphine. The evolved HCl gas was absorbed in water and titrated with NaOH solution.[1] Two to three successive determinations were carried out with the samples.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial reagent, fractionated three times before use, b.p.=124–125 °C.

Estimated Errors:

Solubility: ±3.5% mean dev.
Temperature: ±0.02 K.

References:

[1] R. P. Bell, J. Chem. Soc. 2903 (1932).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K=273–343

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^4 x_2 (compiler)
0	1.44×10^{-2}	1.56	—	—
10	1.46×10^{-2}	1.59	5.3×10^{-3}	4.88
20	1.48×10^{-2}	1.61	7.5×10^{-3}	6.90
25	1.50×10^{-2}	1.63	1.05×10^{-2}	9.66
30	1.55×10^{-2}	1.68	1.1×10^{-2}	10.1
40	1.67×10^{-2}	1.81	—	—
60	2.05×10^{-2}	2.23	—	—
70	2.40×10^{-2}	2.61	—	—

Solubility data as a function of temperature were presented in graphical form only except for data values at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial grade, source not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: Not specified.
Temperature: Not specified.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, Am. Chem. Soc. **7**, 91 (1952).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	2.0×10^{-2}	2.17	1.21×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
20	1.5×10^{-2}	1.5×10^{-2}	1.63

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemicals Co., used as received.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]

Original Measurements:

V. D. Simonov, V. E. Pogulyai, and T. M. Shamsutdinov Russ. J. Phys. Chem. **44**, 1755 (1970).

Variables:

T/K=303–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
30	1.04×10^{-2}	9.56	5.77×10^{-4}
50	2.82×10^{-2}	25.90	1.56×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of tetrachloroethene and water was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Distilled (compiler).

(2) Pure grade, washed with Na_2CO_3 solution and redistilled before use.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]

Original Measurements:

V. D. Simonov *et al.*, Dokl. Neftekim. Sekt., Bashkir. Respub. Pravl. Vses. Khim. Obshchest. **1**, 346 (1971).

Variables:

$T/K = 289-302$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$10^5\ w_1$ Alekseev	Fischer	Spectroscopy	$10^4\ x_1$ Alekseev	Fischer	Spectroscopy
16	5.70	5.73	5.5	5.244	5.272	5.060
18	6.35	—	6.0	5.842	—	5.520
21.3	7.17	—	7.5	6.596	—	6.900
23	7.91	7.95	7.8	7.296	7.313	7.175
29	9.37	9.45	−8.618	8.692	—	

Auxiliary Information

Method/Apparatus/Procedure:

The determination of the solubility of water in tetrachloroethene was based on the infrared spectroscopic method. A UR-20 spectrophotometer was used with 2 cm cuvettes and the windows made of KBr. The spectra were recorded at 3600–810 cm^{-1}, and the absorbance at 3702 cm^{-1} was found by the baseline method. Standard mixtures of tetrachloroethene and water were used for the calibration graphs. The results obtained were compared with measurements made by the method of cloud point[1] and a Karl Fischer titration.

Source and Purity of Materials:

(1) Distilled.
(2) ''Ch'' brand, treated with Na_2CO_3 solution, dried with $CaCl_2$ and P_2O_5 and then distilled before use.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] V. F. Alekseev, Wiad. Ann. **28**, 305 (1886).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972) (VINITI No. 3739-71).

Variables:

$T/K = 288-299$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$100\ w_1$	$10^6\ x_1$ (compiler)	$100\ w_2$	$10^4\ x_2$ (compiler)
15	7.5×10^{-3}	8.15	—	—
18	—	—	5.62×10^{-3}	5.17
20	8.74×10^{-3}	9.50	—	—
22	—	—	6.91×10^{-3}	6.36
26	1.51×10^{-2}	16.41	8.5×10^{-3}	7.82

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of tetrachloroethene and water was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Source not given, treated with Na_2CO_3 solution and further purified by distillation.
(2) Distillation

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 183 (1973).

Variables:

T/K=298–373

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^7 x_1 (compiler)
25	3.080×10^4	7.29×10^{-4}	7.92
50	1.090×10^4	6.91×10^{-3}	7.507×10^1
70	4.760×10^3	3.61×10^{-2}	3.9218×10^2
90	2.370×10^3	1.490×10^{-1}	1.6210×10^3
100	1.760×10^3	2.782×10^{-1}	3.0294×10^3

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

The distribution coefficient was determined by sample distillation in a stream of an inert carrier gas which was employed for the sampling of the equilibrium vapor phase. The concentration of the compound studied in both phases was determined through the use of a ^{36}Cl labeled compound.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]

Original Measurements:

N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 55 (1974).

Variables:

T/K=298–358

Prepared By:

A. L. Horvath

Experimental Data

$$\log_{10} \alpha = \frac{1308.48}{(T/\mathrm{K})} - 0.581,$$

where α=distribution coefficient.

At the normal boiling point of C_2Cl_4 , $\alpha=548$ and the activity coefficient, $\gamma_1=273$.

Auxiliary Information

Method/Apparatus/Procedure:

The water concentration in tetrachloroethene rich phase was determined by a radiometric method using tritium labeled water. The experimental procedure is described in more detail elsewhere (Ref. 1).

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 100 (1973).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. D. Simonov, T. M. Shamsutdinov, V. E. Pogulyai, and L. N. Popova, Russ. J. Phys. Chem. **48**, 1573 (1974).

Variables:

T/K=313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
40	1.66×10^{-2}	1.80	1.66×10^{-2}	1.52

Auxiliary Information

Method/Apparatus/Procedure:

The synthetic method of Alexejew was used. For further details are found elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] V. D. Simonov, L. N. Popova, T. M. Shamsutdinov, V. E. Pogulyai, and F. A. Mamina, Symp. Dokl. Neftekhimicheskoi Sektsii, Ufa, No. 6 (1971).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13-8 (1975).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^6 g_1/g_2	100 w_1 (compiler)	10^5 x_1 (compiler)
20	150	1.50×10^{-2}	1.63

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of tetrachloroethene in water was determined by gas–liquid chromatography (GLC) using an electron capture detector. Where possible, identification was confirmed by a linked mass spectrometer (MS).

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. R. Pearson and G. McConnell, Proc. R. Soc. London Ser. B **189**, 305 (1975).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	150	1.50×10^{-2}	1.63

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with n-pentane and an aliquot of the extract taken for GLC analysis. The gas chromatograph was fitted with a ^{63}Ni electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. L. Archer and V. L. Stevens, I&EC Prod. Res. Dev. **16**, 319 (1977).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100\ g_1/g_2$	$10^5\ x_1$ (compiler)	$100\ g_2/g_1$	$10^4\ x_2$ (compiler)
25	1.5×10^{-2}	1.63	1.0×10^{-2}	9.20

Original source is Ref. 1.

Auxiliary Information

Method/Apparatus/Procedure:

Details are not given.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] News Release from Dow Chemical USA (October 23, 1975).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1997).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	0.2065	2.069×10^{-2}	2.25

Auxiliary Information

Method/Apparatus/Procedure:

Water was saturated with tetrachloroethene in a thermostatted round bottomed flask fitted with a stirrer and a mercury seal. The stirring was continued for several days until equilibrium between the two liquids was established. The analysis of the saturated aqueous solution was carried out using a gas chromatograph. The column was filled with Cromosorb W, impregnated with Apiezon I. The helium carrier gas flow rate was 500 cm^3/min.

Source and Purity of Materials:

(1) Type ''pure'' (METU 6-00 No. 6590-70), redistilled and checked by GLC.
(2) Distilled.

Estimated Errors:

Solubility: ±1.74%.
Temperature: ±0.2 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^5 x_1 (compiler)
37	0.43	1.36×10^{-2}	1.48

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

Tetrachloroethene vapor was equilibrated in an airtight vial between water and the overlying air. When equilibrium was established, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and was injected into a gas chromatograph and analyzed. The peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.17 std. dev.
Temperature: ±0.5 K (compiler).

Components:	Original Measurements:
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4] (2) Water; H_2O; [7732-18-5]	V. H. Freed, C. T. Chiou, D. W. Schmedding, and R. Kohnert, Environ. Sci. Technol. **30**, 75 (1979).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25	400	4.0×10^{-2}	4.35

Auxiliary Information

Method/Apparatus/Procedure:

A known volume of water was mixed with tetrachloroethene in an Erlenmeyer flask. The flask was immersed in a water bath and magnetically stirred. Samples were removed for analyses at regular intervals. All samples were analyzed using a gas–liquid chromatography equipped with an electron capture detector. The solubility given is the average of five consecutive samples with less than 5% variation.

Source and Purity of Materials:

(1) Source not given; analytical grade, purity greater than 95%.
(2) Distilled and run through a resin column.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:	Original Measurements:
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4] (2) Water; H_2O; [7732-18-5]	J. Coca and R. M. Diaz, J. Chem. Eng. Data **25**, 80 (1980).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$100\ w_1$	$10^5\ x_1$ (compiler)	$100\ w_2$	$10^5\ x_2$ (compiler)
25	2.0×10^{-2}	2.17	1.0×10^{-2}	9.20

Auxiliary Information

Method/Apparatus/Procedure:

Saturation was determined by titration. The measurement was performed in an Erlenmeyer flask by adding tetrachloroethene to water until a permanent turbidity was observed. The flask was immersed in a water bath thermostat while maintaining a constant agitation through the use of a magnetic stirrer.

Source and Purity of Materials:

(1) Fluka laboratory grade reagent, further purified by distillation; middle fraction used.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4] (2) Water; H_2O; [7732-18-5]	G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 767, Philadelphia, PA, 1980, pp. 116–29.
Variables:	**Prepared By:**
$T/\mathrm{K}=293$	A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	$n_1 V_2^{-1}/\mathrm{mol\ dm}^{-3}$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	2.66×10^{-3}	4.78×10^{-2}	5.19

Auxiliary Information

Method/Apparatus/Procedure:

An excess of tetrachloroethene was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
$T/\mathrm{K}=298$	A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	$10^{-3}\ c_1\ /\mathrm{mol\ dm}^{-3}$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25	2.92×10^{-3}	4.85×10^{-2}	5.27

Auxiliary Information

Method/Apparatus/Procedure:

An excess of tetrachloroethene was added to a stainless steel tube containing water and then the tube was sealed. The equilibration occurred during shaking for 1 week at 25 °C. After centrifugation, the concentration was obtained from a measurement of radioactivity through liquid scintillation counting. The solubility procedure was carried out at least twice for each sample and the analysis was done in duplicate.

Source and Purity of Materials:

(1) New England Nuclear, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±1.0% std. dev.
Temperature: ±0.3 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
Variables:	**Prepared By:**
T/K=274–299	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^5 x_1 (compiler)
1.0	2.069×10^2	2.676×10^{-2}	2.908
1.0	2.267×10^2	2.442×10^{-2}	2.654
1.2	2.361×10^2	2.346×10^{-2}	2.549
2.5	2.604×10^2	2.339×10^{-2}	2.542
7.0	3.141×10^2	2.566×10^{-2}	2.788
10.0	3.702×10^2	2.609×10^{-2}	2.835
12.0	4.010×10^2	2.711×10^{-2}	2.946
12.0	4.373×10^2	2.486×10^{-2}	2.701
12.9	4.529×10^2	2.545×10^{-2}	2.765
14.0	5.015×10^2	2.435×10^{-2}	2.646
18.0	6.151×10^2	2.492×10^{-2}	2.708
18.0	6.272×10^2	2.444×10^{-2}	2.656
18.0	6.275×10^2	2.443×10^{-2}	2.655
19.0	6.449×10^2	2.513×10^{-2}	2.731
19.2	6.339×10^2	2.557×10^{-2}	2.779
19.5	6.479×10^2	2.512×10^{-2}	2.795
24.3	8.681×10^2	2.518×10^{-2}	2.736
25.2	8.898×10^2	2.523×10^{-2}	2.742
25.3	9.054×10^2	2.546×10^{-2}	2.767
26.0	8.968×10^2	2.639×10^{-2}	2.868
26.0	9.388×10^2	2.521×10^{-2}	2.739
26.1	9.207×10^2	2.570×10^{-2}	2.773

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL tetrachloroethene sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The tetrachloroethene content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±2.3%.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]	K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	2.0×10^{-1}	1.2×10^{-2}	1.10

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 tetrachloroethene in a flask which was then lowered into a thermostat bath. The flask was shaken vigorously until the first cloud (turbidity) appeared. The sample water content was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial JTS extra pure reagent, further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Mackay *et al.*, ‘‘Volatilization of Organic Pollutants from Water,’’ U.S. EPA Report **600/3-82-019**, Athens, Georgia (1982) (PB 82-230939).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	0.400	4.00×10^{-2}	4.347

Auxiliary Information

Method/Apparatus/Procedure:

An aqueous solution with an excess amount of tetrachloroethene was stirred for 1 day before being introduced into a 1 L glass vessel. Nitrogen entered at the bottom of the vessel through a sintered glass disk. The exit gas flow rate was measured by a soap bubble flow meter. The concentration of tetrachloroethene in water was determined by gas chromatography. The GC was equipped with both a dual flame ionization detector and an electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Doubly distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1.0 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. H. Lincoff and J. M. Gossett, in *Gas Transfer at Water Surfaces*, edited by W. Brutsaert and G. H. Jirka (Reidel Dordrecht, 1984), pp. 17–25.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

EPICS method

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	1.30×10^{-2}	2.379×10^{-2}	2.585

$$\log_e H=13.12-5119/(T/\mathrm{K})$$

Batch air stripping method

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	1.16×10^{-2}	2.666×10^{-2}	2.897

$$\log_e H=11.32-4622/(T/\mathrm{K})$$

Auxiliary Information

Method/Apparatus/Procedure:

Henry's law constants were measured by EPICS and Batch Air Stripping Methods. The Equilibrium Partitioning in the Closed Systems technique compares the GC peak heights upon direct injection of headspace samples. In the Batch Air Stripping Method, equal volume samples were placed in serum battles and the equilibrated headspaces contained concentrations proportional to original concentrations in the aqueous samples. Full equilibrium was achieved in a few hours.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5%–10%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4] (2) Water; H_2O; [7732-18-5]	C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
10	3.691×10^{-1}	2.030×10^{-2}	2.206
20	5.816×10^{-1}	2.203×10^{-2}	2.394
30	9.544×10^{-1}	2.201×10^{-2}	2.392

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Matheson Coleman & Bell, OH.; greater than 99.5% pure.
(2) Distilled and deionized.

Estimated Errors:

Solubility: ±0.019 std. dev.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4] (2) Water; H_2O; [7732-18-5]	Y. Yoshioka, Y. Ose, and T. Sato, Ecotoxicol. Environ. Saf. **12**, 15 (1986).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^3\ \rho_1$ /g m^{-3}	$100\ w_1$ (compiler)	$10^7\ x_1$ (compiler)
20	1.8[a]	1.8×10^{-4}	1.96

[a] Cited value in the original paper is in error (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A supersaturated solution of tetrachloroethene in water was agitated for 2 h at 20 °C. After storing for 2 h the water phase was filtered through Whatman No. 2 filter paper before analysis. The concentration of tetrachloroethene in water was determined by gas chromatography or by ultraviolet spectroscopy.

Source and Purity of Materials:

(1) Source not given, analytical grade reagent.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. P. Warner, J. M. Cohen, and J. C. Ireland, ‘‘Determination of Henry’s Law Constants of Selected Priority Pollutants, U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987)

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry’s law constant, H/m^3 atm/mol^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
24.85	2.87×10^{-2}	1.495×10^{-2}	1.624

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry’s law constants, as described by Mackay *et al.*,[1] was used. The general procedure was to add an excess quantity of tetrachloroethene to distilled de-ionized water, place the sample in a thermostat bath, and mix overnight. A portion of this solution was returned to the stripping vessel. Tetrachloroethene was stripped isothermally from the solution mixture at a known gas flow rate. The Henry’s law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used without further purification, stated purity greater than 99%.
(2) Distilled de-ionized.

Estimated Errors:

Solubility: ±6.0% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:

T/K=283–308

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry’s law constant, H/m^3 atm mol^{-1}	CV[a] %	100 w_1 (compiler)	10^5 x_1 (compiler)
9.6	6.82×10^{-3}	3.75	2.553×10^{-2}	2.774
17.5	1.17×10^{-2}	1.28	2.299×10^{-2}	2.498
24.8	1.77×10^{-2}	4.81	2.292×10^{-2}	2.491
34.6	2.82×10^{-2}	1.63	2.405×10^{-2}	2.613

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry’s law constants. A precise quantity of tetrachloroethene was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Alfa Products, ultrapure; greater than 99% pure.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, Report ESL-TR-86-66, Vol. 1, AFESC Tyndall Air Force Base, Florida (September 1987), 86 pp. (AD-A188 571).
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
10	99	9.9×10^{-3}	1.076
20	136	1.36×10^{-2}	1.467
30	116	1.16×10^{-2}	1.260

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. A measured volume of tetrachloroethene was injected into the bottles through each septum using a microliter syringe. Tetrachloroethene was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC response was compared with calibration plots.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% pure, used as received.
(1) Distilled de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4] (2) MQ-Water	C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

8. Tetrachloroethene with MQ-Water

Experimental Data

t/°C	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	6.04×10^{-1}	2.12×10^{-2}	2.305

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Matheson Coleman & Bell, OH.; greater than 99.5% pure.
(2) 0.25 mg total organic carbon/dm^3 and 0.75 mg COD/dm^3.

Estimated Errors:

Solubility: ±0.003 std. dev.
Temperature: ±0.5 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]
(2) Municipal tap water (PASE)

Original Measurements:

C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

Variables:

$T/K=293$

Prepared By:

A. L. Horvath

9. Tetrachloroethene with Municipal Tap Water (PASE)

Experimental Data

$t/°C$	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	6.73×10^{-1}	1.91×10^{-2}	2.072

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were pre-concentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Matheson Coleman & Bell, OH.; greater than 99.5% pure.
(2) 10 mg total organic carbon/dm^3 and 40 mg COD/dm^3.

Estimated Errors:

Solubility: ±0.035 std. dev.
Temperature: ±0.5 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]
(2) Ammonium carbonate; $(NH_4)_2CO_3$; [506-87-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

Variables:

$T/K=293$; concentration/mol $dm^{-3}=1-2$

Prepared By:

A. L. Horvath

10. Tetrachloroethene with Ammonium Carbonate and Water

Experimental Data

$t/°C$	$10^{-3}\ c_2$ /mol dm^{-3}	$10^3\ \rho_1$ /g m^{-3}	$100\ w_1$ (compiler)
20	1.00	100.0 ± 5.6	9.6×10^{-3}
	1.62	78.8 ± 1.3	7.5×10^{-3}
	2.10	77.2 ± 1.8	7.0×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tertachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''chemically pure.''
(3) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Hydrogen chloride; HCl; [7647-01-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

Variables:

T/K=293; concentration/mol dm^{-3}=0.2–2

Prepared By:

A. L. Horvath

11. Tetrachloroethene with Hydrogen Chloride and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	0.20	198.5±6.8	1.98×10^{-2}
	1.00	199.0±6.1	1.95×10^{-2}
	1.64	199.1±12.9	1.93×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flask fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''chemically pure.''
(3) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Hydrogen chloride; HCl; [7647-01-0]
(3) Sodium chloride; NaCl; [7647-14-5]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

Variables:

T/K=293; concentration/mol dm^{-3}=0.3–2

Prepared By:

A. L. Horvath

12. Tetrachloroethene with Hydrogen Chloride, Sodium Chloride, and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^{-3} c_3 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	0.27	0.17	89.8±1.3	8.94×10^{-3}
	0.96	0.17	85.5±4.7	8.41×10^{-3}
	1.64	0.17	82.5±8.0	8.01×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) and (3) Type ''chemically pure.''
(4) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Nitric acid; HNO_3; [7697-37-2]
(3) Ammonium nitrate; NH_4NO_3; [6484-52-2]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

Variables:

T/K=293; concentration/mol dm^{-3}=0–4

Prepared By:

A. L. Horvath

13. Tetrachloroethene with Nitric Acid, Ammonium Nitrate, and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^{-3} c_3 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	0.08	1.25	160.0±3.0	1.58×10^{-2}
	0.80	1.25	232.5±8.0	2.26×10^{-2}
	2.40	1.25	292.0±9.4	2.70×10^{-2}
	3.20	1.25	297.5±6.5	2.69×10^{-2}
	4.00	1.25	334.0±9.4	2.96×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''chemically pure.''
(3) Type ''chemically pure.''
(4) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4]
(2) Phosphoric acid; H_3PO_4; [7664-38-2]
(3) Sulfuric acid; H_2SO_4; [7664-93-9]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

Variables:

T/K=293; concentration/mol dm^{-3}=1–3

Prepared By:

A. L. Horvath

14. Tetrachloroethene with Phosphoric Acid, Sulfuric Acid, and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^{-3} c_3 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	1.0	0.2	163.1±4.6	1.53×10^{-2}
	1.7	0.2	146.9±3.1	1.35×10^{-2}
	2.0	0.2	144.1±8.0	1.31×10^{-2}
	2.6	0.2	130.5±2.2	1.14×10^{-2}
	3.0	0.2	129.7±2.6	1.12×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''analysis pure.''
(3) Type ''chemically pure.''
(4) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).
Variables:	**Prepared By:**
T/K=293; concentration/mol dm^{-3}=0.2–2	A. L. Horvath

15. Tetrachloroethene with Sodium Chloride and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	0.17	139.2±6.8	1.38×10^{-2}
	1.70	73.1±1.5	6.84×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''chemically pure.''
(3) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:	**Original Measurements:**
(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4; [127-18-4] (2) Sulfuric acid; H_2SO_4; [7664-93-9] (3) Water; H_2O; [7732-18-5]	L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).
Variables:	**Prepared By:**
T/K=293; concentration/mol dm^{-3}=0–1	A. L. Horvath

16. Tetrachloroethene with Sulfuric Acid and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	0.05	194.9±6.2	1.94×10^{-2}
	1.00	168.6±6.8	1.58×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''chemically pure.''
(3) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:

(1) Tetrachloroethene (tetrachloroethylene); C_2Cl_4 ; [127-18-4]
(2) Sulfuric acid; H_2SO_4 ; [7664-93-9]
(3) Ammonium sulfate; $(NH_4)_2SO_4$; [7783-20-2]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

L. M. Moiseeva, G. G. Stepanova, and A. N. Pukhonto, Sov. Chem. Ind. **9**, 453 (1977).

Variables:

T/K=293; concentration/mol dm^{-3}=0.1–2

Prepared By:

A. L. Horvath

17. Tetrachloroethene with Sulfuric Acid, Ammonium Sulfate, and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	10^{-3} c_3 /mol dm^{-3}	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)
20	0.10	0.75	89.2±5.7	8.44×10^{-3}
	0.50	0.75	72.0±0.0	6.82×10^{-3}
	1.50	0.75	92.0±2.1	8.39×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirrers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals to check for equilibrium. The concentration of tetrachloroethene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials:

(1) Type ''pure'' (MRTU 6-00 No. 6590-70), redistilled and checked by GC before use.
(2) Type ''chemically pure.''
(3) Type ''analysis pure.''
(4) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.2 K.

Components:

(1) 1,1,2,2-tetrachloro-1,2-difluoroethane; $C_2Cl_4F_2$; [76-12-0]; R-112
(2) Water; H_2O; [7732-18-5]

Original Measurements:

du Pont de Nemours & Company, ''Solubility Relationships between Fluorocarbons and Water,'' Tech. Bull. B-43, Wilmington, Del. (1966), 17 pp.

Variables:

T/K=300–301

Prepared By:

A. L. Horvath

18. 1,1,2,2-Tetrachloro-1,2-Difluoroethane and Water

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
27	1.58×10^{-1}	1.40	—	—
28	—	—	9.9×10^{-3}	1.12

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source not given, 0.8% CCl_3 .$CClF_2$ content.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) Hexachloroethane; C_2Cl_6 ; [67-72-1]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

19. Hexachloroethane and Water

Critical Evaluation

All the available data for the solubility of hexachloroethane (1) in water (2) are summarized in Table 1.

The data are in very poor agreement and in the absence of other independent studies it is not possible to determine which of the values are most reliable. Further studies will be necessary before even tentative values can be selected.

TABLE 1. Reported solubility of hexachloroethane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^6 x_1	References
10	283.15	0.00231	1.758	1
		0.0041	3.120	2
20	293.15	0.0272	20.69	3
		0.00275	2.093	1
		0.000771	0.587	4
		0.0037	2.816	2
22.3	295.45	0.005	3.81	5
		0.005	3.81	6
24.85	298.00	0.00112	0.855	7
25	298.15	0.005	3.81	8
30	303.15	0.00324	2.465	1
		0.0041	3.120	2

References:

[1] C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

[2] G. B. Howe, M. E. Mullins, and T. N. Rogers, Report ESL-TR-86-66, *Vol. 1*, AFESC Tyndall Air Force Base, Florida (September 1987), 86 pp. (AD-A188 571).

[3] G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 707, Philadelphia, 1980, pp. 116–29.

[4] C. D. Munz and P. V. Roberts, Environ. Sci. Technol. **20**, 830 (1986).

[5] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

[6] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

[7] H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

[8] W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

Components:

(1) Hexachloroethane [67-72-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Amer. J. Hyg. **16**, 325 (1932).

Variables:

$T/\text{K}=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\text{C}$	$V_2\ g_1^{-1}/\text{cm}^3\ \text{g}^{-1}$	100 w_1 (compiler)	10^6 x_1 (compiler)
25	2.0×10^4	5.0×10^{-3}	3.81

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of hexachloroethane with a large volume of water and measuring the volume of the undissolved portion.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and then redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Hexachloroethane; C_2Cl_6; [67-72-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=295

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	100 g_1/g_2	100 w_1 (compiler)	$10^6\ x_1$ (compiler)
22.3	5.0×10^{-3}	5.0×10^{-3}	3.81

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Hexachloroethane; C_2Cl_6; [67-72-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K=295

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	100 w_1	$10^6\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
22.3	5.0×10^{-3}	3.81	2.11×10^{-5}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial grade, source not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Hexachloroethane; C_2Cl_6 ; [67-72-1] (2) Water; H_2O; [7732-18-5]	G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 707, Philadelphia, PA, 1980, pp. 116–29.
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	1.148×10^{-4}	2.72×10^{-2}	2.069

Auxiliary Information

Method/Apparatus/Procedure:

An excess of hexachloroethane was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:	**Original Measurements:**
(1) Hexachloroethane; C_2Cl_6 ; [67-72-1] (2) Water; H_2O; [7732-18-5]	C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/dimensionless	10^3 ρ_1 /g m^{-3}	100 w_1 (compiler)	10^6 x_1 (compiler)
10	6.12×10^{-2}	23.1	2.31×10^{-3}	1.758
20	1.17×10^{-1}	27.5	2.75×10^{-3}	2.093
30	2.13×10^{-1}	32.4	3.24×10^{-3}	2.465

Auxiliary Information

Method/Apparatus/Procedure:

An excess amount of hexachloroethane with water was introduced into 30 cm^3 centrifuge tubes that were closed with a screw cap. The tubes were rotated for 3 days inside a temperature controlled chamber at 10, 20, and 30° C, respectively. Samples were taken from the tubes and analyzed by gas chromatography after liquid–liquid extraction. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Supelco, Inc., PA., contained 3%–5% C_2Cl_4 as a contaminant.
(2) Distilled and de-ionized

Estimated Errors:

Solubility: $\pm8.5\times10^{-3}$ std. dev.
Temperature: ±0.5 K.

Components:
(1) Hexachloroethane; C_2Cl_6 ; [67-72-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
C. D. Munz and P. V. Roberts, Environ. Sci. Technol. **20**, 830 (1986).

Variables:
$T/K=293$

Prepared By:
A. L. Horvath

Experimental Data

$t/°C$	$g_1V_2^{-1}/g\ m^{-3}$	$100\ w_1$ (compiler)	$10^7\ x_1$ (compiler)
20	7.7	7.71×10^{-4}	5.87

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibration technique of a closed system with analysis of the aqueous phase using ^{14}C liquid scintillation counting yielded the best result as described in a Ph.D. thesis.[1] Duplicate experiments were carried out for the solubility measurements.

Source and Purity of Materials:

(1) Supelco, Inc., PA., contained about 3% C_2Cl_4 as a contaminant.
(2) Distilled and further purified in Milli-Q reagent grade system.

Estimated Errors:

Solubility: ±1%–2%.
Temperature: ±0.1 K.

References:

[1] C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

Components:
(1) Hexachloroethane; C_2Cl_6 ; [67-72-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants, U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

Variables:
$T/K=298$

Prepared By:
A. L. Horvath

Experimental Data

$t/°C$	Henry's law constant, $H/m^3\ atm\ mol^{-1}$	$100\ w_1$ (compiler)	$10^7\ x_1$ (compiler)
24.85	9.85×10^{-3}	1.123×10^{-3}	8.547

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants, as described by Mackay *et al.*,[1] was used. The general procedure was to add an excess quantity of hexachloroethane to distilled de-ionized water, place the sample in a waterbath thermostat, and mix overnight. A portion of this solution was returned to the stripping vessel. Hexachloroethane was stripped isothermally from the solution mixture at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, greater than 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) Hexachloroethane; C_2Cl_6 ; [67-72-1]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, Report ESL-TR-86-66, Vol. 1, ''AFESC Tyndall Air Force Base,'' Florida (September 1987), 86 pp. (AD-A188 571).

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^6\ x_1$ (compiler)
10	41	4.1×10^{-3}	3.12
20	37	3.7×10^{-3}	2.82
30	41	4.1×10^{-3}	3.12

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. A measured volume of hexachloroethane was injected into the bottles through each septum using a microliter syringe. Hexachloroethane was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC response was compared with calibration plots.

Source and Purity of Materials:

(1) Probably a commercial reagent, at least 99% pure, used as received.
(2) Distilled and de-ionizes.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

20. 2-Bromo-2-Chloro-1,1,1-Trifluoroethane with Water

Critical Evaluation

The 2-bromo-2-chloro-1,1,1-trifluoroethane (1) and water (1) binary system is discussed in two parts; part 1 is 2-bromo-2-chloro-1,1,1-trifluoroethane (1) in water (1) and part 2 is water (2) in 2-bromo-2-chloro-1,1,1-trifluoroethane (1).

Part 1. The solubility of 2-bromo-2-chloro-1,1,1-trifluoroethane (1) in water (2) has been reported by 14 laboratories with reasonably consistent results. The only measurement by Saidman *et al.*[1] resulted in a higher value than the likely solubility and has been rejected. The remaining data of 13 laboratories were compiled or used for the smoothing equation. These determinations were reported by Raventos,[2] Larson*et al.*,[3] Duncan,[4] Berndt,[5] Lowe,[6] Okuda,[7] Lowe and Hagler,[8] Laasberg and Hedley-Whyte,[9] Ikeda,[10] Stoelting and Longshore,[11] Halliday *et al.*,[12] Lauven *et al.*,[13] and Horvath.[14] These measurements are sufficiently reliable for use in the smoothing equation and they are shown in Fig. 4 below.

The combined mass percent data covering the temperature interval from 283 to 313 K were correlated to obtain the following mass percent equation:

$$\text{Solubility } [100w_1]=22.0805-0.14127(T/\text{K})+2.300\times10^{-4}(T/\text{K})^2$$

which yielded a standard deviation of 3.80×10^{-2}. The tentative solubility at 5 K intervals for 2-bromo-2-chloro-1,1,1-trifluoroethane in water are presented in the following table.

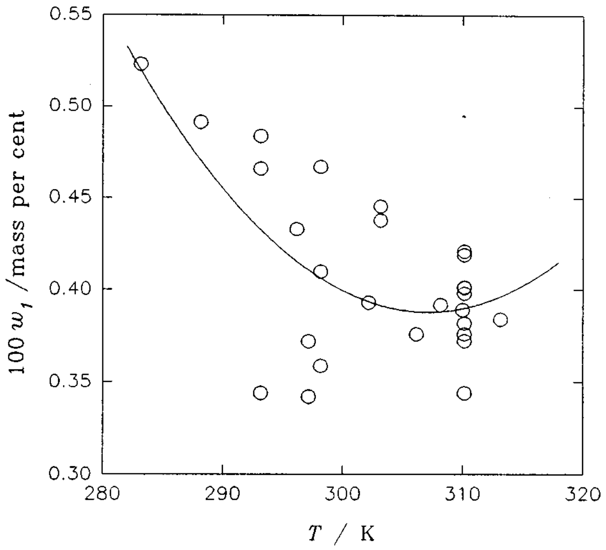

FIG. 4. Solubility of 2-bromo-2-chloro-1,1,1-trifluoroethane (1) in water (2).

TABLE 1. Tentative solubility of 2-bromo-2-chloro-1,11-trifluoroethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
10	283.15	0.521	4.78
15	288.15	0.472	4.33
20	293.15	0.434	3.98
25	298.15	0.407	3.73
30	303.15	0.392	3.59
35	308.15	0.389	3.56
40	313.15	0.397	3.64

Part 2. The solubility of water (2) in 2-bromo-2-chloro-1,1,1-trifluoroethane (1) has been measured by Lees and Sarem[15] and Horvath.[14] The two determinations at 297 and 298 K compare favorably with a recommended (100 w_2) value of 0.035 at 298.15 K.

References:

[1] L. J. Saidman, E. I. Eger, E. S. Munson, and J. W. Severinghaus, Anesthesiology **27**, 180 (1996).

[2] J. Raventos, Brit. J. Pharmacol. **11**, 394 (1956).

[3] C. P. Larson, E. I. Eger, and J. W. Severinghaus, Anesthesiology **23**, 349 (1962).

[4] W. A. M. Duncan, in *Uptake and Distribution of Anesthetic Agents*, edited by E. M. Papper and R. J. Kitz (McGraw-Hill, New York, 1963), pp. 17–9.

[5] P. Berndt, Pharm. Prax. 277 (1964).

[6] H. J. Lowe, in *Theory and Application of Gas Chromatography*, edited by H. S. Kroman and S. R. Bender (Grune and Stratton, New York, 1968), pp. 194–209.

[7] Y. Okuda, Arch. Jap. Chir. **37**, 700 (1968).

[8] H. J. Lowe and K. Hagler, in *Gas Chromatography, Biology and Medicine*, edited by R. Poster (Churchill, London, 1969), pp. 86–112.

[9] L. H. Laasberg and J. Hedley-Whyte, Anesthesiology **32**, 351 (1970).

[10] S. Ikeda, Anesthesiology **37**, 87 (1972).

[11] R. K. Stoelting and R. N. Longshore, Anesthesiology **36**, 503 (1972).

[12] M. M. Halliday, I. MacDonald, and M. H. G. MacGregor, Br. J. Anaest. **49**, 413 (1977).

[13] P. M. Lauven, G. Hack, and H. Stoeckel, Anaesthesist **28**, 104 (1979).

[14] A. L. Horvath, *Halogenated Hydrocarbons* (Marcel Dekker, New York, 1982), 889 pp.

[15] F. P. Lees and P. Sarram, J. Chem. Eng. Data, **16**, 41 (1971).

Components:	Original Measurements:
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7] (2) Water; H_2O; [7732-18-5]	J. Raventos, Br. J. Pharmac. **11**, 394 (1956).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10 ^{4} x_1 (compiler)
20	0.345	0.344	3.15

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Imperial Chemical Industries Limited, Widnes, used as received.

(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. P. Larson, E. I. Eger, and J. W. Severinghaus, Anesthesiol. **23**, 349 (1962).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
37	0.345	0.344	3.15

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by equilibrating water with 2-bromo-2-chloro-1,1,1-trifluoroethane in closed flasks and analyzing the concentration of the overlying gas phase with an infrared halothane analyzer. The flasks were shaken vigorously until identical readings were obtained from the Beckman infrared analyzer. All samples attained equilibrium within 2–4 h. Eleven determinations were carried out.

Source and Purity of Materials:

(1) Supplied by Ayerst Laboratories, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±7%.
Temperature: ±0.5 K.

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. A. M. Duncan, in *Uptake and Distribution of Anesthetic Agents*, edited by E. M. Papper and R. J. Kitz (McGraw-Hill, New York, 1963), pp. 17–9.

Variables:

T/K=283–310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient L/dimensionless	ρ_1 /kg m^3	100 w_1 (compiler)	10^4 x_1 (compiler)
10	3.05	5.23	0.523	4.80
23	1.45	4.32	0.433	3.97
37	0.79	3.95	0.398	3.65

Auxiliary Information

Method/Apparatus/Procedure:

2-bromo-2-chloro-1,1,1-trifluoroethane was added to a measured volume of water in a flask of known volume. The flask was sealed and the contents allowed to equilibrate at the desired temperature. After equilibration, a sample of the liquid phase was withdrawn for analysis using the Burns and Snow modification method for halothane

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7] (2) Water; H_2O; [7732-18-5]	P. Berndt, Pharm. Prax., 277 (1964).

Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	400 V_1 /V_2	100 w_1 (compiler)	10^4 x_1 (compiler)
20	1.0	0.466	4.27

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial reagent from VEB Arzneimittelverk Drezden, contained 0.01% thymol as a stabilizer.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7] (2) Water; H_2O; [7732-18-5]	L. J. Saidman, E. I. Eger, E. S. Munson, and J. W. Severinghaus, Anesthesiol. **27**, 180 (1966)

Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	1.04	0.566	5.19

Auxiliary Information

Method/Apparatus/Procedure:

The conventional Scholander apparatus[1] was used with the reaction chamber unit surrounded by a water bath. A carrier gas containing 2-2-bromo-2-chloro-1,1,1-trifluoroethane was absorbed in water. The change in volume of the original gas sample divided by the original gas volume gave the percentage of 2-bromo-2-chloro-1,1,1-trifluoroethane that was present in the original gas sample. The carrier gas was nitrogen containing 10% 2-bromo-2-chloro-1,1,1-trifluoroethane.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.211 std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] P. F. Schlolander, J. Biol. Chem. **167**, 235 (1947).

Components:	**Original Measurements:**
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7] (2) Water; H_2O; [7732-18-5]	H. J. Lowe, in *Theory and Application of Gas Chromatography*, edited by H. S. Kroman and S. R. Bender (Grune and Stratton, New York, 1968), pp. 194–209.
Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	0.88	0.376	3.44

Auxiliary Information

Method/Apparatus/Procedure:

The direct injection technique was used for the determination of the solubility of 2-bromo-2-chloro-1,1,1-trifluoroethane in water. Ostwald coefficients were determined by equilibration of 2-bromo-2-chloro-1,1,1-trifluoroethane with water in a capped system. After thoroughly mixing, a sample was withdrawn and analyzed in a gas chromatograph equipped with a hydrogen flame detector. The concentration was proportional to the recorded signal peak height.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7] (2) Water; H_2O; [7732-18-5]	Y. Okuda, Arch. Jpn. Chir. **37**, 700 (1968).
Variables:	**Prepared By:**
T/K=288–313	A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
15	2.27±0.22	0.491	4.505
20	1.83±0.13	0.484	4.435
25	1.46±0.07	0.467	4.28
30	1.14±0.04	0.438	4.01
35	0.87±0.04	0.392	3.59
37	0.82±0.03	0.401	3.68
40	0.71±0.04	0.384	3.52

Auxiliary Information

Method/Apparatus/Procedure:

A gas chromatographic analysis combined with a crushed ampoule technique was used. The solubility values were determined by equilibrating 2-bromo-2-chloro-1,1,1-trifluoroethane with water in a sealed ampoule. Then, after the ampoules were broken, the samples were analyzed using a gas chromatograph equipped with a flame ionization detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: see above.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. J. Lowe and K. Hagler, in *Gas Chromatography, Biology and Medicine*, edited by R. Poster (Churchill, London, 1969), pp. 86–112.

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	0.86	0.421	3.86

Auxiliary Information

Method/Apparatus/Procedure:

The direct sample injection method was used. The samples containing the equilibration mixture were injected into a chromasorb column equipped with an ionization detector. The response areas were compared with those of gas standards analyzed under similar conditions.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. H. Laasberg and J. Hedley-Whyte, Anesthesiol. **32**, 351 (1970).

Variables:

T/K=298–310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.28±0.01	0.410	3.75
30	1.16±0.01	0.446	4.08
37	0.78±0.01	0.382	3.50

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 sample of water was equilibrated with an equal volume of 2-bromo-2-chloro-1,1,1-trifluoroethan vapor in air for 4 h in a temperature controlled water bath. After equilibration both the liquid and gas phases were analyzed using a Hewlett-Packard Research gas chromatograph. The instrument was equipped with a hydrogen flame ionization detector. The reproducibility of the determinations was ±2%.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]

Original Measurements:

F. P. Lees and P. Sarram, J. Chem. Eng. Data **16**, 41 (1971).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	3.0×10^{-2}	3.28	1.7×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

An apparatus containing the mixture of 2-bromo-2-chloro-1,1,1-trifluoroethane and water was placed in a waterbath thermostat. The stirring of the mixture was accomplished by using a glass rod rotated by a horseshoe magnet for about 48 h. The concentration of water in the organic liquid phase was determined by the Karl Fisher titration method.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given. Analytical grade, used as received but degassed.

Estimated Errors:

Solubility: ±7%.
Temperature: ±0.1 K.

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. Ikeda, Anesthesiol. **37**, 87 (1972).

Variables:

T/K=298–310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	1.12±0.02	0.359	3.28
29	1.06±0.04	0.393	3.60
33	0.88±0.05	0.376	3.44
37	0.76±0.03	0.372	3.41

Auxiliary Information

Method/Apparatus/Procedure:

Sample equilibration was done in a bubble tonometer which included a humidifying chamber. The entire system was circulated by a stirring pump temperature controlled water bath. The equilibration time for 10 cm^3 distilled water volumes was 30-min at every temperature tested. The concentrations of 2-bromo-2-chloro-1,1,1-trifluoroethane in the liquid and gas phases were analyzed by gas chromatography. Ten determinations were performed at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.5 K (compiler).

Components:
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
R. K. Stoelting and R. N. Longshore, Anesthesiol. **36**, 503 (1972).

Variables:
T/K=310

Prepared By:
A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	0.82	0.401	3.67

Auxiliary Information

Method/Apparatus/Procedure:
Mixtures of 5 μL 2-bromo-2-chloro-1,1,1-trifluoroethane and 5 cm^3 distilled water were added to 300 cm^3 Erlenmeyer flasks which were then placed in a water bath thermostat and agitated for 120 min. After equilibration, samples were taken and analyzed for 2-bromo-2-chloro-1,1,1-trifluoroethane by gas chromatography. Concentrations were calculated by comparing sample signal peak heights with those of known standards. The result is the average of six determinations.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled.

Estimated Errors:
Solubility: ±0.03 std. dev.
Temperature: ±0.5 K (compiler).

Components:
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
M. M. Halliday, I. MacDonald, and M. H. G. MacGregor, Br. J. Anaesth. **49**, 413 (1977).

Variables:
T/K=310

Prepared By:
A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
36.85	0.80	0.389	3.56

Auxiliary Information

Method/Apparatus/Procedure:
A steady flow of anaesthetic vapor was bubbled through water, allowing 45 min for equilibration. The concentration in the gas mixture was in the range 1–3% (v/v) 2-bromo-2-chloro-1,1,1,-trifluoroethane. A Riken 18A refractometer provided accurate estimations of the gaseous concentrations of 2-bromo-2-chloro-1,1,1-trifluoroethane. Five samples of aqueous solutions were analyzed by gas chromatography. The chromatograph was equipped with a flame ionization detector and a potentiometric recorder.

Source and Purity of Materials:
(1) ICI Pharmaceuticals, used as received.
(2) Distilled.

Estimated Errors:
Solubility: ±0.01 SEM.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Lauven, G. Hack, and H. Stoeckel, Anaesth. **28**, 104 (1979).

Variables:

T/K=297–310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
24	1.07	0.342	3.13
37	0.77	0.419	3.84

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 2-bromo-2-chloro-1,1,1-trifluoroethane in water was determined by a gas chromatographic analysis using the direct injection method. After equilibration, the sample was injected into the column containing Chromosorb W and the chromatograms were displayed on a strip chart recorded. Five parallel determinations were carried out.

Source and Purity of Materials:

(1) ICI Pharmaceuticals, used as received.
(2) Demineralized.

Estimated Errors:

Solubility: ±5%.
Temperature: ±0.5 K (compiler).

Components:

(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $C_2HBrClF_3$; [151-67-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. L. Horvath, *Halogenated Hydrocarbons* (Marcel Dekker, New York, 1982), 889 pp.

Variables:

T/K=297

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
24	0.372	3.406	3.5×10^{-2}	3.82

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 2-bromo-2-chloro-1,1,1-trifluoroethane and water was introduced into an equilibration flask which was then lowered into a waterbath thermostat. The assembly was shaken mechanically for 3 days at constant temperature. When equilibrium was reached, the two phases were separated and filtered. The aqueous and organic phases were analyzed using a gas chromatograph fitted with an electron capture detector. The determination was checked by a linked mass spectrometer.

Source and Purity of Materials:

(1) ICI Limited, 99.9% pure; checked by GC.
(2) Distilled.

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.2 K.

Components:

(1) 2,2-dichloro-1,1,1-trifluoroethane; $C_2HCl_2F_3$; [306-83-2]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

21. 2,2-Dichloro-1,1,1-Trifluoroethane with Water

Critical Evaluation

The solubility of 2,2-dichloro-1,1,1-trifluoroethane (1) in water (2) and that of water (2) in 2,2-dichloro-1,1,1-trifluoroethane (1) have been studied by two research groups. Details are not available on the experimental methods, apparatus, and procedures for the measurements. The binary system is treated in two parts; part 1 is 2,2-dichloro-1,1,1-trifluoroethane (1) in water (2) and part 2 is water (2) in 2,2-dichloro-1,1,1-trifluoroethane (1).

Part 1. The solubility of 2,2-dichloro-1,1,1-trifluoroethane (1) in water (2) has been reported in a du Pont bulletin[1] and by Sukornick[2] at 298.15 K only. There is a serious discrepancy between the two values and in the absence of other independent studies, it is not possible to determine which value is more reliable. Further studies will be necessary before even tentative values can be chosen.

Part 2. Uncertainties regarding the solubility of water (2) in 2,2-dichloro-1,1,1-trifluoroethane (1) are similar to those concluded for the reciprocal system as drawn from the available solubility data. All the available solubility data are summarized in Table 1:

TABLE 1. Reported mutual solubility between 2,2-dichloro-1,1,1-trifluoroethane (1) and water (2)

Temperature		Solubility				
°C	K	100 w_1	$10^4\ x_1$	100 w_2	$10^3\ x_2$	Reference
21	294.15	—	—	0.047	3.98	1
25	298.15	0.46	5.44	—	—	2
		0.21	2.48	0.0662	5.59	3

References:

[1] du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon Compounds,'' Technical Bulletin B-7, Wilmington, Del. (1966), 16 pp.

[2] B. Sukornick, B. Int. J. Thermophys. **10**, 553 (1989).

[3] du Pont de Nemours & Company, ''Solubility Relationships between Fluorocarbons and Water,'' Technical Bulletin B-43, Wilmington, Del. (1966), 17 pp.

Components:

(1) 2,2-dichloro-1,1,1-trifluoroethane; $C_2HCl_2F_3$; [306-83-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon Compounds,'' Tech. Bull. B-7, Wilmington, Del. (1966), 16 pp.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	0.46	5.44	3.0×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The original report is not obtainable; therefore, the solubility data were taken from a secondary source.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] P. A. Sanders, *Handbook of Aerosol Technology*, 2nd ed. (Van Nostrand Reinhold Co., New York, 1979), p. 184.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 2,2-dichloro-1,1,1-trifluoroethane; $C_2HCl_2F_3$; [306-83-2]

Original Measurements:

du Pont de Nemours & Company, ''Solubility Relationships between Fluorocarbons and Water,'' Tech. Bull. B-43, Wilmington, Del., (1966), 17 pp.

Variables:

T/K=294

Prepared by:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
21	4.7×10^{-2}	3.98	2.6×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).

(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 2,2-dichloro-1,1,1-trifluoroethane; $C_2HCl_2F_3$; [306-83-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. Sukornick, Int. J. Thermophys. **10**, 553 (1989).

Variables:

T/K=298

Prepared by:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	2.10×10^{-1}	2.48	6.62×10^{-2}	5.59

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Allied-Signal Inc., Buffalo, N. Y., used as received.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

22. Trichloroethene with Water

Critical Evaluation

The trichloroethene (1) and water (2) binary system is discussed in two parts; part 1 is trichloroethene (1) in water (2) and part 2 is water (2) in trichloroethene (1).

Part 1. The solubility of trichloroethene (1) in water (2) has been studied by 34 groups of workers; their reports are summarized in the Compilation Sheets immediately following this Critical Evaluation.

The experimental data of most investigators in the temperature range of 273–333 K are sufficiently reliable to use in a smoothing equation. The experimental values are shown in Fig. 5. Even so, the experimental work from several workers was not used for the smoothing equation for a variety of reasons. The solubility data of Salkowski,[1] Wright and Schaffer,[2] Newman *et al.*,[3] Soucek,[4] and Orlandini *et al.*[5] are markedly higher than other results and, therefore, have been rejected. The data of Reiley *et al.*,[6] Sedmerova and Novak,[7] Prosyanov *et al.*,[8] Coca and Diaz,[9] McNally and Grob,[10] and Yoshioka *et al.*[11] appear to be several percent lower than the smoothed solubility values and they also have been rejected.

It may be noted that only two investigators[12,13] showed the appearance of a solubility minimum over the reported temperature interval. In several studies the solubility steadily increases[14–16] or decreases[17–20] with increasing temperature. The solubility data of Wright *et al.*[21] actually show a maximum at 303 K, which is inconsistent with the observations concerning the aqueous solubility behavior given in the Preface.

The solubility data of McGovern,[14] Powell,[15] Tettamanti *et al.*,[22] O'Connell,[23] Lowe and Hagler,[24] Antropov *et al.*,[16] McConnell *et al.*,[25] Pearson and McConnell,[26] Chiou and Freed,[17] Archer and Stevens,[27] Halliday *et al.*,[28] Sato and Nakijima,[29] Gossett,[18] Banerjee *et al.*,[30] Leighton and Calo,[19] Tewari *et al.*,[31] Lincoff and Gossett,[32] Munz,[20] Miller *et al.*,[33] Gossett,[12] Warner *et al.*,[34] Howe *et al.*,[13] and Wright *et al.*[21] are in reasonable agreement, although further studies are required before any particular values can be recommended. The tentative solubility values in mass percent for trichloroethene (1) in water (2) over the temperature range of 273–333 K were used to obtain the following mass percent (1) equation:

$$\text{Solubility}\ [100\ w_1] = 1.4049 - 8.2223\times10^{-3}(T/\text{K}) + 1.3218\times10^{-5}(T/\text{K})^2.$$

This equation represents the combined data values from 23 studies which yielded a standard deviation of 1.59×10^{-2}.

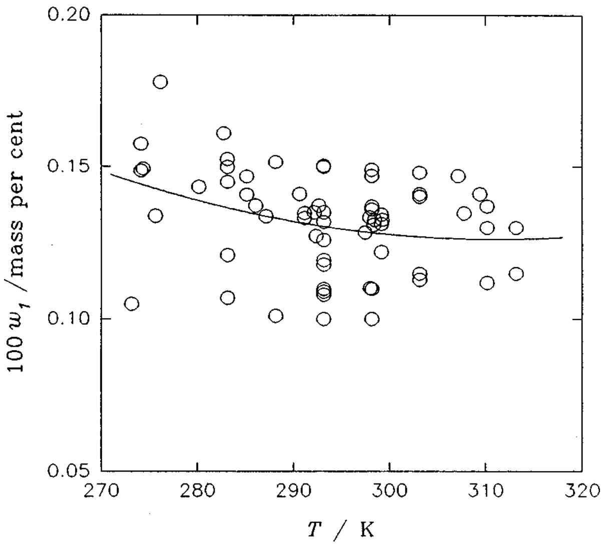

FIG. 5. Solubility of trichloroethene (1) in water (2).

The tentative values of solubility at 5 K intervals for trichloroethene (1) in water (2) are presented in Table 1. The curve obtained from the smoothing equation, shown in Fig. 5 as a solid line, indicates a distinct minimum at 311.0 K. The appearance of the solubility minimum is discussed in the Preface.

Part 2. The solubility of water (2) in trichloroethene (1) has been reported by researchers from 16 laboratories since 1932. The solubility measurements fall in the temperature range from 253 to 353 K. Figure 6 presents the resulting data.

Some reported data, mostly at a single temperature, are rather uncertain and have not been considered for the smoothing equation. The data of Eberius,[35] Sedmerova and Novak,[7] and Prosyanov *et al.*[36] are substantially lower than all other studies and are rejected. The data of Tettamanti *et al.*,[22] Archer and Stevens,[27] and Orlandini *et al.*[5] are significantly higher than the likely solubility and are also rejected. The remaining data mainly due to Carlisle and Levine,[37] Marins,[38] Reilly *et al.*,[6] Hutchison and Lyon,[39] McGovern,[14] O'Connell,[23] Lees and Sarram,[40] Antropov *et al.*,[16] Coca and Diaz,[9] and Ohtsuka and Kazama[41] are in good agreement as shown in Fig. 6. The combined measured mole fraction solubilities of water (2) in trichloroethene between 253 and 353 K were used to obtain the following equation:

$$\log_{10} x_2 = 1.6410 - 1291.0/(T/\text{K}).$$

This equation yielded a standard deviation of 5.75×10^{-2}. The recommended solubility values at 5 K intervals for water (2) in trichloroethene (1) are presented in Table 2.

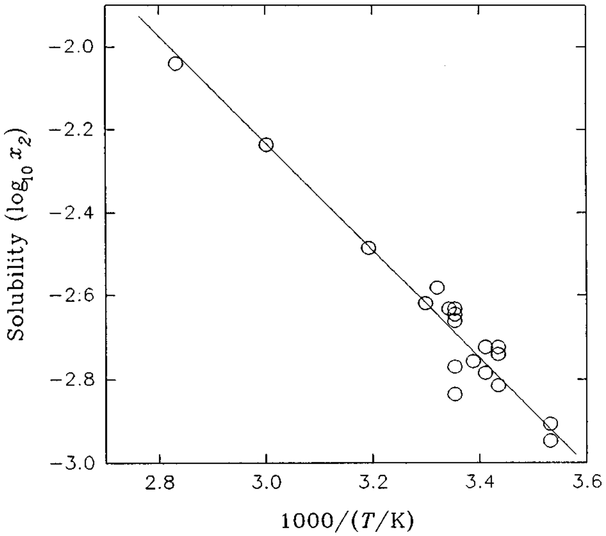

FIG. 6. Solubility of water (2) in trichloroethene (1).

TABLE 1. Tentative solubility of trichloroethene (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 w_1
0	273.15	0.145	1.99
5	278.15	0.141	1.94
10	283.15	0.137	1.88
15	288.15	0.133	1.83
20	293.15	0.131	1.80
25	298.15	0.128	1.76
30	303.15	0.127	1.74
35	308.15	0.126	1.73
40	313.15	0.126	1.73
45	318.15	0.127	1.74
50	323.15	0.128	1.76
55	328.15	0.130	1.78
60	333.15	0.133	1.82

TABLE 2. Recommended solubility of water (2) in trichloroethene (1)

Temperature		Solubility	
°C	K	100 w_2	10^4 x_2
−20	253.15	0.00477	3.477
−15	258.15	0.00599	4.366
−10	263.15	0.00745	5.433
−5	268.15	0.00920	6.707
0	273.15	0.0113	8.216
5	278.15	0.0137	9.991
10	283.15	0.0166	12.066
15	288.15	0.0199	14.478
20	293.15	0.0237	17.263
25	298.15	0.0281	20.463
30	303.15	0.0331	24.120
35	308.15	0.0389	28.280
40	313.15	0.0454	32.989
45	318.15	0.0527	38.297
50	323.15	0.0609	44.254
55	328.15	0.0701	50.912
60	333.15	0.0804	58.327
65	338.15	0.0918	66.553
70	343.15	0.104	75.648
75	348.15	0.118	85.670
80	353.15	0.134	96.678

References:

[1] E. Salkowski, Biochem. Z. **107**, 191 (1920).

[2] W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

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Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. Salkowski, Biochem. Z. **107**, 191 (1920).

Variables:

T/K=293

Prepared by:

A. L. Horvath

Experimental Data

t/°C	$10^3\ V_1/V_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	1.8	0.263	3.61

Auxiliary Information

Method/Apparatus/Procedure:

A volumetric method similar to that introduced by Alexejew[1] was used. Trichloroethene was gradually added to water from a pipet under constant agitation. The appearance of clouding was the indication of saturation.

Source and Purity of Materials:

(1) Kahlbaum solvent, used as received.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±2 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared by:

A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	5.50×10^2	0.182	2.50

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of trichloroethene with a large volume of water and measuring the volume of the undissolved trichloroethene.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and then redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]

Original Measurements:

P. J. Carlisle and A. A. Levine, Ind. Eng. Chem. **24**, 1164 (1932).

Variables:

Temperature

Prepared by:

A. L. Horvath

Experimental Data

The results of the solubility determination were presented in graphical form only.

Auxiliary Information

Method/Apparatus/Procedure:

The water content was found by determining the temperature where tichloroethene was saturated with water, that is, determining the cloud point. The relationship between the cloud point and the percentage moisture in the saturated sample provided the solubility values as a function of temperature.

Source and Purity of Materials:

(1) Distilled.
(2) Factory grade, first dried and followed by fractional distillation.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.2 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]

Original Measurements:

G. Marins, Riv. Ital. Essenze Profumi **19**, 263 (1937), and XXX–XXXI.

Variables:

T/K=283–301

Prepared by:

A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
10	1.7×10^{-2}	1.7×10^{-2}	1.24
18	2.6×10^{-2}	2.6×10^{-2}	1.89
28	3.6×10^{-2}	3.6×10^{-2}	2.62

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled.

(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Reilly, D. F. Kelly, and M. O'Connor, J. Chem. Soc. 275 (1941).

Variables:

T/K=289–291

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
16	8.1×10^{-2}	1.11	—	—
18	—	—	2.5×10^{-2}	1.820

Auxiliary Information

Method/Apparatus/Procedure:

A cloud point method was used for the quantitative determination of mutual solubility. Water was added to the liquid sample drop by drop from a burette and the cloud point was found by visual observation. The determination of the solubility of trichloroethene in water was accomplished by a quantitative hydrolysis reaction with aqueous KOH solution for 3 h at 150 °C in a sealed Carius tube. The chlorine content was determined by the Volhard method.

Source and Purity of Materials:

(1) Imperial Chemical Industries limited, further purified and free from basic substances.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1M^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.30×10^{-3}	2.34×10^{-2}	1.70

Auxiliary Information

Method/Apparatus/Procedure:

A 1 to 15 volume ratio mixture of water and trichloroethene was introduced into an equilibration flask and then lowered into the waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. The description of procedure was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given, purified and dried before use.

Estimated Errors:

Solubility: $\pm1.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1995), p. 129.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K = 253–353

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4 x_1$ (compiler)	100 w_2	$10^4 x_2$ (compiler)
−20	—	—	3.9×10^{-3}	2.84
0	0.105	1.44	9.8×10^{-3}	7.14
10	0.107	1.47	1.55×10^{-2}	11.3
20	0.108	1.48	2.25×10^{-2}	16.4
25	0.110	1.51	3.2×10^{-2}	23.3
30	0.113	1.55	3.3×10^{-2}	24.0
40	0.115	1.58	4.5×10^{-2}	32.7
60	0.125	1.72	8.0×10^{-2}	58.1
80	—	—	1.26×10^{-1}	91.2

Solubility data as a function of temperature were presented in graphical form only except for data values at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source not given, commercial grade.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. F. Powell, Br. J. Ind. Med. **4**, 233 (1947).

Variables:

T/K = 293–310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	$10^4 x_1$ (compiler)
20	3.0	0.126	1.72
37	1.6	0.137	1.89

Auxiliary Information

Method/Apparatus/Procedure:

The trichloroethene and air mixtures were prepared in gas cylinders under pressure. An Oxford vaporizer was used to produce a high concentration of trichloroethene. Water was equilibrated with the gas mixture by a simple bubbling technique. The saturated aqueous solution was treated with pyridiene and HCl solution to generate a yellow color which was measured spectrophotometrically using a filter transmitting at 430 m. u.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±3.0%.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	M. Newman, C. B. Hayworth, and R. E. Treybal, Ind. Eng. Chem. **41**, 2039 (1949).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	0.40	5.5	3.0×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium between trichloroethene and water was established in a constant temperature water bath with sufficient agitation. The usual procedures were followed;[1] the specific gravity was used as a means of analysis.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] J. C. Smith, Ind. Eng. Chem. **34**, 234 (1942).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]	E. Eberius, *Wasserbestimmung mit Karl-Fischer-Lösung*, (GMBH, Weinheim, 1954), p. 67.
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	0.011±0.002	8.02	6.10×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

50 g trichloroethene was shaken with pure water in a 100 mL Erlenmeyer flask. When equilibrium was attained and the two phases separated, the organic phase was analyzed for water using the Karl Fischer titration method. Five determinations were performed.

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: see above.
Temperature: ±0.5 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. Soucek, Prakt. Lek. **7**, 86 (1955).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	2.3	0.197	2.71

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

K. Tettamanti, M. Nogradi, and J. Sawinsky, Period. Polytech. **4**, 201 (1960).

Variables:

T/K=293

Prepared By:

Z. Maczynska

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
20	0.10	1.37	8.0×10^{-2}	5.80

Auxiliary Information

Method/Apparatus/Procedure:

Turbidimetric titrations were used for both the aqueous and the organic phases. First, the trichloroethene was titrated with water from a microburet up to the appearance of turbidity. Then, afterwards, the water was titrated with trichloroethene. The amounts of water or trichloroethylyne in the flasks were weighted to an accuracy of 0.01 g. The temperature was maintained constant using an ultrathermostat.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±10%.
Temperature: ±0.1 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
20	0.11	1.51	2.0×10^{-2}	1.46

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemicals Co., used as received.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. Sedmerova and J. P. Novak, Chem. Prum. **16**, 270 (1966).

Variables:

T/K=293–313

Prepared By:

Z. Maczynska

Experimental Data

t/°C	100 w_1	10^6 x_1 (compiler)	100 w_2	10^5 x_2 (compiler)
19.85	1.0×10^{-3}	1.4	7.0×10^{-4}	5.0
29.85	1.5×10^{-3}	2.1	1.0×10^{-3}	7.0
39.85	2.0×10^{-3}	2.7	1.2×10^{-3}	8.7

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. Water was titrated with trichloroethene from a burette. The mixture was kept at constant temperature under vigorous stirring until the appearance of turbidity.

Source and Purity of Materials:

(1) Source not given, technical grade, distilled and dried over $CaCl_2$ before use, b.p.=87.20 °C, d^{20}=1.4662.
(2) Twice distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. J. Lowe and K. Hagler, in *Gas Chromatography, Biology and Medicine*, edited by R. Poster (Churchill, London, 1969), pp. 86–112.

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	1.51	0.130	1.784

Auxiliary Information

Method/Apparatus/Procedure:

The direct sample injection method was used. The sample containing the equilibration mixture was injected into a Chromosorb column equipped with an ionization detector. The response areas were compared with those of the gas standards analyzed under similar conditions.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]

Original Measurements:

F. P. Lees and P. Sarram, J. Chem. Eng. Data **16**, 41 (1971).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	2.0×10^{-2}	1.46	1.1×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus containing the organic-water system was held in a thermostatic bath. The stirring of the mixture was accomplished by using a glass rod rotated by a horseshoe magnet for about 48 h. The concentration of water in the organic phase was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given, analytical grade, degassed and used without further purification.

Estimated Errors:

Solubility: ±12%.
Temperature: ±0.1 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972) (VINITI No. 3739-71).

Variables:

T/K = 288–299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
15	1.01×10^{-1}	1.39	—	—
18	—	—	2.1×10^{-2}	1.53
20	1.09×10^{-1}	1.50	—	—
22	—	—	2.4×10^{-2}	1.75
26	1.22×10^{-1}	1.67	3.2×10^{-2}	2.33

Auxiliary Information

Method/Apparatus/Procedure:

Alexejew's synthetic solubility method of solubility determination was used.[1] A fixed weight of trichloroethene and water was sealed in a tube and the mixture was subjected to gradually increasing temperature with constant agitation. The appearance of opalescence or clouding was the indication of the saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, of the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 183 (1973).

Variables:

T/K = 287–373

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
14	1.196×10^{4}	3.469×10^{-3}	4.757×10^{-2}
21	9.42×10^{3}	6.217×10^{-3}	8.525×10^{-2}
32	6.75×10^{3}	1.440×10^{-2}	1.974×10^{-1}
50	4.36×10^{3}	4.696×10^{-2}	6.442×10^{-1}
60	3.06×10^{3}	9.74×10^{-2}	1.334×10^{0}
70.3	2.07×10^{3}	2.06×10^{-1}	2.836×10^{0}
80	1.45×10^{3}	4.05×10^{-1}	5.571×10^{0}
90.3	1.13×10^{3}	7.12×10^{-1}	9.825×10^{0}
96.6	1.08×10^{3}	8.95×10^{-1}	1.237×10^{1}
100	9.80×10^{2}	1.085×10^{0}	1.502×10^{1}

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

The distribution coefficient was determined by by distillation. An inert carrier gas stream was used to take samples from the equilibrium vapor phase. The concentration of the trichloroethene in both liquid and vapor phases was determined by using ^{36}Cl labeled compound.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]	N. N. Prosynaov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. **55** (1974).
Variables:	**Prepared By:**
T/K=298–355	A. L. Horvath

Experimental Data

$$\log_{10} \alpha = \frac{917.18}{(T/\mathrm{K})} - 0.958,$$

where α=distribution coefficient. At the normal boiling point of C_2HCl_3, $\alpha=39$ and the activity coefficient, $\gamma_1=63$.

Auxiliary Information

Method/Apparatus/Procedure:

The water concentration in the trichloroethene rich phase was determined by a radiometric method using tritium labeled water. The experimental procedure is described in more detail elsewhere.[1]

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 100 (1973).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Water; H_2O; [7732-18-5]	G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

$t/°C$	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	1.1×10^3	0.1099	0.1508

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of the trichloroethene in water was determined by gas–liquid chromatography (GLC) using an electron capture detector. Where possible, identification was confirmed by a linked mass spectrometer (MS).

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. R. Pearson and G. McConnell, Proc. Roy. Soc., London Ser. B **189**, 305 (1975).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	1.1×10^3	0.1099	1.508

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with *n*-pentane and an aliquot of the extract taken for gas–liquid chromatographic analysis. The gas chromatograph was fitted with a ^{63}Ni electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. T. Chiou and V. H. Freed, ‘‘Chemodynamic Studies on Bench Mark Industrial Chemicals,’’ U. S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).

Variables:

T/K=276–307

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
3	1.78	0.178	2.44
20	1.50	0.150	2.06
34	1.46	0.147	2.02

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5–10 g trichloroethene was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on determination and evaluation of the procedure are found elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou and D. W. Schmedding, Test. Protec. Environ. Fate Mov. Toxicants, Proc. Symp., 1980, pp. 28–42 (Publ. 1981).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	W. L. Archer and V. L. Stevens, I&EC Prod. Res. Dev. **16**, 319 (1977).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	$10^4\,x_1$ (compiler)	100 g_2/g_1	$10^3\,x_2$ (compiler)
25	0.10	1.37	4.0×10^{-2}	2.91

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The data were adopted from a related source.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] News Release from Dow Chemical USA (October 23, 1975).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	M. M. Halliday, I. MacDonald, and M. H. G. MacGregor, Br. J. Anaesth. **49**, 413 (1977).
Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	$10^4\,x_1$ (compiler)
36.85	1.64	0.141	1.94

Auxiliary Information

Method/Apparatus/Procedure:

A constant flow of trichloroethene vapor was bubbled through water, allowing 45 min for equilibration. The concentration in the gas mixture was in the range 0.5%–2% (v/v) trichloroethene. A Riken 18A refractometer provided accurate estimations of gaseous concentrations of trichloroethene. Five samples of aqueous solutions were analyzed by gas chromatography. The chromatograph was equipped with a flame ionization detector and potentiometric recorder.

Source and Purity of Materials:

(1) ICI Pharmaceuticals, used as received.
(2) Distilled.

Estimated errors:

Solubility: ±0.02 SEM.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	1.3	0.112	1.53

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

Trichloroethene vapor was equilibrated in an airtight vial with water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and this sample was injected into a gas chromatograph for analysis. The chromatogram peak height was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.1 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Coca and R. M. Diaz, J. Chem. Eng. Data **25**, 80 (1980).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	1.0×10^{-2}	1.37	3.0×10^{-2}	2.18

Auxiliary Information

Method/Apparatus/Procedure:

The titration was performed in an Erlenmeyer flask by adding trichloroethene to water until a permanent turbidity was observed. The flask was immersed in a thermostat bath while maintaining a constant agitation by means of a magnetic stirrer.

Source and Purity of Materials:

(1) Fluka reagent, laboratory grade, further purified by distillation; middle fraction was used.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	J. M. Gossett, ''Packed Tower Air Stripping of Trichloroethylene from Dilute Aqueous Solutions,'' Engineering & Services Laboratory Report TR-81-38, Tyndall Air Force Base, Florida (August 1980) AD A129727.
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
10	4.01×10^{-3}	0.1526	2.095
15	5.22×10^{-3}	0.1516	2.081
20	6.74×10^{-3}	0.1504	2.065
25	8.62×10^{-3}	0.1491	2.047
30	1.09×10^{-2}	0.1481	2.033

Auxiliary Information

Method/Apparatus/Procedure:

Henry's law constants were determined by a method similar to that described by Mackay *et al.*[1] A water sample containing trichloroethene was placed in the sample vessel. Water saturated air was bubbled through the solution. Samples from the equilibrium experiments were assayed using the head space gas chromatographic technique.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, de-ionized and carbon-treated.

Estimated Errors:

Solubility: 0.99 coef. of determ.
Temperature: ±0.5 K (compiler).

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.12×10^{-2}	0.147	2.02

Auxiliary Information

Method/Apparatus/Procedure:

An excess of trichloroethene was added to a stainless steel tube containing water and the tube was sealed. It was allowed to equilibrate during shaking for 1 week at 25 °C. After centrifugation, the sample was analyzed for radioactivity using a liquid scintillation counting. The solubility determination was repeated at least twice for each sample and the analysis was done in duplicate.

Source and Purity of Materials:

(1) New England Nuclear, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±3.5% std. dev.
Temperature: ±0.3 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

T/K=274–299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
1.0	1.316×10^2	0.1576	2.164
1.0	1.395×10^2	0.1487	2.041
1.2	1.388×10^2	0.1494	2.051
2.5	1.684×10^2	0.1339	1.838
7.0	2.009×10^2	0.1434	1.968
10.0	2.327×10^2	0.1450	1.991
12.0	2.548×10^2	0.1468	2.016
12.0	2.658×10^2	0.1408	1.933
12.9	2.870×10^2	0.1372	1.884
14.0	3.099×10^2	0.1337	1.836
18.0	3.750×10^2	0.1348	1.851
18.0	3.796×10^2	0.1332	1.329
18.0	3.750×10^2	0.1340	1.851
19.0	3.935×10^2	0.1350	1.853
19.2	4.173×10^2	0.1273	1.749
19.5	3.965×10^2	0.1372	1.884
24.3	5.371×10^2	0.1285	1.764
25.2	5.399×10^2	0.1309	1.797
25.3	5.457×10^2	0.1325	1.819
26.0	5.511×10^2	0.1343	1.844
26.0	5.638×10^2	0.1313	1.802
26.1	5.581×10^2	0.1326	1.820

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL trichloroethene sample was injected into a 2.3 L equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The trichloroethene content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±2.1%.
Temperature: ±0.5 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Y. B. Tewari, M. M. Miller, S. P. Wasik, and D. E. Martire, J. Chem. Eng. Data **27**, 451 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25.0	1.04×10^{-2}	0.136	1.87

Auxiliary Information

Method/Apparatus/Procedure:

The modified generator column method was used. A chromatographic column was coated with liquid trichloroethene. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by a high pressure liquid chromatographic procedure, which has been described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. At least 99% pure by GC analysis.
(2) Baker-analyzed HPLC grade.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.1 K.

References:

[1] H. DeVoe, M. M. Miller, and S. P. Wasik, J. Res. Natl. Bur. Stand. **86**, 361 (1981).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]	K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$g_1 V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	0.45	3.1×10^{-2}	2.26

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 trichloroethene in a flask which was then lowered into a thermostat bath. The flask was shaken vigorously until the first cloud (turbidity) appeared. The sample water content was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial JIS extra pure reagent, further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Water; H_2O; [7732-18-5]	M. Orlandini, M. Fermeglia, I. Kikic, and P. Alessi, Chem. Eng. J. **26**, 245 (1983).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^4\ x_1$	$10^3\ x_2$	100 w_1 (compiler)	100 w_2 (compiler)
20	5.5	9.9	0.400	0.137

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of trichloroethene and water was agitated overnight and left at equilibrium for 24 h. Three samples were withdrawn for each phase with a syringe and analyzed by gas chromatography. The gas chromatograph (C. Erba ATc/t) was equipped with a Shimadzu Chromatopac E-1A integrator. A stainless column packed with 100–120 mesh Chromosorb W DMCD coated with heptadecane nitrile was used for analysis.

Source and Purity of Materials:

(1) Fluka reagent, purified by distillation before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Water; H_2O; [7732-18-5]	A. H. Lincoff and J. M. Gossett, in *Gas Transfer at Water Surfaces*, edited by W. Brutsaert and G. H. Jirka (Reidel, Dordrecht, 1984), pp. 17–25.

Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

EPICS method

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	7.64×10^{-3}	0.1319	1.810

$$\log_e H = 11.94 - 4929/(T/K)$$

Batch air stripping method

20	6.74×10^{-3}	0.1495	2.052

$$\log_e H = 9.703 - 4308/(T/K)$$

Auxiliary Information

Method/Apparatus/Procedure:

Henry's law constants were measured by EPICS and Batch Air Stripping Methods. The Equilibrium Partitioning in the Closed Systems technique compares the GC peak heights upon direct injection of headspace samples. In the Batch Air Stripping Method, equal volume samples were placed in serum battles and the equilibrated headspaces contained concentrations proportional to original concentrations in the aqueous samples. Full equilibrium was achieved in a few hours.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5%–10%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Water; H_2O; [7732-18-5]	M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:	**Prepared By:**
T/K=303	A. L. Horvath

Experimental Data

t/°C	$g_1 V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	7.431×10^2	7.458×10^2	1.023

Auxiliary Information

Method/Apparatus/Procedure:

Standard trichloroethene solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±3.2% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. D. Munz, Ph. D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/dimensionless	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
10	0.192	1.21	0.1210	1.661
20	0.326	1.18	0.1180	1.620
30	0.535	1.15	0.1150	1.578

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibration technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) J. T. Baker Chemicals Co., N. J., greater than 99.5% pure.
(2) Distilled and deionizes.

Estimated Errors:

Solubility: ±0.0077 std. dev.
Temperature: ±0.5 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. M. Miller, S. P. Wasik, G.-L. Huang, W.-Y. Shiu, and D. Mackay, Environ. Sci. Technol. **19**, 522 (1985).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.04×10^1	0.1369	1.879

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution was prepared by passing of water through a column which was packed with glass beads coated with trichloroethene. The saturated solution was then pumped through an extractor column and trichloroethene was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both an UV absorbance and a fluorescence detector with excitation filters. The peak area was established using a Hewlett–Packard recorder.

Source and Purity of Materials:

(1) Eastman Kodak Co., commercial quality, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Water; H_2O; [7732-18-5]	Y. Yoshioka, Y. Ose, and T. Sato, Ecotoxicol. Environ. Saf. **12**, 15 (1986).

Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

$t/°C$	$10^3\ \rho_1$ /g m^{-3}	100 w_1 (compiler)	$10^7\ x_1$ (compiler)
20	2.5[a]	2.5×10^{-4}	3.43

[a] Cited value in the original paper is in error (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A supersaturated solution of trichloroethene in water was agitated for 2 h above 20 °C. After stirring for 2 h, the water phase was filtered with Whatman No. 2 filter paper and then analyzed. The concentration of trichloroethene in water was determined by gas chromatography or by ultraviolet spectrometry.

Source and Purity of Materials:

(1) Source not given, analytical grade.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Water; H_2O; [7732-18-5]	J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:	**Prepared By:**
T/K=283–308	A. L. Horvath

Experimental Data

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	CV[a] %	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
9.6	3.78×10^{-3}	3.52	0.1611	2.212
17.5	6.32×10^{-3}	1.32	0.1410	1.934
24.8	9.58×10^{-3}	3.81	0.1334	1.832
34.6	1.49×10^{-2}	2.89	0.1347	1.849

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of trichloroethene was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The head-space concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Fluka AG Chemicals Fab., greater than 99.5%, stabilized with 0.01% triethylamine.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987)
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
24.85	1.17×10^{-2}	0.1102	1.511

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants are described elsewhere.[1] The general procedure was to add an excess quantity of trichloroethene to distilled de-ionized water, place the sample in a thermostat bath, and provide overnight mixing. A portion of this solution was returned to the stripping vessel. Trichloroethene was stripped isothermally from the solution at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available and was used without further purification, stated greater than 99% purity.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3 ; [79-01-6] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987); 86 pp. (AD-A188 571).
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	10^6 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
10	1.499×10^3	0.1499	2.0574
20	1.194×10^3	0.1194	1.6388
30	1.401×10^3	0.1401	1.9233

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. A measured volume of trichloroethene was injected into the bottles through each septum using a microliter syringe. Trichloroethene was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopac Column and a FID detector. The GC response was compared with calibration plots.

Source and Purity of Materials:

(1) Probably a commercial grade at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^4\ x_1$	100 w_1 (compiler)
20	5410±160	1.85	0.135
30	5180±195	1.93	0.141
40	5580±290	1.79	0.130

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of trichloroethene (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. Trichloroethene was injected into the mixture cells and a magnetic stirrer was turned on. Then, the cells were allowed to equilibrate. Later, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered and de-ionized.

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:

(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]
(2) MQ-Water

Original Measurements:

C. D. Munz, Ph. D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

Variables:

T/K=293

Prepared by:

A. L. Horvath

23. Trichloroethene with MQ-Water

Experimental Data

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	0.424	9.84×10^{-2}	1.350

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibration technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. Known volumes of liquid and gas were introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) J. T. Baker Chemicals Co., N. J., greater than 99.5% pure.
(2) 0.25 mg total organic carbon/dm^3; 0.75 mg COD/dm^3.

Estimated Errors:

Solubility: ±0.015 std. dev.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6] (2) Municipal tap water (PASE)	C. D. Munz, Ph.D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

24. Trichloroethene with Municipal Tap Water (PASE)

Experimental Data

t/°C	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	0.509	8.21×10^{-2}	1.127

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibration technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. Known volumes of liquid and gas were introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) J. T. Baker Chemicals Co., N.J., greater than 99.5% pure.
(2) 10 mg total organic carbon/dm^3; 40 mg COD/dm^3.

Estimated Errors:

Solubility: ±0.035 std. dev.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) Water-d_2; D_2O; [7789-20-0] (2) Trichloroethene (trichloroethylene); C_2HCl_3; [79-01-6]	C. A. Hutchison and A. M. Lyon, Columbia University Report **A-745** (July 1, 1943).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

25. Trichloroethene with Water-d_2

Experimental Data

t/°C	$100\ w_1 M_1^{-1}$/mol g^1	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	1.12×10^{-3}	2.24×10^{-2}	1.47

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and trichloroethene was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source not given, purified and dried before use.

Estimated Errors:

Solubility: $\pm1.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:	**Evaluator:**
(1) Pentachloroethane; C_2HCl_5; [76-01-7] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

26. Pentachloroethane with Water

Critical Evaluation

The pentachloroethane (1) and water (2) binary system is treated in two parts; Part 1 is pentachloroethane (1) in water (2) and Part 2 is water (2) in pentachloroethane (1).

Part 1. The solubility of pentachloroethane (1) in water (2) has been studied by seven work groups. All the experimental data were reported at only 293.15 and 298.15 K. The datum of Wright and Schaffer[1] at 298.15 K is lower than other results and is rejected. The datum of Veith *et al.*[2] at 293.15 K is also significantly higher than other results and is therefore rejected.

The remaining data of van Arkel and Vles,[3] McGovern,[4] O'Connell,[5] Walraevens *et al.*,[6] and Hutchinson *et al.*[7] at 293.15 and 298.15 K are in reasonable agreement. Walraevens *et al.*[6] expressed the solubility between 283 and 353 K in an empirical equation; this work is summarized in the Compilation Sheet. The tentative solubility values in weight percent and mole fraction are given in Table 1.

TABLE 1. Tentative solubility of pentachloroethane (1) in Water (2)

Temperature		Reported solubility	
°C	K	100 w_1	10^5 x_1
20	293.15	0.047	4.18
25	298.15	0.049	4.37

Regardless of the above tentative values, further studies are required to establish more accurate values and to extend the temperature range of the solubility data.

Part 2. The solubility of water (2) in pentachloroethane (1) between 273 and 303 K has been measured by five groups of researchers with reasonable agreement. The datum of O'Connell[5] is markedly higher than other results and is therefore rejected.

The solubility measurements at 298.15 K have been studied by four workers[4,8–10] with good agreement. The temperature dependence of the solubility of water in pentachloroethane between 273 and 303 K was studied only by Staverman.[8] Consequently, Table 2 summarizes the tentative solubility of water in pentachloroethane at 5 K intervals. (Because it is not possible to say which of the four data are more accurate, it is suggested that the arithmetic mean of the four reported measurements is probably the most accurate at 298.15 K.)

TABLE 2. Tentative solubility of water (1) in pentachloroethane (1)

Temperature		Reported solubility	
°C	K	100 w_2	10^3 x_2
0	273.15	0.0162	1.82
5	278.15	0.0189	2.12
10	283.15	0.0221	2.48
15	288.15	0.0257	2.88
20	293.15	0.0300	3.36
25	298.15	0.0347	3.91
30	303.15	0.0414	4.65

References:

[1] W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

[2] G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, *Proceedings of the 3rd Annual Symposium on Aquatic Toxicology* (ASTM, Philadelphia, PA, 1980), pp. 116–29.

[3] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

[4] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

[5] W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

[6] R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).

[7] T. C. Hutchinson *et al.*, *Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment* (Plenum, New York, 1980), pp. 577–86.

[8] A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

[9] K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

[10] C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Components:	**Original Measurements:**
(1) Pentachloroethane; C_2HCl_5; [76-01-7] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables: T/K=298	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	2.90×10^3	3.46×10^{-2}	3.08

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of pentachloroethane with a large volume of water and measuring the volume of the undissolved pentachloroethane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with $NaHCO_3$ solution and then redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Pentachloroethane; C_2HCl_5 ; [76-01-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
20	4.7×10^{-2}	4.7×10^{-2}	4.19

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Pentachloroethane; C_2HCl_5 ; [76-01-7]

Original Measurements:

A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
0	1.62×10^{-2}	1.82	8.99×10^{-4}
25	3.47×10^{-2}	3.91	1.93×10^{-3}
30	4.14×10^{-2}	4.65	2.30×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Water was shaken with pentachloroethane for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. The result is an average of two measurements. A full description of the method used is given in a thesis.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, Belgium, 1838.

Components:

(1) Water; H_2O; [7732-18-5]
(2) Pentachloroethane; C_2HCl_5 ; [76-01-7]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.86×10^{-3}	3.35×10^{-2}	3.75

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of water and pentachloroethane was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given, purified and dried before use.

Estimated Errors:

Solubility: $\pm2.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) Pentachloroethane; C_2HCl_5 ; [76-01-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	5.0×10^{-2}	4.45	3.0×10^{-2}	3.36

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source not given, commercial reagent.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Pentachloroethane; C_2HCl_5; [76-01-7] (2) Water; H_2O; [7732-18-5]	W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^2 x_2 (compiler)
20	4.7×10^{-2}	4.18	0.24	2.63

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemicals Co., used as received.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Pentachloroethane; C_2HCl_5; [76-01-7] (2) Water; H_2O; [7732-18-5]	R. Walraevens, P.Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).
Variables:	**Prepared By:**
T/K=283–353	A. L. Horvath

Experimental Data

The temperature dependence of the solubility of pentachloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}\ (S/\text{mol dm}^{-3})=\frac{2070}{(T/\text{K})}-16.412+0.0230\ (T/\text{K}),$$

where S=solubility, and T=absolute temperature.
The temperature interval covered by the above equation is from 283 to 353 K. For example, the calculated solubility derived from the above equation is 4.96×10^{-2} (100 w_1) at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of pentachloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated and the equilibrium was maintained by vigorous stirring. The concentration of pentachloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Solvay reagent, rectified before use, purity was 99.9% by GLC.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:

(1) Pentachloroethane; C_2HCl_5; [76-01-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, *Proceedings of the 3rd Annual Symposium on Aquatic Toxicology* (ASTM Philadelphia, PA, 1980), p. 116–29.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1 V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
20	3.80×10^{-3}	7.69×10^{-2}	6.85

Auxiliary Information

Method/Apparatus/Procedure:

An excess of pentachloroethane was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) Pentachloroethane; C_2HCl_5; [76-01-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

T. C. Hutchinson *et al.*, *Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment* (Plenum, New York, 1980), pp. 577–586.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
25	0.480	4.81×10^{-2}	4.28

Auxiliary Information

Method/Apparatus/Procedure:

An excess quantity of pentachloroethane was added to water and stirred vigorously for 24 h. After the sample was allowed to settle at 25 °C for 48 h, the solution was extracted with cyclohexane. The samples were analyzed by an Aminco-Bowman spectrophotofluorometer. A detailed description of the method has been reported elsewhere.[1]

Source and Purity of Materials:

(1) Aldrich Chemicals, highest grade, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.2 K (compiler).

References:

[1] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Pentachloroethane; C_2HCl_5 ; [76-01-7]

Original Measurements:

K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi, **22**, 197 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	0.62	3.7×10^{-2}	4.14

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 pentachloroethane in a flask which was then lowered into a thermostatic bath. The flask was shaken vigorously until the first cloud (turbidity) appeared. The sample water content was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial JIS extra pure reagent, further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water-d_2 ; D_2O; [7789-20-0]
(2) Pentachloroethane; C_2HCl_5 ; [76-01-7]

Original Measurements:

C. A. Hutchison, and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

27. Pentachloroethane with Water-d_2

Experimental data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.63×10^{-3}	3.26×10^{-2}	3.28

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and pentachloroethane was introduced into an equilibration flask and then lowered into a water bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source not given. Purified and dried before use.

Estimated Errors:

Solubility: $\pm1.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dibromo-1,2-dichloroethane; $C_2H_2Br_2Cl_2$; [683-68-1]

Original Measurements:

W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:

T/K=293

Prepared By:

A. L. Horvath

28. 1,2-Dibromo-1,2-Dichloroethane with Water

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
20	7.0×10^{-2}	7.0×10^{-2}	9.88

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).

(2) Dow Chemicals Co., used as received.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

29. 1,1,2,2-Tetrabromoethane with Water

Critical Evaluation

The 1,1,2,2-tetrabromoethane (1) and water (2) binary system is treated in two parts; part 1 is 1,1,2,2-tetrabromoethane (1) in water (2) and part 2 is water (2) in 1,1,2,2-tetrabromoethane (1).

Part 1. The solubility of 1,1,2,2-tetrabromoethane (1) in water (2) has been studied by five groups of workers. The Compilation Sheets immediately follow this Critical Evaluation. The approximate datum of Booth and Everson[1] is rejected because the reported solubility is somewhat low as well as only approximate. The datum of Blumberg and Melzer[2] is also rejected because it is significantly higher than the other measurements.

Because the measurements were made at more than one temperature, the solubility data of Gooch *et al.*[3] are believed to be more reliable than the other data by Gross *et al.*[4] and O'Connell.[5] All the data are classified as tentative and listed in Table 1 at 5 K intervals. The solubility values of Gooch *et al.*[3] were smoothed by least squares regression to give the following equation:

$$\text{Solubility}\ [100\ g_1/g_2]=1920.55\ \exp(9.92396-1.07375\times10^4/(T/\text{K})+1.4079217\times10^6/(T/\text{K})^2)$$

TABLE 1. Tentative solubility of 1,1,2,2-tetrabromoethane (1) in water (2)

Temperature		Reported Solubility	
°C	K	100 w_1	10^5 x_1
0	273.15	0.0521	2.71
5	278.15	0.0539	2.81
10	283.15	0.0556	2.95
15	288.15	0.0594	3.10
20	293.15	0.0630	3.28
25	298.15	0.0678	3.54
30	303.15	0.0724	3.77
35	308.15	0.0794	4.14
40	313.15	0.0876	4.56
45	318.15	0.0948	4.95
50	323.15	0.106	5.52
55	328.15	0.115	6.00
60	333.15	0.126	6.57
65	338.15	0.141	7.38
70	343.15	0.156	8.13
75	348.15	0.175	9.15
80	353.15	0.194	10.1
85	358.15	0.219	11.4
90	363.15	0.246	12.8
95	368.15	0.274	14.3
100	373.15	0.307	16.1

Part 2. A small difference exists between the data of Hutchison and Lyon[6] at 298.15 K and that of Blumberg and Melzer[2] at 302.15 K and O'Connell[5] at 293.15 K. Because it is not possible to say which of the two values is more accurate; therefore, it is suggested that the average of the two is possibly the most accurate, that is, 0.039 (100 w_2) at 298.15 K.

References:

[1] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).
[2] R. Blumberg and P. Melzer, TBE Bull. **2**, 5 (1960).
[3] J. P. Gooch, E. K. Landis, and J. S. Browning, U.S. Dept. of Interior Bur. of Mines, Bull. R. I. 7656 (1972), 24 pp. (CA. 78:34523y).
[4] P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).
[5] W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).
[6] C. A. Hutchison and A. M. Lyon, Columbia University Report **A-745**, (July 1, 1943).

Components:

(1) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
30	0.651	6.51×10^{-2}	3.39

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solution was prepared in a flask and placed in a waterbath thermostat. The samples were analyzed using a Zeiss combination liquid and gas interferometer described elsewhere.[1] A detailed description of the complete procedure is given in a M. A. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Co., purified by fractional distillation before use, b. p. range 124.6–125.0 °C.
(2) Distilled.

Estimated Errors:

Solubility: ±2.0%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
[2] M. A. Gorman, M. A. thesis, Duke University, Durham, 1932.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report **A-745** (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	2.113×10^{-3}	3.807×10^{-2}	7.254

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of water and 1,1,2,2-tetrabromoethane was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given. Purified and dried before use.

Estimated Errors:

Solubility: $\pm3.0\times10^{-6}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by, M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	10^5 x_1 (compiler)
25.0	$<2.0\times10^{-2}$	$<5.9\times10^{-2}$	<3.1

Auxiliary Information

Method/Apparatus/Procedure:

The sample equilibrium was established and ensured through repeated shaking and centrifuging of the sample mixture in a stoppered Goetz tube and returned the tube to a constant temperature water bath. The difference between the total amount of 1,1,2,2-tetrabromoethane which was added and the amount remaining in excess at equilibrium was taken as the amount of solute dissolved in the known volume of water. The determination of the excess amount of solute added has been described elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, C.P. grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] R. S. Hanslick, Ph.D. thesis, Columbia University, New York, N. Y., 1935.

Components:

(1) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. Blumberg and P. Melzer, TBE Bull. **2**, 5 (1960).

Variables:

T/K=302–324

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (complier)	100 w_2	10^3 x_2 (compiler)
29	—	—	0.04±0.01	7.62
51	0.30±0.07	1.57	0.15±0.04	28.0

Auxiliary Information

Method/Apparatus/Procedure:

The only available information refers to the determination of water in the organic phase by the Karl Fischer titration method. The overall experimental error was about ±20%.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: see above.
Temperature: ±1 K.

Components:

(1) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:

T/K=293–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	$10^5\ x_1$ (compiler)	100 g_2/g_1	$10^3\ x_2$ (compiler)
20	—	—	4.0×10^{-2}	7.62
30	6.5×10^{-2}	3.39	—	—

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemical Co., used as received.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. P. Gooch, E. K. Landis, and J. S. Browning, U.S. Dept. of Interior, Bur. of Mines Bull. R. I. **7656** (1972), 24 pp. (CA. 78:34523y).

Variables:

T/K=274–370

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	100 g_1/g_2	$10^5\ x_1$
1.0	5.23×10^{-2}	5.23×10^{-2}	2.72
10.0	5.56×10^{-2}	5.56×10^{-2}	2.95
20.0	6.30×10^{-2}	6.30×10^{-2}	3.28
25.0	6.76×10^{-2}	6.76×10^{-2}	3.52
30.0	7.24×10^{-2}	7.24×10^{-2}	3.77
40.0	8.76×10^{-2}	8.76×10^{-2}	4.56
50.0	1.06×10^{-1}	1.06×10^{-1}	5.52
60.0	1.26×10^{-1}	1.26×10^{-1}	6.57
70.0	1.56×10^{-1}	1.56×10^{-1}	8.13
80.0	1.94×10^{-1}	1.94×10^{-1}	10.1
90.0	2.46×10^{-1}	2.47×10^{-1}	12.8
97.0	2.87×10^{-1}	2.88×10^{-1}	15.0

Auxiliary Information

Method/Apparatus/Procedure:

The equilibration between 1,1,2,2-tetrabromoethane and water was established in a flask with a stirrer. The entire apparatus was immersed in a thermostat. After equilibrium was established, samples of the mixture were taken for an x-ray spectroscopic determination of bromine and a gas chromatograph analysis using a flame ionization detector. The values presented are averages from duplicate experiments at each temperature. The determination was also reported in a Ph.D. thesis.[1]

Source and Purity of Materials:

(1) Fisher's reagent grade, used as received. $d_4=2.9632$ g/cm^3 and $n_D=1.6363$ both at 20°C.
(2) Distilled.

Estimated Errors:

Solubility: ±1.0%.
Temperature: ±0.2 K.

References:

[1] J. P. Gooch, Ph.D. thesis, Univ. of Alabama, Birmingham, AL, 1971, 68 pp.

Components:

(1) Water-d_2 ; D_2O; [7789-20-0]
(2) 1,1,2,2-tetrabromoethane; $C_2H_2Br_4$; [79-27-6]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

30. 1,1,2,2-Tetrabromoethane with Water-d_2

Experimental Data

t/°C	100 $w_1 M_1^{-1}$/mol g^1	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.786×10^{-3}	3.58×10^{-2}	6.142

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and 1,1,2,2-tetrabromoethane was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source not given, purified and dried before use.

Estimated Errors:

Solubility: $\pm1.5\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., April 1993.

31. 1,1-Dichloroethene with Water

Critical Evaluation

The 1,1-dichloroethene (1) and water (2) binary system is treated in two parts; part 1 is 1,1-dichloroethene (1) in water (2) and part 2 is water (2) in 1,1-dichloroethene.

Part 1. The solubility of 1,1-dichloroethene (1) in water (2) has been reported in 13 publications with only partially consistent results. The original data in these publications are compiled in the Compilation Sheets immediately following this Critical Evaluation. Among the 13 publications there are three secondary sources,[1–3] which do not include details on the origin of data, method of experimental determinations, and the purity of the components. Nevertheless, these three sources of information cannot be disregarded. The likely origin of the solubility data are from industrial reports, bulletins, or brochures.

The data reported in the early publications[1,2] together with that of McConnell *et al.*,[4] Pearson and McConnell,[5] and Howe *et al.*[6] are substantially lower than all other studies and are rejected. The datum of Warner *et al.*[7] at 298.15 K is substantially higher than the selected value and is therefore rejected. The data of Wiener[8] at 298.15 K and at two difference pressures (450 and 590 mm Hg) must be classified as tentative pending further studies. The interested reader is referred to the relevant Compilation Sheet for the experimentally determined solubility values.

The remaining data of Jaeger and Stringer,[9] DeLassus and Schmidt,[10] Leighton and Calo,[11] Kirk-Othmer,[3] McNally and Grob,[12] and Gossett[13] in the temperature range between 275.65 and 363.65 K are generally in reasonable agreement.

The available solubility data of 1,1-dichloroethene in water were first evaluated by DeLassus and Schmidt[10] in 1981. They found that the solubility has been measured only for a narrow temperature interval of 277.15–298.15 K and the scatter of the data was considerable. Consequently, they have determined the solubility between 288.15 and 363.65 K. They found that the solubility is nearly constant over the measured temperature interval.

The measured data are shown, along with the regression curve, in Fig. 7 as a function of temperature.

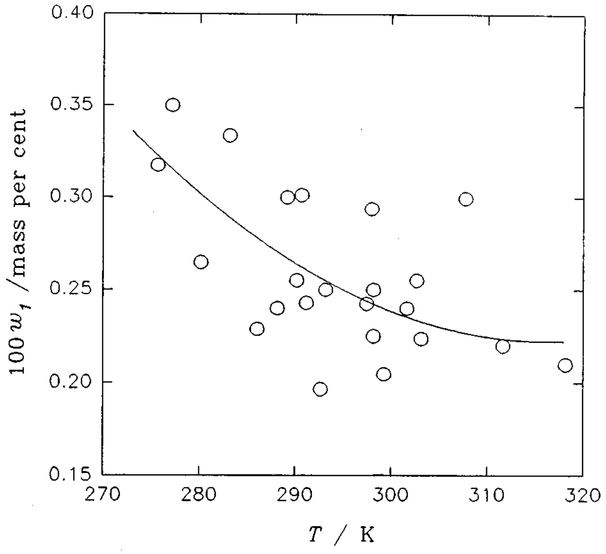

FIG. 7. Solubility of 1,1-dichloroethene (1) in water (2).

The experimental data discussed above[9–13] have been correlated, with equal weight for each of the data points, using a normal polynomial equation to give the following mass percent (1) relation:

$$\text{Solubility } [100 \ w_1] = 6.27413 - 3.8257\times10^{-2}(T/\text{K}) + 6.04607\times10^{-5}(T/\text{K})^2.$$

The above equation, representing the combined data, yielded a standard deviation of 3.13×10^{-2}. The curve obtained from the smoothing equation shows a distinct minimum at 316.44 K as seen in Fig. 7. The recommended mass percent and mole fraction solubility values at 5 K intervals for 1,1-dichloroethene in water are presented in Table 1.

TABLE 1. Recommended solubility of 1,1-dichloroethylene (1) in water (2)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^4\ x_1$
5	278.15	0.310	5.77
10	283.15	0.289	5.38
15	288.15	0.270	5.03
20	293.15	0.255	4.75
25	298.15	0.242	4.51
30	303.15	0.233	4.35
35	308.15	0.226	4.21
40	313.15	0.223	4.15
45	318.15	0.222	4.13
50	323.15	0.225	4.19
55	328.15	0.230	4.28
60	333.15	0.239	4.45
65	338.15	0.251	4.67
70	343.15	0.265	4.94
75	348.15	0.283	5.27
80	353.15	0.304	5.66
85	358.15	0.328	6.11
90	363.15	0.355	6.62

Part 2. The solubility of water (2) in 1,1-dichloroethene (1) has been reported in three secondary sources[1–3] only. They neither disclosed the original sources nor described the experimental methods and purity of components. Two sources[2,3] reported identical solubilities of 0.035 $[100\ w_2]$ at 298.15 K, while the third reference (Ref. 1) gives the solubility of 0.4 $[100\ w_2]$ at 293.15 K. This latter value is too high and consequently it is rejected. The solubility values of 0.035 $[100\ w_2]$ at 298.15 K is classified as tentative.

There are no other experimental data for comparison. It is difficult to assess the deviation of this value from the true solubility, however, it may be considerably in excess of 10%.

References:

[1] *Kirk-Othmer Encyclopedia of Chemical Technology*, 2nd ed. (Wiley, New York, 1964), Vol. 5, p. 178.
[2] *Encyclopedia of Polymer Science and Technology*, 1st ed. (Wiley, New York, 1971), Vol. 14, p. 542.
[3] *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed. (Wiley, New York, 1983), Vol. 23, p. 765.
[4] G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13-8 (1975).
[5] C. R. Pearson and G. McConnell, Proc. R. Soc. London, Ser. B. **189**, 305 (1975).
[6] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).
[7] H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U. S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).
[8] H. Wiener, J. Polymer Sci. **7**, 1 (1951).
[9] J. Jaeger and W. Stringer, in ''Vinylidene Chloride Monomer'' Dow Chemical U.S.A., Circular (1972), No. 102-232-72.
[10] P. T. DeLassus and D. D. Schmidt, J. Chem. Eng. Data **26**, 274 (1981).
[11] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
[12] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
[13] J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Components:	**Original Measurements:**
(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4] (2) Water; H_2O; [7732-18-5]	H. Wiener, J. Polym. Sci. **7**, 1 (1951).
Variables:	**Prepared By:**
T/K=298 and P/cm Hg=45–59	A. L. Horvath

Experimental Data

t/°C	p_1 /cm Hg	$10^{-3}\ c_1$ /mol dm^3	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	45	2.7×10^{-2}	0.262	0.489
25	59	6.6×10^{-2}	0.642	1.20

Auxiliary Information

Method/Apparatus/Procedure:

Small known quantities of 1,1-dichloroethene vapor were added to a closed vessel containing a known amount of water and headspace. The equilibrium vapor pressure above the solution was monitored after each addition. At the equilibrium pressure, the added 1,1-dichloroethene was adjusted for the headspace volume, and the remainder was assumed to have dissolved in water.

Source and Purity of Materials:

(1) ICI Limited, fractionally distilled, washed with aqueous solutions of $FeSO_4$ and NaOH and dried over silica gel.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Kirk-Othmer Encyclopedia of Chemical Technology, 2nd ed. (Wiley, New York, 1964), Vol. 5, p. 178.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^2 x_2 (compiler)
20	4.0×10^{-2}	7.4	0.4	1.7

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given, b.p.=31.8 °C.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

Encyclopedia of Polymer Science and Technology, 1st ed. (Wiley, New York, 1971), Vol. 14, p. 542.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	2.1×10^{-2}	3.9	3.5×10^{-2}	1.88

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given, b.P.=31.56 °C.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Jaeger and W. Stringer, ''Vinylidene Chloride Monomer,'' Dow Chemical U. S. A., Circular (1972), No. 102-232-72.

Variables:

T/K=277–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
4	0.35	6.52	3.61×10^{-3}
16	0.30	5.59	3.09×10^{-3}
25	0.25	4.65	2.58×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^6 g_1/g_2	100 w_1 (compiler)	10^5 x_1 (compiler)
25	4.0×10^{2}	4.0×10^{-2}	7.44

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of the 1,1-dichloroethene in water was determined by gas–liquid chromatography (GLC) using an electron capture detector. Where possible, identification was confirmed by a linked mass spectrometer (MS) method.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. R. Pearson and G. McConnell, Proc. R. Soc. London, Ser. B **189**, 305 (1975).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	4.0×10^2	4.0×10^{-2}	7.44

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with *n*-pentane and an aliquot of the extract taken for gas–liquid chromatographic analysis. The gas chromatograph was fitted with a ^{3}Ni electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. T. DeLassus and D. D. Schmidt, J. Chem. Eng. Data **26**, 274 (1981).

Variables:

T/K=288–364

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1 M_1^{-1}$/mol g^{-1} (compiler)
15	0.24	4.47	2.47×10^{-3}
17	0.255	4.75	2.63×10^{-3}
20.5	0.25	4.65	2.58×10^{-3}
25	0.225	4.19	2.32×10^{-3}
28.5	0.24	4.47	2.47×10^{-3}
29.5	0.255	4.75	2.63×10^{-3}
38.5	0.22	4.09	2.27×10^{-3}
45	0.21	3.91	2.17×10^{-3}
51	0.23	4.28	2.37×10^{-3}
55	0.21	3.91	2.17×10^{-3}
60	0.24	4.47	2.47×10^{-3}
65	0.225	4.19	2.32×10^{-3}
71	0.295	5.49	3.04×10^{-3}
74.5	0.25	4.65	2.58×10^{-3}
81	0.295	5.49	3.04×10^{-3}
85.5	0.37	6.90	3.82×10^{-3}
90.5	0.35	6.52	3.61×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Approximately 60 cm^3 each of 1,1-dichloroethene and water was placed in a steel bomb and immersed in a thermostat bath. After 6–24 h mechanical shaking, samples were taken from the water phase using a syringe and injected into a measured aliquot of dimethylacetamide. The solutions were then analyzed using a gas chromatograph technique. Three or more samples were taken at each temperature.

Source and Purity of Materials:

(1) Source not given, stabilized with monomethyl ether and hydroquinone.
(2) Distilled.

Estimated Errors:

Solubility: ±5%.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
Variables:	**Prepared By:**
T/K=276–299	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
2.5	5.335×10^2	0.3174	5.9132
7.0	7.801×10^2	0.2647	4.9299
12.9	1.1618×10^3	0.2288	4.2589
18.0	1.3364×10^3	0.2429	4.5227
19.5	1.7520×10^3	0.1965	3.6572
24.3	1.7145×10^3	0.2425	4.5158
26.1	2.1468×10^3	0.2047	3.8113

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,1-dichloroethene sample was injected into a 2.3 L equilibration cell containing distilled water. After the liquid sample was shaken vigorously for about 5 min, its homogeneity was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,1-dichloroethene content was extracted and measured using a gas chromatograph which was equipped with a dual flame ionization detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±14.0%.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4] (2) Water; H_2O; [7732-18-5]	*Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed. (Wiley, New York, 1983), Vol 23, p. 765.
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	0.25	4.65	3.5×10^{-2}	1.88

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/ gm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	2232	0.2237	4.165

Auxiliary Information

Method/Apparatus/Procedure:

Standard 1,1-dichloroethene solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph for analysis. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA, purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±3.67% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:

T/K=283–308

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	CV[a] %	100 w_1 (compiler)	10^4 x_1 (compiler)
10.0	1.27×10^{-2}	1.86	0.3336	6.216
17.5	1.91×10^{-2}	2.11	0.3012	5.612
24.8	2.61×10^{-2}	2.86	0.2938	5.473
34.6	3.66×10^{-2}	2.50	0.2995	5.579

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of 1,1-dichloroethene was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Riedel-De Haen AG., greater than 99.9% by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U. S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
24.85	1.50×10^{-2}	0.5046	9.410

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants are described elsewhere.[1] The general procedure was to add an excess quantity of 1,1-dichloroethene to distilled deionized water, place the sample in a thermostat bath, and provide overnight mixing. A portion of this solution was returned to the stripping vessel. The 1,1-dichloroethene was stripped isothermally from the solution at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used as received, stated purity greater than 99%.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) 1,1-dichloroethene (1,1-dichloroethylene); $C_2H_2Cl_2$; [75-35-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188571).

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^6 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
10	6.30×10^2	6.30×10^{-2}	1.171
20	7.50×10^2	7.50×10^{-2}	1.395
30	6.56×10^2	6.56×10^{-2}	1.220

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. A measured volume of 1,1-dichloroethene was injected into the bottles through each septum using a microliter syringe. The 1,1-dichloroethene was in excess of the anticipated solubility limit. The bottles were shaken for 1 h our with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopac Column and a FID detector. The GC response was compared with calibration plots.

Source and Purity of Materials:

(1) Probably a commercial reagent, at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

32. Cis-1,2-Dichloroethene with Water

Critical Evaluation

The cis-1,2-dichloroethene (1) and water (2) binary system is treated in two parts; part 1 is cis-1,2-dichloroethene (1) in water (2) and part 2 is water (2) in cis-1,2-dichloroethene (1).

Part 1. The solubility of cis-1,2-dichloroethene (1) in water (2) has been investigated by five groups of workers in the narrow temperature range from 283.15 to 313.15 K. The data of Howe *et al.*[1] are markedly lower than other results and are therefore rejected. The solubility determinations of Howe *et al.*[1] have been found to give lower values in general, as discussed in the critical evaluation of solubilities of CCl_3F, CCl_4, $CHBr_2Cl$, $CHCl_3$, and CH_2Cl_2 in water. Both the measured values of McGovern[2] and those of Sato and Nakijima[3] are noticeably low and were not used for the smoothing equation.

The combined data of Gossett[4] and Wright *et al.*[5] were correlated to obtain the following mass percent (1) equation:

$$\text{Solubility }[100\ w_1]=27.7353-0.178316(T/\text{K})+2.93282\times10^{-4}(T/\text{K})^2,$$

which yielded a standard deviation of 5.32×10^{-2} in the temperature range from 283.15 to 313.15 K. The above equation represents the combined data with maximum deviation of 12%, usually less, and may be considered tentative for solubility of cis-1,2-dichloroethene in water. The tentative values for this system are given in Table 1, as smoothed values at 5 K intervals. The curve obtained from the smoothing equation shows a distinct minimum at 304 K as shown in Fig. 8 which presents the data and calculated values versus temperature. The appearance of the solubility minimum is discussed in the Preface.

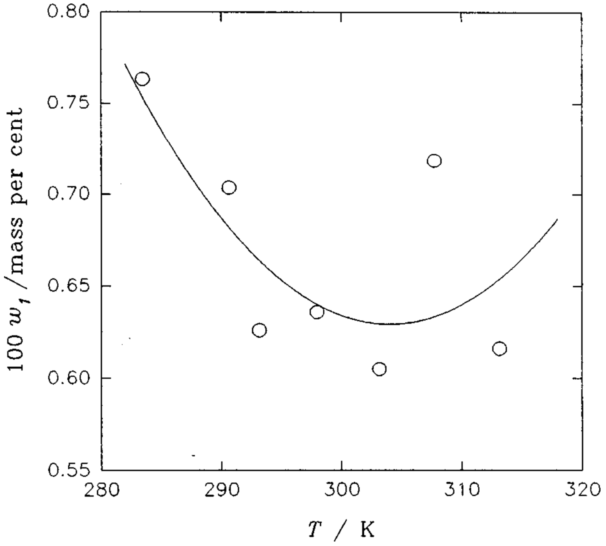

FIG. 8. Solubility of cis-1,2-dichloroethene (1) in water (2).

TABLE 1. Tentative solubility of cis-1,2-dichloroethene (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^3\ x_1$
10	283.15	0.755	1.41
15	288.15	0.705	1.32
20	293.15	0.667	1.25
25	298.15	0.641	1.20
30	303.15	0.631	1.18
35	308.15	0.636	1.19
40	313.15	0.656	1.23

Part 2. The solubility of water (2) in cis-1,2-dichloroethene (1) has been studied by McGovern[2] and Ohtsuka and Kazama[6] between 273.15 and 298.15 K. The solubility data of McGovern[2] are believed to be more reliable than that of Ohtsuka and Kazama[6] because McGovern made measurements at more than one temperature. However, the datum at 298.15 K is a misprint, and it should be read as 0.055 [100 w_2]. These data are classified as tentative and are listed in Table 2.

TABLE 2. Tentative solubility of water (2) in cis-1,2-dichloroethene (1)

Temperature		Solubility	
°C	K	100 w_2	$10^3\ x_2$
0	273.15	0.019	1.02
5	278.15	0.024	1.29
10	283.15	0.028	1.50
15	288.15	0.034	1.83
20	293.15	0.039	2.10
25	298.15	0.055	2.95

References:

[1] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).
[2] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).
[3] A. Sato and T. Nakijima, Arch. Environ. Health. **34**, 69 (1979).
[4] J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).
[5] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).
[6] K. Ohtsuka and K. Kazama, Sen't Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Components:

(1) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K=273–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
0	—	—	1.9×10^{-2}	1.02
10	—	—	2.8×10^{-2}	1.50
20	—	—	3.9×10^{-2}	2.10
25	3.5×10^{-1}	6.52	5.5×10^{-1}	28.9

Solubility data as a function of temperature were presented in graphical form only except for data values at 25 °C.
It is apparent that the solubility datum at 25 °C for (2) under the 100 w_2 column is a misprint and should be 5.5×10^{-2}.

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source not given of the commercial grade.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
37	2.9	0.483	9.01

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A cis-1,2-dichloroethene vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height on the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.4 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]

Original Measurements:

K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Variables:

$T/K=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$g_1V_2^{-1}$ /g dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.17	9.1×10^{-2}	4.88

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 cis-1,2-dichloroethene in a flask and it was lowered into a thermostat bath. The flask was then shaken vigorously until the first cloud (turbidity) appeared. The water content in the sample was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial JIS extra pure solvent, further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:

$T/K=283-308$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	CV^a %	100 w_1 (compiler)	10^3 x_1 (compiler)
10.3	1.72×10^{-3}	3.59	0.7632	1.427
17.5	2.65×10^{-3}	2.44	0.7037	1.315
24.8	4.08×10^{-3}	6.32	0.6359	1.188
34.6	5.45×10^{-3}	5.04	0.7186	1.343

^{a}CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of cis-1,2-dichloroethene was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Aldrich Chemical Co., 97% pure.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:

(1) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188571).

Variables:

T/K = 283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
10	1.52×10^2	1.52×10^{-2}	2.825
20	2.73×10^2	2.73×10^{-2}	5.075
30	1.76×10^2	1.76×10^{-2}	3.271

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. A measured volume of cis-1,2-dichloroethene was injected into the bottles through each septum using a microliter syringe. The cis-1,2-dichloroethene was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopac Column and a FID detector. The GC response was compared with calibration plots.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) cis-1,2-dichloroethene (cis-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-59-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K = 293–313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^3\ x_1$	$100\ w_1$ (compiler)
20	856 ± 44	1.17	0.626
30	884 ± 43	1.13	0.605
40	866 ± 65	1.15	0.616

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of cis-1,2-dichloroethene (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. The cis-1,2-dichloroethene was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered, and de-ionized.

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:	**Evaluator:**
(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

33. Trans-1,2-dichloroethene with Water

Critical Evaluation

The binary system of trans-1,2-dichloroethene (1) and water (2) binary system is treated in two parts; part 1 is trans-1,2-dichloroethene (1) in water (2) and part 2 is water (2) in trans-1,2-dichloroethene (1).

Part 1. The solubility of trans-1,2-dichloroethene (1) in water (2) has been studied by six groups of workers in the narrow temperature range from 283.15 to 313.15 K. Both the measurements of McGovern[1] and those of Sato and Nakijima[2] are noticeably higher than the likely solubility and are rejected. The solubility determinations of Howe *et al.*[3] tend to appear low in general, as discussed in the critical evaluation of solubilities of CCl_3F, CCl_4 , $CHBr_2Cl$, $CHCl_3$, CH_2Cl_2 , and cis-1,2-CHCl=CHCl in water, and they are also rejected.

The remaining solubility data of Gossett,[4] Warner *et al.*,[5] and Wright *et al.*[6] were used to obtain by regression the following mass percent (1) equation:

$$\text{Solubility}\ [100\,w_1]=7.803\,906-4.5457\times10^{-2}(T/\text{K})+6.96755\times10^{-5}(T/\text{K})^2.$$

This equation represents the combined data points and it yields a standard deviation of 2.72×10^{-2} in the temperature range from 283.15 to 313.15 K. The tentative values of solubility at 5 K intervals for trans-1,2-dichloroethene (1) in water (2) are presented in Table 1 on the following page.

The weight percent (1) observed values and the curve obtained from the smoothing equation are shown in Fig. 9.

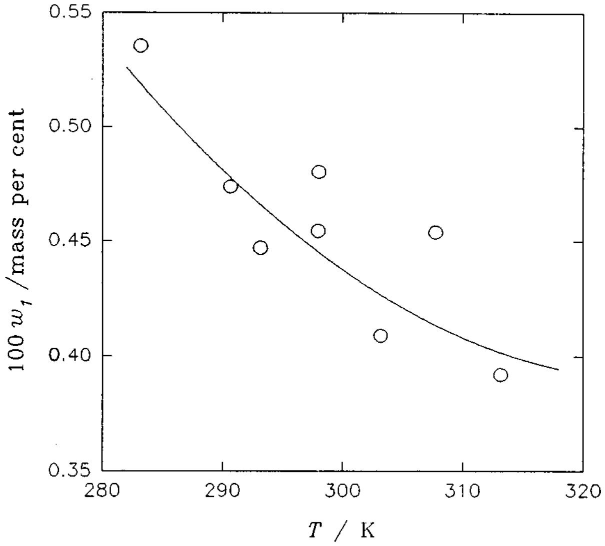

FIG. 9. Solubility of trans-1,2-dichloroethene (1) in water (2).

TABLE 1. Tentative solubility of trans-1,2-dichloroethene (1) in water (2)

Temperature		Solubility	
°C	K	$100\,w_1$	$10^4\,x_1$
10	283.15	0.525	9.80
15	288.15	0.497	9.27
20	293.15	0.472	8.81
25	298.15	0.452	8.43
30	303.15	0.433	8.08
35	308.15	0.419	7.81
40	313.15	0.408	7.61

Part 2. The solubility of water (2) in trans-1,2-dichloroethylene (1) has been studied only by McGovern[1] and there are no other measurements for comparison. Therefore, it is not possible to perform a critical evaluation. The reader is referred to the Compilation Sheet for further details.

References:

[1] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

[2] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

[3] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

[4] J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

[5] H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' USA EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

[6] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Components:	**Original Measurements:**
(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5] (2) Water; H_2O; [7732-18-5]	E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:	**Prepared By:**
T/K=273–298	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
0	—	—	1.9×10^{-2}	1.02
10	—	—	2.8×10^{-2}	1.50
20	—	—	3.9×10^{-2}	2.10
25	6.3×10^{-1}	1.18	5.5×10^{-1}	28.9

Solubility data as a function of temperature were presented in graphical form only except for data values at 25 °C.
It is apparent that the solubility datum at 25 °C for (2) under the 100 w_2 column is a misprint and should be 5.5×10^{-2}.

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial grade, source not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5] (2) Water; H_2O; [7732-18-5]	A. Sato and T. Nakijama, Arch. Environ. Health **34**, 69 (1979).

Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
37	2.1	0.556	1.04

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A sample of trans-1,2-dichloroethene vapor was equilibrated in an airtight vial between water and the overlying air. When equilibrium was established, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and was injected into a gas chromatograph and analyzed. The peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.4 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:

T/K=283–308

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	CV[a] %	100 w_1 (compiler)	10^4 x_1 (compiler)
10.0	4.20×10^{-3}	1.76	0.5354	9.993
17.5	6.60×10^{-3}	2.27	0.4738	8.839
24.8	9.38×10^{-3}	2.07	0.4544	8.475
34.6	1.38×10^{-2}	1.75	0.4539	8.466

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of trans-1,2-dichloroethene was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Riedel-De Haen AG., greater than 99.9% pure.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:

(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U. S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
24.85	5.32×10^{-3}	0.4804	8.967

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants, as described by Mackay *et al.*,[1] was used. The general procedure was to add an excess quantity of trans-1,2-dichloroethene to distilled de-ionized water, place the sample in a thermostat bath, and mix overnight. A portion of this solution was returned to the stripping vessel. The trans-1,2-dichloroethene was stripped isothermally from the solution mixture at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, stated purity greater than 99%, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6.0% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188571).

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
10	4.188×10^3	0.4188	7.810
20	3.590×10^3	0.3590	6.691
30	3.861×10^3	0.3861	7.198

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled and de-ionized water and sealed. A measured volume of trans-1,2-dichloroethene was injected into the bottles through each septum using a microliter syringe. The trans-1,2-dichloroethene was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopac Column and a FID detector. The GC response was compared with calibration plots.

Source and Purity of Materials:

(1) Probably a commercial reagent, at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) trans-1,2-dichloroethene (trans-1,2-dichloroethylene); $C_2H_2Cl_2$; [156-60-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^4\ x_1$	$100\ w_1$ (compiler)
20	200±60	8.33	0.447
30	1310±65	7.63	0.409
40	1370±75	7.30	0.392

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of trans-1,2-dichloroethene (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. The trans-1,2-dichloroethene was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered and de-ionized.

Estimated Errors:

Solubility: See above.
Temperature: ±0.05 K.

Components:

(1) 1,2-dichloro-1,1-difluoroethane; $C_2H_2Cl_2F_2$; [1649-08-7]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon Compounds,'' Tech. Bull. B-7, Wilmington, Del. (1996), 16 pp.

Variables:

T/K=297

Prepared By:

A. L. Horvath

34. 1,2-Dichloro-1,1-Difluoroethane with Water

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
24	0.49	6.57	8.5×10^{-2}	6.33

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. The original report is not obtainable; therefore, the solubility data were taken from a secondary source.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] P. A. Sanders, *Handbook of Aerosol Technology*, 2nd ed. (Van Nostrand Reinhold, New York, 1979), p. 184.

Components:

(1) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

35. 1,1,1,2-Tetrachloroethane with Water

Critical Evaluation

The 1,1,1,2-tetrachloroethane (1) and water (2) binary system is treated in two parts; part 1 is 1,1,1,2-tetrachloroethane (1) in water (2) and part 2 is water (2) in 1,1,1,2-tetrachloroethane (1).

Part 1. The solubility of 1,1,1,2-tetrachloroethane (1) in water (2) has been studied by five groups of workers in the temperature range from 273.15 to 323.15 K. There is a reasonable agreement among the reported results except for those of Chiou and Freed[1] whose measurements are markedly lower than other data and are therefore rejected.

The combined data of van Arkel and Vles,[2] Walraevens *et al.*,[3] Sato and Nakijima,[4] and Weight *et al.*[5] were correlated to obtain the following mass percent (1) equation:

$$\text{Solubility }[100\ w_1]=2.17896-1.3966\times10^{-2}\ (T/\text{K})+2.35307\times10^{-5}(T/\text{K})^2,$$

which shows a standard deviation of 4.97×10^{-3} in the temperature range from 273.15 to 323.15 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 10. The curve shows a distinct minimum at 296.76 K. The appearance of the solubility minimum for aqueous hydrocarbon systems is discussed in the Preface.

The recommended solubility values at 5 K intervals for 1,1,1,2-tetrachloroethane (1) in water (2) are presented in Table 1.

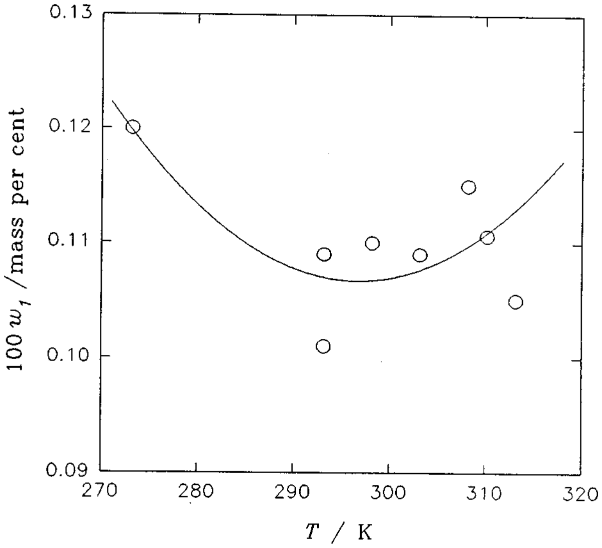

FIG. 10. Solubility of 1,1,1,2-tetrachloroethane (1) in water (2).

TABLE 1. Recommended solubility of 1,1,1,2-tetrachloroethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
0	273.15	0.120	1.289
5	278.15	0.115	1.236
10	283.15	0.111	1.192
15	288.15	0.108	1.160
20	293.15	0.107	1.150
25	298.15	0.107	1.150
30	303.15	0.108	1.160
35	308.15	0.110	1.182
40	313.15	0.113	1.214
45	318.15	0.117	1.257
50	323.15	0.123	1.322

Part 2. The solubility of water (2) in 1,1,1,2-tetrachloroethane has been reported in one paper. Only the data of Staverman[6] are available for the solubility of water in 1,1,1,2-tetrachloroethane and so no critical evaluation is possible. These data are classified as tentative. For further details the reader is referred to the relevant Compilation.

References:

[1] C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U. S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).
[2] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
[3] R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).
[4] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
[5] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).
[6] A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Components: (1) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
Variables: T/K$=273-323$	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
0	0.120	0.120	1.29
20	0.109	0.109	1.17
35	0.115	0.115	1.23
50	0.125	0.125	1.34

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6]

Original Measurements:

A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:

$T/\mathrm{K}=273-303$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	$100\ w_1$	$10^5\ x_1$	$100\ w_1M_1^{-1}/\mathrm{mol\ g}^{-1}$ (compiler)
0	2.30×10^{-2}	2.14×10^{2}	1.28×10^{-3}
25	5.55×10^{-2}	5.13×10^{2}	3.08×10^{-3}
30	6.08×10^{-2}	5.66×10^{2}	3.37×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,1,2-tetrachloroethane and water was shaken for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. A full description of the method used is given elsewhere.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph. D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).

Variables:

$T/\mathrm{K}=283-353$

Prepared By:

A. L. Horvath

Experimental Data

The temperature dependence of the solubility of 1,1,1,2-tetrachloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/\mathrm{mol\ dm}^{-3})=\frac{2070}{(T/\mathrm{K})}-16.165+0.0236(T/\mathrm{K}),$$

where S = solubility, and T = absolute temperature.

The temperature interval covered by the above equation is from 283 to 353 K. For example, the calculated solubility derived from the above equation is 1.10×10^{-1} [$100\ w_1$] at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,1,2-tetrachloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated and the equilibrium was maintained by vigorous stirring. The concentration of 1,1,1,2-tetrachloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Prepared from MVC, rectified before use, purity was 99.9% by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:

(1) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U.S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1997).

Variables:

T/K=276–307

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
3	0.215	2.15×10^{-2}	2.31
20	0.200	2.00×10^{-2}	2.15
34	0.201	2.02×10^{-2}	2.17

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5–10 g 1,1,1,2-tetrachloroethane was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on determination and evaluation of the procedure are found elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou and D. W. Schmedding, Test. Protec. Environ. Fate Mov. Toxicants, Proc. Symp., 1980, pp. 28–42 (1981).

Components:

(1) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

T/K=310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L /dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	5.5	0.1106	1.188

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A 1,1,1,2-tetrachloroethane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.4 std. dev.
Temperature: ±0.5 K (compiler).

Components: (1) 1,1,1,2-tetrachloroethane; $C_2H_2Cl_4$; [630-20-6] (2) Water; H_2O; [7732-18-5]	**Original Measurements:** D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).
Variables: T/K=293–313	**Prepared By:** A. L. Horvath

Experimental Data

t/°C	γ_1^{∞}	$10^4\ x_1$	100 w_1 (compiler)
20	9280±730	1.08	0.101
30	8530±635	1.17	0.109
40	8830±645	1.13	0.105

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,1,1,2-tetrachloroethane (γ_1^{∞}) in water. Cells containing degassed water were submerged in a thermostat water bath. The 1,1,1,2-tertachloroethane was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered, and de-ionized.

Estimated Errors:

Solubility: See above.
Temperature: ±0.05 K.

Components: (1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	**Evaluator:** A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

36. 1,1,2,2-Tetrachloroethane with Water

Critical Evaluation

The 1,1,2,2-tetrachloroethane (1) and water (2) binary system is treated in two parts; part 1 is 1,1,2,2-tetrachloroethane (1) in water (2) and part 2 is water (2) in 1,1,2,2-tetrachloroethane (1).

Part 1. The solubility of 1,1,2,2-tetrachloroethane (1) in water (2) has been studied by 19 groups of workers in the temperature range from 276.15 to 419.35 K. Despite the large number of investigations, the solubility values are very uncertain above 323.15 K.

Most of the solubility measurements provide relatively consistent results with the exception of those by Hollo and Lengyel[1] and Prosyanov *et al.*[2] These data appear erratic when compared with other measurements. Furthermore, they appear inconsistent in that they do not show comparable effects with increasing temperature and are therefore rejected. The remaining solubility data of Wright and Schaffer,[3] van Arkel and Vles,[4] Othmer *et al.*,[5] McGovern,[6] Walraevens *et al.*,[7] Chiou and Freed,[8] Sato and Nakijima,[9] Schwarz,[10] Veith *et al.*,[11] Banerjee *et al.*,[12] Schwarz and Miller,[13] Leighton and Calo,[14] McNally and Grob,[15] Barr and Newsham,[16] Howe *et al.*,[17] Vogel,[18] and Wright *et al.*[19] were used to obtain the following mass percent (1) equation:

$$\text{Solubility}\ [100\ w_1]=4.87975-3.0937\times10^{-2}(T/\text{K})+5.20513\times10^{-5}(T/\text{K})^2,$$

which shows a standard deviation of 4.54×10^{-2} in the temperature range from 276.15 to 323.15 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 11. A solubility minimum appears at 297.18 K. Additional details concerning the solubility minimum for aqueous hydrocarbon systems are provided in the Preface.

The recommended solubility values at 5 K intervals for 1,1,2,2-tetrachloroethane (1) in water (2) are presented in Table 1.

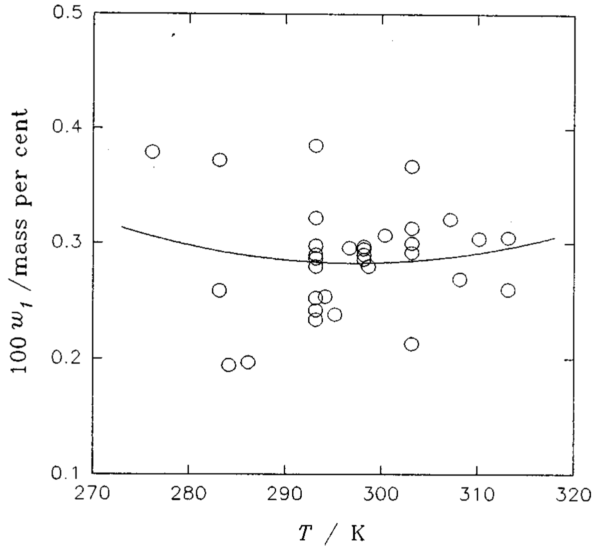

FIG. 11. Solubility of 1,1,2,2-tetrachloroethane (1) in water (2).

TABLE 1. Recommended solubility of 1,1,2,2-tetrachloroethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
5	278.15	0.302	3.25
10	283.15	0.293	3.15
15	288.15	0.287	3.09
20	293.15	0.284	3.06
25	298.15	0.283	3.05
30	303.15	0.285	3.07
35	308.15	0.289	3.11
40	313.15	0.296	3.18
45	318.15	0.306	3.29
50	328.15	0.318	3.42

Part 2. The solubility of water (2) in 1,1,2,2-tetrachloroethane (1) has been studied by 11 groups of workers, mostly at 298.15 K. The datum of Lees and Sarram[20] is markedly lower than other results and is therefore rejected. The measurements of Othmer *et al.*,[5] McGovern,[6] and Zielinski[21] are several percent higher than the smoothed solubility values and are also rejected. The solubilities calculated from the distribution coefficients of Prosyanov *et al.*[22] are in very poor agreement, giving no confidence in the values which are regarded as dubious.

The remaining data of Staverman,[23] Hutchison and Lyon,[24] Johnson *et al.*,[25] Johnson,[26] Christian *et al.*,[27] and Barr and Newsham[16] were compiled or used for the smoothing equation. The fitting equation used was:

$$\log_{10} x_2 = 1.3175 - 974.642/(T/\mathrm{K}).$$

This equation represents the combined data with a standard deviation of 3.36×10^{-2} in the 273–323 K temperature range.

The recommended solubilities at 5 K intervals for water in 1,1,2,2-tetrachloroethane are given in Table 2.

TABLE 2. Recommended solubility of water (2) in 1,1,2,2-tetrachloroethane (1)

Temperature		Solubility	
°C	K	$100 w_2$	10^2 x_2
0	273.15	0.0605	0.561
5	278.15	0.0703	0.651
10	283.15	0.0811	0.751
15	288.15	0.0931	0.861
20	293.15	0.107	0.984
25	298.15	0.121	1.12
30	303.15	0.138	1.27
35	308.15	0.155	1.43
40	313.15	0.174	1.60
45	318.15	0.195	1.79
50	323.15	0.219	2.00

Measured values and the curve obtained from the smoothing equation for solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature are shown in Fig. 12.

It may be noted that all studies show a general increase in solubility with temperature which is consistent with the theory of water solubility for halogenated hydrocarbons as discussed in the Preface. As a common practice, the temperature dependence of solubility is often plotted on a Cox chart, that is, $\log_{10} x_2$ versus $1/(T/\mathrm{K})$, in which case a straight line usually represents the data, at least over some limited temperature range.

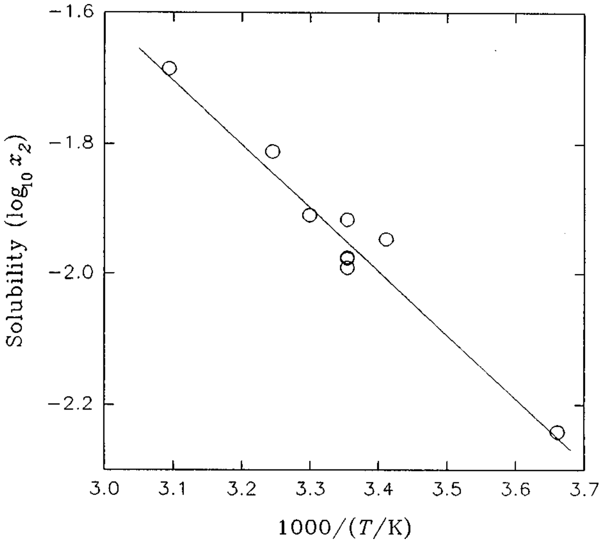

FIG. 12. Solubility of water (2) in 1,1,2,2-tetrachloroethane (1); log x_2 vs 1000/(T/K).

References:

[1] J. Hollo and T. Lengyel, Period. Polytech. **4**, 125 (1960).

[2] N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Teckhnol. Inst. 183 (1973).

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[4] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

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[18] A. I. Vogel, rev. by B. S. Furniss *et al. Vogel's Textbook of Practical Organic Chemistry*, 5th ed. (Longman, London, 1989), p. 1442.

[19] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

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[21] A. Zielinski, Z. Chem. Stosowana **3**, 377 (1955).

[22] N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 55 (1974).

[23] A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

[24] C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1943).

[25] J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Soc. A. 77 (1966).

[26] J. R. Johnson, Ph.D. thesis, University of Oklahoma, Norman, Oklahoma, 1966.

[27] S. D. Christian, H. E. Affsprung, W. J. A. Hunter, W. S. Gillam, and W. H. McCoy, ''Solute Properties of Water,'' U.S. Office of Saline Water Research and Development Program, Report No. 301 (1968).

Components:	**Original Measurements:**
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Amer. J. Hyg. **16**, 325 (1932).

Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/dm^3 kg^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	3.50×10^2	0.286	3.08

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,1,2,2-terachloroethane with a large volume of water and measuring the volume of the undissolved 1,1,2,2-terachloroethane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with a $NaCHO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
Variables:	**Prepared By:**
T/K=293–329	A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
20	0.288	0.287	3.09
55.5	0.336	0.335	3.61

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]	A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).
Variables:	**Prepared By:**
T/K=273–303	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	5.84×10^{-2}	5.73×10^{2}	3.24×10^{-3}
25	1.095×10^{-1}	1.02×10^{3}	6.08×10^{-3}
30	1.32×10^{-1}	1.23×10^{3}	7.33×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,2,2-tetrachloroethane and water was shaken for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. A full description of the method used is given elsewhere.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. F. Othmer, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1513 (1941).

Variables:

T/K=299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
25.5	<0.28	<3.01	0.13	1.2

Auxiliary Information

Method/Apparatus/Procedure:

The determination of the solubility was carried out in a 125 cm^3 Erlenmeyer flask, containing about 15 cm^3 of water.[1] The 1,1,2,2-tetrachloroethane was added to a sample from a buret and the flask was agitated until the solution becomes turbid. The amounts were converted to appropriate units using known densities of the pure components from volume to weight measurements.

Source and Purity of Materials:

(1) du Pont de Nemours & Company, purified to show a distillation range of 1–2 °C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ± 0.5 K.

References:

[1] D. F. Othmer, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $w_1 M_1^{-1}$/mol g^{-1}	$10^2\ x_1$ (compiler)	100 w_1 (compiler)
25	6.41×10^{-3}	1.06	0.115

Auxiliary Information

Method/Apparatus/Procedure:

A 1 to 15 volume ratio mixture of 1,1,2,2-tetrachloethane and water was introduced into an equilibration flask and then lowered into the water-bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given, purified and dried before use.

Estimated Errors:

Solubility: $\pm3.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:
T/K=293–323

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^2 x_2 (compiler)
20	2.8×10^{-1}	3.01	—	—
25	2.9×10^{-1}	3.12	1.13	9.62
30	3.0×10^{-1}	3.23	—	—
40	3.05×10^{-1}	3.28	—	—
50	3.1×10^{-1}	3.34	—	—

Solubility data as a function of temperature were presented in graphical form only except for data values at 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Source not given, commercial grade, used as received.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Original Measurements:
A. Z. Zielinski, Chem. Stosow. **3**, 377 (1959).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^2 x_1 (compiler)
25	2.08	0.131	1.21

Auxiliary Information

Method/Apparatus/Procedure:
The concentration of water in the organic phase was determined by the Karl Fischer titration method. Additional details are reported elsewhere.[1]

Source and Purity of Materials:
(1) Distilled (compiler).
(2) Gliwice Chemical, washed and redistilled before use.

Estimated Errors:
Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] J. Mitchell and D. M. Smith, *Aquametry: A Treatise on Methods for the Determination of Water* (Wiley, New York, 1952), pp. 73, 260.

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Hollo and T. Lengyel, Period. Polytech. **4**, 125 (1960).

Variables:

T/K=371–419

Prepared By:

A. L. Horvath

Experimental Data

t/°C	mole % (1)	100 w_1 (compiler)	10^2 x_1 (compiler)
97.9	1.0	8.60	1.0
94.5	5.1	33.37	5.1
94.0	17.79	66.85	17.79
93.4	37.0	84.55	37.0
94.1	53.1	91.34	53.1
94.1	85.87	98.26	85.87
94.0	91.8	99.05	91.8
95.3	96.85	99.65	96.85
116.0	96.9	99.66	96.9
131.5	99.01	99.89	99.01
146.2	100.0	100.0	100.0

Auxiliary Information

Method/Apparatus/Procedure:

The measurements were carried out in an apparatus for measuring equilibrium developed in the authors' institution.[1]

Source and Purity of Materials:

(1) Source not given; distilled before use, 90%–97% pure, b. p.=141–148 °C.
(2) Industrial water.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] J. Hollo and T. Lengyel, Comm. of the Inst. of Agricult. Chem. Techn., Polytechn. University, Budapest (1958).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Original Measurements:

J. R. Johnson, S. D. Christian, and H. E. Affsprung, J. Chem. Soc. A 77 (1966).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^2 x_1 (compiler)
25	0.101	0.115	1.06

Auxiliary Information

Method/Apparatus/Procedure:

Samples of the organic-water solutions were equilibrated in isothermal waterbaths. A solute isopiestic apparatus was used which has been described elsewhere.[1] The water solubilities were determined using a Beckman Model KF-3 Aquameter.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source not given. Reagent grade, distilled in an Oldershaw column before use.

Estimated Errors:

Solubility: ±0.0012.
Temperature: ±0.1 K.

References:

[1] S. D. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Original Measurements:

J. R. Johnson, Ph.D. thesis, University of Oklahoma, Norman, Oklahoma, 1966.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^2 x_1 (compiler)
25	0.101	0.115	1.06

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium between 1,1,2,2-tetrachloroethane and water took place in a well stirred water bath. The experimental samples were allowed to equilibrate for 2 or more days before analysis. The concentration of water in the organic phase was analyzed with a Beckman Aquameter using a Karl Fischer reagent. Full details are available in the thesis.

Source and Purity of Materials:

(1) Distilled.
(2) Allied Chemical Corp., purified by distillation before use.

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.1 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Original Measurements:

S. D. Christian, H. E. Affsprung, W. J. A. Hunter, W. S. Gillam, and W. H. McCoy, ‘‘Solute Properties of Water,’’ U.S. Office of Saline Water Research and Development Program, Report No. 301 (1968), p. 71.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	0.1010±0.0012	0.1143	10.55

Auxiliary Information

Method/Apparatus/Procedure:

The solute isopiestic method was used without modification. The apparatus employed consisted of a closed vessel divided into two compartments, one for water and the other for the organic solvent. Equilibrium was attained after a period of 6–8 h. Samples of the solution were analyzed for water with the Beckman KH-3 Aquameter. The Karl Fischer reagent was standardized against crystalline sodium tartarate dihydrate.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given, certified or reagent grade, distilled through a 30-plate Oldershaw column before use.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]	F. P. Lees and P. Sarram, J. Chem. Eng. Data **16**, 41 (1971).

Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	4.0×10^{-2}	3.71	2.2×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

An apparatus containing the mixture of 1,1,2,2-tetrachloroethane and water was placed in a water-bath thermostat. The stirring of the mixture was accomplished by using a glass rod rotated by a horseshoe magnet for about 48 h. The concentration of water in the organic liquid phase was determined by the Karl Fisher titration method.

Source and Purity of Materials:

(1) Distilled.

(2) Source not given, analytical grade, degassed and used without further purification.

Estimated Errors:

Solubility: ±7%.

Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 183 (1973).

Variables:	**Prepared By:**
T/K=287–373	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
14	1.360×10^3	1.95×10^{-3}	2.094×10^{-2}
32	8.80×10^2	1.00×10^{-2}	1.077×10^{-1}
50	5.90×10^2	4.20×10^{-2}	4.509×10^{-1}
60	5.50×10^2	7.50×10^{-2}	8.061×10^{-1}
70	4.50×10^2	1.47×10^{-1}	1.579×10^0
80	4.40×10^2	2.32×10^{-1}	2.500×10^0
90	3.35×10^2	4.57×10^{-1}	4.926×10^0
90.4	2.95×10^2	6.61×10^{-1}	7.142×10^0
100	2.80×10^2	7.95×10^{-1}	8.591×10^0

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

The distribution coefficient was determined by distillation. An inert carrier gas stream was used to take samples from the equilibrium vapor phase. The concentration of the 1,1,2,2-tetrachloroethane in both liquid and vapor phases was determined by using a ^{36}Cl labeled compound.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.

Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

Original Measurements:

N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 55 (1974).

Variables:

T/K = 298–363

Prepared By:

A. L. Horvath

Experimental Data

$$\log_{10} \alpha = \frac{1317.16}{(T/\mathrm{K})} - 1.7423,$$

where α = distribution coefficient.

At the normal boiling point of $CHCl_2$–$CHCl_2$, $\alpha = 25$ and the activity coefficient, $\gamma_1 = 19$.

Auxiliary Information

Method/Apparatus/Procedure:

The water concentration in 1,1,2,2-tetrachloroethane rich phase was determined by radiometric method using tritium labeled water. The experimental procedure is described in more detail elsewhere.[1]

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 100 (1973).

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. Walraevens, P.Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).

Variables:

T/K = 283–353

Prepared By:

A. L. Horvath

Experimental Data

The temperature dependence of the solubility of 1,1,2,2-tetrachloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/\mathrm{mol\ dm^{-3}}) = \frac{2070}{(T/\mathrm{K})} - 15.316 + 0.0222(T/\mathrm{K}),$$

where S = Solubility, and T = absolute temperature

The temperature interval covered is between 283 and 353 K. For example, the calculated solubility derived from the above equation is 2.95×10^{-1} [100 w_1] at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,2,2-tetrachloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated and the equilibrium was maintained by vigorous stirring. The concentration of 1,1,2,2-tetrachloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Solvay chemical, rectified before use, purity was 99.9% by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [7934-5] (2) Water; H_2O; [7732-18-5]	C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U. S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).
Variables:	**Prepared By:**
T/K=276–307	A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
3	3.80	0.379	4.08
20	3.23	0.322	3.47
34	3.21	0.321	3.46

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5-10 g 1,1,2,2-tetrachloroethane was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on determination and evaluation of the procedure are found elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou and D. W. Schmedding, Test. Protec. Environ. Fate Mov. Toxicants, Proc. Symp., 1980, pp. 28–42 (Publ. 1981).

Components:	**Original Measurements:**
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Partition coefficient[a], K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	3.57×10^1	0.3041	3.273

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A 1,1,2,2-tetrachloroethane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height on the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±1.4 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Variables:

T/K=297

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
23.5	0.296	3.18	1.76×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous solubility was determined by elution chromatography. The solute columns (3 mm o.d., 2 mm i.d., and 40 cm long) were filled with Chromosorb P. The analysis consisted of removing a segment of the column packing and placing it into a test tube containing *n*-octane. Then, samples were injected into a gas chromatograph for analysis. The average deviations were calculated from several measurements on different samples.

Source and Purity of Materials:

(1) Commercial reagent of spectral grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±3.0% std. dev.
Temperature: ±1.5 K.

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. **767**, Philadelphia, Pa., 1980, pp. 116–29.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1 V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	1.78×10^{-2}	0.298	3.21

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,1,2,2-tetrachloroethane was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^{-3}\ c_1$ /mol dm^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	1.77×10^{-2}	0.297	3.20

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,1,2,2-tetrachloroethane was added to a stainless steel tube containing water and the tube was sealed. It was allowed to equilibrate during shaking for 1 week at 25 °C. After centrifugation, the sample was analyzed for radioactivity using a liquid scintillation counter. The solubility determination was repeated at least twice for each sample and the analysis was done in duplicate.

Source and Purity of Materials:

(1) New England Nuclear, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±0.6% std. dev.
Temperature: ±0.3 K.

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. P. Schwarz and J. Miller, Anal. Chem. **52**, 2162 (1980).

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
10.0	0.372 ± 0.007	4.01	2.22×10^{-3}
20.0	0.385 ± 0.017	4.15	2.19×10^{-3}
30.0	0.367 ± 0.007	3.95	2.19×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous solubility was determined by elution chromatography. The solute columns (3 mm o.d., 1.8 mm i.d.) were positioned vertically in a waterbath thermostat. The measurement time interval ranged from 1 day to 2 weeks. The average deviations were calculated from several measurements on different samples. The elution chromatography method has been described elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: 4%.
Temperature: ±0.5 K.

References:

[1] F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

T/K=284–300

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient[a], D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
11.0	10.94	0.1943	2.0892
13.0	12.52	0.1967	2.1150
21.0	17.03	0.2538	2.7305
22.0	19.40	0.2384	2.5647
27.2	20.94	0.3069	3.3030

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,1,2,2-tetrachloroethane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,1,2,2-tetrachloroethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5.6.
Temperature: ±0.5 K.

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1 V_2^{-1}$/g m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	2.915×10^3	0.2919	3.141

Auxiliary Information

Method/Apparatus/Procedure:

Standard 1,1,2,2-tetrachloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±5.43% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:	Original Measurements:
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	R. S. Barr and D. M. T. Newsham, Fluid Phase Equilib. **35**, 189 (1987).

Variables:	Prepared By:
T/K=293–323	A. L. Horvath

Experimental Data

t/°C	$10^4\ x_1$	$100\ w_1$ (compiler)	$10^3 x_2$	$100\ w_2$ (compiler)
20	2.52	0.234	11.3	0.123
35	2.89	0.269	15.4	0.168
50	3.32	0.308	20.6	0.225

Mole fraction of 1,1,2,2-tetrachloroethane (x_1) was calculated from the activity coefficients at infinite dilution (γ_1^∞) using the relation $x_1=1/\gamma_l^\infty$.

Auxiliary Information

Method/Apparatus/Procedure:

The water-rich mixture was studied using gas–liquid chromatography in which a mixture of methane and 1,1,2,2-tetrachloroethane vapor passed through the sampling loop. The eluted 1,1,2,2-tetrachloroethane was determined with a flame ionization detector. The organic-rich mixture was studied using an isopiestic method in which $CaCl_2$ solution controlled the partial pressure of water. The water concentration of the organic phase was determined by using a Karl Fischer titration apparatus.

Source and Purity of Materials:

(1) BDH Chemicals Limited, redistilled in a glass sieve tray column.
(2) Doubly-distilled tap water.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:	Original Measurements:
(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida, (September 1987), 86 pp. (AD-A188 571).

Variables:	Prepared By:
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
10	2588	0.2588	2.7841
20	2526	0.2526	2.7173
30	2131	0.2131	2.2916

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled, de-ionized water and sealed. Measured volumes of 1,1,2,2-tetrachloroethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC responses were compared with calibration plots to establish concentrations

Source and Purity of Materials:

(1) Probably a commercial reagent, at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. I. Vogel, rev. by B. S. Furniss *et al.*, *Vogel's Textbook of Practical Organic Chemistry*, 5th ed. (Longman, London, 1989), p. 1442.

Variables:

$T/\mathrm{K}=293$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1M_1^{-1}/\mathrm{mol\ g}^{-1}$ (compiler)
20.0	0.29	3.12	1.73×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The solubility determination was carried out in small test tubes (e.g., 100×12 mm) to permit vigorous shaking of the solvent and solute mixtures. During the experiment, 0.20 cm^3 1,1,2,2-tetrachloroethane was added to 3.0 cm^3 of water and agitated. The concentration of 1,1,2,2-tetrachloroethane in water was analyzed by passing the sample through a chromatographic column.

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

$T/\mathrm{K}=293-313$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	γ_1^{∞}	$10^4\ x_1$	$100\ w_1$ (compiler)
20	3850±660	2.60	0.242
30	2970±625	3.37	0.313
40	3570±245	2.80	0.260

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,1,2,2-tetrachloroethane (γ_1^{∞}) in water. Cells containing degassed water were submerged in a thermostat water bath. The 1,1,2,2-tetrachloroethane was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered and de-ionized.

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:	**Original Measurements:**
(1) Water-d_2 ; D_2O; [7789-20-0] (2) 1,1,2,2-tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]	C. A. Hutchison and A. M. Lyon, Columbia University Report **A-745** (July 1, 1943).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

37. 1,1,2,2-Tetrachloroethane with Water-d_2

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	10^3 x_1 (compiler)	100 w_1 (compiler)
25	5.56×10^{-3}	9.23	0.111

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and 1,1,2,2-tetrachloroethane was introduced into an equilibration flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source is not given, purified and dried before use.

Estimated Errors:

Solubility: ±1.0×10^{-5} av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:	**Original Measurements:**
(1) cis-1,2-diiodoethene (cis-1,2-diiodoethylene); $C_2H_2I_2$; ; [590-26-1] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **75**, 5733 (1951).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

38. Cis-1,2-Diiodoethene with Water

Experimental Data

t/°C	c_1 /mol m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25.0	1.65	4.63×10^{-2}	2.98

Auxiliary Information

Method/Apparatus/Procedure:

Water was mixed with cis-1,2-diiodoethene in a glass stoppered Erlenmeyer flask which was then placed in a constant temperature bath and rotated for 30 h. The organic halide content of the aqueous phase was extracted with *n*-hexane. The optical density of the extract was measured against a blank pure *n*-hexane sample using a Beckman spectrophotometer as described elsewhere.[1]

Source and Purity of Materials:

(1) Prepared by isomerization of crude trans-1,2-diiodoethylene at 160 °C. The cis- and trans-isomers were separated by filtration and then centrifugation.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.3 K (compiler).

References:

[1] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).

Components:	**Original Measurements:**
(1) trans-1,2-diiodoethene (trans-1,2-diiodoethylene); $C_2H_2I_2$; [590-27-2] (2) Water; H_2O; [7732-18-5]	L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **73**, 5733 (1951).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

39. Trans-1,2-Diiodoethene with Water

Experimental Data

t/°C	c_1 /mol m^{-3}	100 w_1 (compiler)	10^6 x_1 (compiler)
25.0	0.527	1.48×10^{-2}	9.53

Auxiliary Information

Method/Apparatus/Procedure:

Water was mixed with trans-1,2-diiodoethene in a glass stoppered Erlenmeyer flask which was then placed in a constant temperature bath and rotated for 30 h. The organic halide content of the aqueous phase was extracted with *n*-hexane. The optical density of the extract was measured against a pure *n*-hexane blank using a Beckman spectrophotometer as described elsewhere.[1]

Source and Purity of Materials:

(1) Prepared by passing commercial acetylene into a solution of iodide in 95% ethyl alcohol and purified by repeated crystallization.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.3 K (compiler).

References:

[1] L. J. Andrews and R. M. Keefer, J. Am. Chem. Soc. **71**, 3644 (1949).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dibromo-1-chloroethane; $C_2H_3Br_2Cl$; [598-20-9]	W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

40. 1,2-Dibromo-1-Chloroethane with Water

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
20	6.0×10^{-2}	6.0×10^{-2}	7.35

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).

(2) Dow Chemical Co., used as received.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2-tribromoethane; $C_2H_3Br_3$; [78-74-0]

Original Measurements:

W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:

T/K=293

Prepared By:

A. L. Horvath

41. 1,1,2-Tribromoethane with Water

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	5.0×10^{-2}	5.0×10^{-2}	7.35

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).

(2) Dow Chemical Co., used as received.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1-dichloro-1-fluoroethane; $C_2H_3Cl_2F$; [1717-00-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. Sukornick, Int. J. Thermophys. **10**, 553 (1989).

Variables:

T/K=298

Prepared By:

A. L. Horvath

42. 1,1-Dichloro-1-Fluoroethane with Water

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
25	6.60×10^{-2}	1.02	4.20×10^{-2}	2.72

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Allied-Signal Inc., Buffalo, N. Y. Purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

43. 1,1,1-Trichloroethane with Water

Critical Evaluation

The 1,1,1,-trichloroethane (1) and water (2) binary system is treated in two parts; part 1 is 1,1,1-trichloroethane (1) in water (2) and part 2 is water (2) in 1,1,1-trichloroethane (1).

Part 1. The solubility of 1,1,1-trichloroethane (1) in water (2) has been studied by 25 groups of workers over the temperature interval from 273.15 to 323.15 K. The experimental data of most investigators are sufficiently reliable to use in the smoothing equation. However, the data of some workers were not used for the smoothing equation for a variety of reasons. The measured solubility of McConnell *et al.*,[1] Pearson and McConnell,[2] Archer and Stevens,[3] Coca and Diaz,[4] Hutchinson *et al.*,[5] and McNally and Grob[6] are markedly lower than the solubility values calculated from the smoothing equation and are therefore rejected. The measurements of Schwarz and Miller[7] and Warner *et al.*[8] are several percent higher than the smoothed solubility values and are also rejected.

The remaining data of van Arkel and Vles,[9] O'Connell,[10] Walraevens *et al.*,[11] Chiou and Freed,[12] Sato and Nakijima,[13] Schwarz,[14] Veith *et al.*,[15] Banerjee *et al.*,[16] Leighton and Calo,[17] Hunter-Smith *et al.*,[18] Orlandini *et al.*,[19] Lincoff and Gossett,[20] Munz,[21] Barr and Newsham,[22] Gossett,[23] Howe *et al.*,[24] and Wright *et al.*,[25] were compiled or used for the smoothing equation. The combined data of 17 laboratories were used to obtain the following mass percent (1) equation:

$$\text{Solubility } [100\ w_1] = 1.09092 - 6.52776\times10^{-3}\ (T/\text{K}) + 1.10747\times10^{-5}(T/\text{K})^2,$$

which showed a standard deviation of 1.71×10^{-2} in the temperature range from 273 to 323 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 13. A solubility minimum calculated from the above regression equation is 0.129 [100 w_1] at 294.71 K. Additional details concerning the solubility minimum for aqueous hydrocarbon systems are discussed in the Preface.

The recommended solubility values at 5 K intervals for 1,1,1-trichloroethane (1) in water (2) are presented in Table 1.

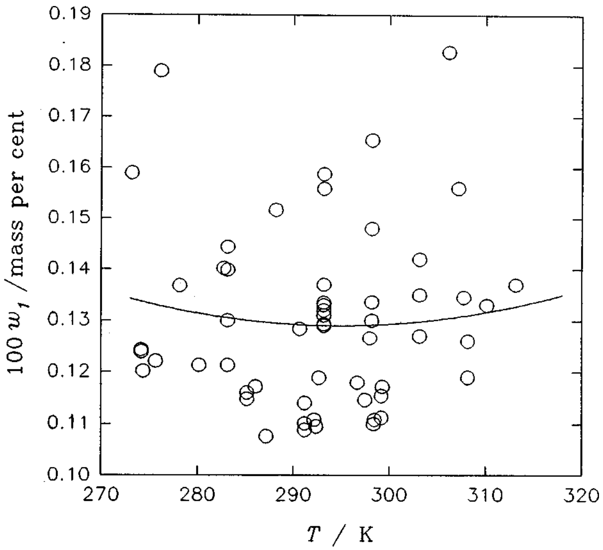

FIG. 13. Solubility of 1,1,1-trichloroethane (1) in water (2).

TABLE 1. Recommended solubility of 1,1,1-trichloroethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^4\ x_1$
0	273.15	0.134	1.81
5	278.15	0.132	1.78
10	283.15	0.130	1.76
15	288.15	0.129	1.74
20	293.15	0.129	1.74
25	298.15	0.129	1.74
30	303.15	0.130	1.76
35	308.15	0.131	1.77
40	313.15	0.133	1.80
45	318.15	0.135	1.82
50	323.15	0.138	1.87

Part 2. The solubility of water (2) in 1,1,1-trichloroethane (1) has been measured by eight groups of workers with reasonably consistent results. The reported solubilities cover the temperature range from 273.15 to 323.15 K.

All the available data for water solubility in 1,1,1-trichloroethane are considered for fitting a correlating equation with the following exclusions. Both results of Lees and Sarram[26] and Archer and Stevens[3] are rejected because they are significantly higher than later studies. The remaining data of six laboratories are in good agreement and the correlated values are recommended. These data of Staverman,[27] Coca and Diaz,[4] O'Connell,[10] Ohtsuka and Kazama,[28] Orlandini *et al.*,[19] and Barr and Newsham,[22] were used for the smoothing equation:

$$\log_{10} x_2 = 0.43885 - 909.536/(T/\text{K}).$$

This equation represents the combinad data with a standard deviation of 9.62×10^{-2} in the temperature range from 273 to 323 K. The recommended values of solubility at 5 K intervals for water (2) in 1,1,1-trichloroethane (1) are presented in Table 2.

TABLE 2. Recommended solubility of water (2) in 1,1,1-trichloroethane (1)

Temperature		Solubility	
°C	K	100 w_2	$10^3\ x_2$
0	273.15	0.0174	1.285
5	278.15	0.0199	1.475
10	283.15	0.0228	1.685
15	288.15	0.0259	1.916
20	293.15	0.0294	2.170
25	298.15	0.0331	2.445
30	303.15	0.0371	2.743
35	308.15	0.0416	3.072
40	313.15	0.0464	3.423
45	318.15	0.0515	3.802
50	323.15	0.0571	4.214

Measured values and the curve obtained from the smoothing equation for solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature are shown in Fig. 14.

The linear relation between the solubility expressed as $\log_{10} x_2$ versus $1/(T/\text{K})$ is illustrated in Fig. 14. Such straight line plots are characteristic for water solubility in halogenated hydrocarbons as discussed in the Preface.

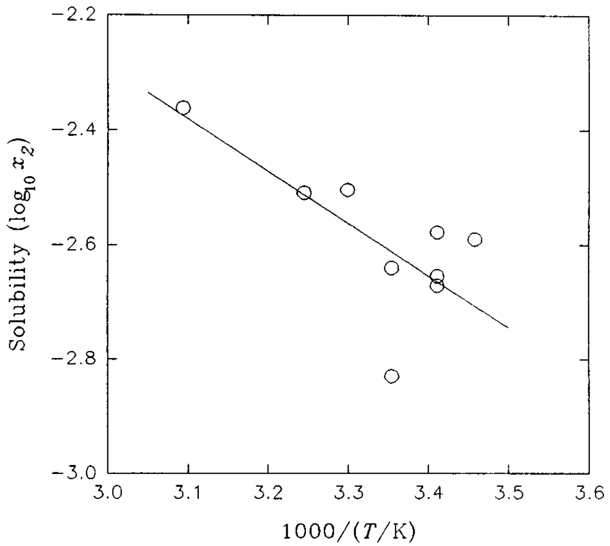

FIG. 14. Solubility of water (2) in 1,1,1-trichloroethane (1); log x_2 vs 1000/(T/K).

References:

[1] G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).

[2] C. R. Pearson and G. McConnell, Proc. R. Soc. London, Ser. B **189**, 305 (1975).

[3] W. L. Archer and V. L. Stevens, I&EC Prod. Res. Dev. **16**, 319 (1977).

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[5] T. C. Hutchinson *et al. Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment* (Plenum, New York, 1980), pp. 577–86.

[6] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

[7] F. P. Schwarz and J. Miller, Anal. Chem. **52**, 2162 (1980).

[8] H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

[9] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

[10] W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

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[18] R. J. Hunter-Smith, P. W. Balls, and P. S. Liss, Tellus **35B**, 170 (1983).

[19] M. Orlandini, M. Fermeglia, I. Kikic, and P. Alessi, Chem. Eng. J. **26**, 245 (1983).

[20] A. H. Lincoff and J. M. Gossett, in *Gas Transfer at Water Surface*, edited by W. Brutsaert and G. H. Jirka (Reidel, Dordrecht, 1984), pp. 17–25.

[21] C. D. Munz, Ph. D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

[22] R. S. Barr and D. M. T. Newsham, Fluid Phase Equilibr. **35**, 189 (1987).

[23] J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

[24] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

[25] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

[26] F. P. Lees and P. Sarram, J. Chem. Eng. Data **16**, 41 (1971).

[27] A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

[28] K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Components:	**Original Measurements:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
Variables:	**Prepared By:**
T/K=273–323	A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
0	0.159	0.159	2.15
20	0.132	0.132	1.78
35	0.126	0.126	1.70
50	0.128	0.128	1.73

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]

Original Measurements:

A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	1.62×10^{-2}	1.19×10^{2}	8.99×10^{-4}
25	3.39×10^{-2}	2.57×10^{2}	1.88×10^{-3}
30	4.22×10^{-2}	3.13×10^{2}	2.34×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,1-trichloroethane and water was shaken for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. A full description of the method used is given elsewhere.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph. D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:

T/K=293–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
20	—	—	3.0×10^{-2}	2.22
25	1.30×10^{-1}	1.75	—	—

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Dow Chemicals Co., used as received.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]	F. P. Lees and P. Sarram, J. Chem. Eng. Data **16**, 41 (1971).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	5.0×10^{-2}	3.69	2.8×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The apparatus containing the organic-water system was held in a waterbath thermostat. The stirring of the mixture was effected by a glass rod rotated by a horseshoe magnet for about 48 h. The concentration of water in the organic phase was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given. Analytical grade, degassed and used without further purification.

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).
Variables:	**Prepared By:**
T/K=283–353	A. L. Horvath

Experimental Data

The temperature dependence of the solubility of 1,1,1-trichloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/\text{mol dm}^{-3})=\frac{2070}{(T/\text{K})}-14.860+0.0200(T/\text{K}),$$

where S=solubility, and T=absolute temperature.

For example, the calculated solubility derived from the above equation is 1.48×10^{-1} [100 w_1] at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,1-trichloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated and the equilibrium was maintained by vigorous stirring. The concentration of 1,1,1-trichloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Solvay, rectified before use, the purity was was 99.9% by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

$t/°C$	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	4.80×10^2	4.80×10^{-2}	6.48

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of the 1,1,1-trichloroethane in water was determined by gas–liquid chromatography (GLC) using an electron capture detector. Where possible, identification was confirmed by a linked mass spectrometer (MS) method.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.2 K (compiler).

Components:	**Original Measurements:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	C. R. Pearson and G. McConnell, Proc. Roy. Soc. London, Ser. B **189**, 305 (1975).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

$t/°C$	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	4.80×10^2	4.80×10^{-2}	6.48

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with *n*-pentane and an aliquot of the extract taken for gas–liquid chromatographic analysis. The gas chromatograph was fitted with a ^{63}Ni electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.2 K (compiler).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U.S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1997).

Variables:

T/K=276–307

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
3	1.79	0.179	2.42
20	1.37	0.137	1.85
34	1.55	0.156	2.11

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5–10 g 1,1,1-trichloroethane was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on determination and evaluation of the procedure are found elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou and D. W. Schmedding, Test. Protec. Environ. Fate Mov. Toxicants, Proc. Symp., 1980, pp. 28–42 (Publ. 1981).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. L. Archer and V. L. Stevens, I&EC Prod. Res. Dev. **16**, 319 (1977).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^5 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	7.0×10^{-2}	9.46	5.0×10^{-2}	3.69

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available. Data were reported elsewhere.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] News Release from Dow Chemical USA (October 23, 1975).

Components:	Original Measurements:
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:	Prepared By:
T/K=310	A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L /dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	0.93	0.133	1.798

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A 1,1,1-trichloroethane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height of the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.14 std. dev.
Temperature: ±0.5 K (compiler).

Components:	Original Measurements:
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Variables:	Prepared By:
T/K=297	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
23.5	0.120	1.62	8.99×10^{-4}
	0.115	1.55	8.62×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous solubility was determined by elution chromatography. The solute columns (3 mm o.d., 2 mm i.d., and 40 cm long) were filled with Chromosorb P. The analysis consisted of removing a segment of the column packing and placing it into a test tube containing *n*-octane. Then, samples were injected into a gas chromatograph for analysis. The average deviations were calculated from several measurements on different samples.

Source and Purity of Materials:

(1) Commercial reagent of spectral grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±3.0% std. dev.
Temperature: ±1.5 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Coca and R. M. Diaz, J. Chem. Eng. Data **25**, 80 (1980).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
25	1.0×10^{-2}	1.35	2.0×10^{-2}	1.48

Auxiliary Information

Method/Apparatus/Procedure:

A titration was performed in an Erlenmeyer flask by adding 1,1,1-trichloroethane to water until a permanent turbidity was observed. The flask was immersed in a waterbath thermostat while maintaining a constant agitation using a magnetic stirrer.

Source and Purity of Materials:

(1) Fluka reagent, laboratory grade, further purified by distillation; middle fraction used.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 707, Philadelphia, Pa., 1980, pp. 116–29.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	1.0×10^{-2}	0.1335	1.805

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,1,1-trichloroethane was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

T. C. Hutchinson, *et al.*, *Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment* (Plenum, New York, 1980), pp. 577–86.

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	0.720	7.22×10^{-2}	9.76

Auxiliary Information

Method/Apparatus/Procedure:

An excess quantity of 1,1,1-trichloroethane was added to water and stirred vigorously for 24 h. After settling at 25 °C for 48 h, the solution was extracted with cyclohexane. The samples were analyzed using an Aminco-Bowman spectrophotofluorometer. A detailed description of the method has been reported elsewhere.[1]

Source and Purity of Materials:

(1) Aldrich Chemicals, highest grade, used as received.
(2) Double distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.2 K (compiler).

References:

[1] D. Mackay and W. Y. Shiu, J. Chem. Eng. Data **22**, 399 (1977).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	1.00×10^{-2}	0.1336	1.81

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,1,1-trichloroethane was added to a stainless steel tube containing water and the tube was sealed. It was allowed to equilibrate during shaking for 1 week at 25 °C. After centrifugation, the sample was analyzed for radioactivity using a liquid scintillation counting. The solubility determination was repeated at least twice for each sample and the analysis was done in duplicate.

Source and Purity of Materials:

(1) New England Nuclear, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±2.1% std. dev.
Temperature: ±0.3 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

F. P. Schwarz and J. Miller, Anal. Chem. **52**, 2162 (1980).

Variables:

$T/\mathrm{K}=283-303$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1M_1^{-1}/\mathrm{mol\ g}^{-1}$ (compiler)
10.0	0.180±0.003	2.43	1.35×10^{-3}
20.0	0.185±0.001	2.50	1.39×10^{-3}
30.0	0.159±0.001	2.15	1.19×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The aqueous solubility was determined by elution chromatography. The solute columns (3 mm o.d., 1.8 mm i.d.) were positioned vertically in a water-bath thermostat. The measurement time interval ranged from 1 day to 2 weeks. The average deviations were calculated from several measurements on different samples. The elution chromatography method has been described elsewhere.[1]

Source and Purity of Materials:

(1) Source not given. Commercial reagent, 98 wt. % pure, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±4%.
Temperature: ±0.5 K.

References:

[1] F. P. Schwarz, Anal. Chem. **52**, 10 (1980).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

$T/\mathrm{K}=274-299$

Prepared By:

A. L. Horvath

Experimental Data

$t/°\mathrm{C}$	Distribution coefficient,[a] D_L /dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
1.0	2.970×10^2	0.1243	1.680
1.0	2.979×10^2	0.1239	1.675
1.2	3.070×10^2	0.1202	1.625
2.5	3.278×10^2	0.1221	1.651
7.0	4.185×10^2	0.1213	1.640
10.0	5.040×10^2	0.1213	1.640
12.0	5.568×10^2	0.1160	1.587
12.0	5.696×10^2	0.1148	1.552
12.9	5.862×10^2	0.1172	1.584
14.0	6.527×10^2	0.1076	1.494
18.0	7.667×10^2	0.1140	1.541
18.0	7.934×10^2	0.1101	1.489
18.0	8.029×10^2	0.1088	1.472
19.0	8.283×10^2	0.1108	1.495
19.2	8.367×10^2	0.1095	1.480
19.5	7.881×10^2	0.1189	1.608
24.3	1.0276×10^3	0.1146	1.549
25.2	1.0943×10^3	0.1100	1.487
25.3	1.1107×10^3	0.1108	1.498
26.0	1.0902×10^3	0.1154	1.540
26.0	1.1314×10^3	0.1112	1.504
26.1	1.0738×10^3	0.1172	1.584

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,1,1-trichloroethane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,1,1-trichloroethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±2.5%.
Temperature: ±0.5 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]

Original Measurements:

K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	0.42	3.1×10^{-2}	2.29

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 1,1,1-trichloroethane in a flask and it was lowered into a thermostatic bath. The flask was then shaken vigorously until the first cloud (turbidity) appeared. The water content in the sample was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled.
(2) Commercial JIS extra pure reagent, further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. J. Hunter-Smith, P. W. Balls, and P. S. Liss, Tellus **35B**, 170 (1983).

Variables:

T/K=278–306

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
5	0.2645	0.1368	1.849
10	0.3183	0.1444	1.952
15	0.3805	0.1517	2.051
20	0.4522	0.1588	2.147
25	0.5342	0.1655	2.238
33	0.6897	0.1838	2.486

[a] The Henry's law constant (H, dimensionless) was derived from a van't Hoff plot best-fit equation: $\log_e H=9.15-2915/(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibration technique was used to measure the Henry's law constant as described elsewhere.[1] A known volume of water in a syringe was shaken with a known volume of pure 1,1,1-trichloroethane. After equilibration the headspace was separated and analyzed for the compound of interest. A gas chromatograph fitted with an electron capture detector was used for the analysis.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5.5% std. dev.
Temperature: ±0.2 K.

References:

[1] C. D. McAuliffe, Chem. Techn. **1**, 46 (1971).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. Orlandini, M. Fermeglia, I. Kikic, and P. Alessi, Chem. Eng. J. **26**, 245 (1983).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^4\ x_1$	$100\ w_1$ (compiler)	$10^3\ x_2$	$100\ w_2$ (compiler)
20	1.8	0.133	2.14	2.90×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,1-trichloroethane and water was agitated overnight and left at equilibrium for 24 h. Three samples were withdrawn for each phase with a syringe and analyzed by gas chromatography. The gas chromatograph (C. Erba ATc/t) was equipped with a Shimadzu Chromatopac E-1A integrator. A stainless column packed with 100-120 mesh Chromosorb W DMCD coated with heptadecane nitrile was used for analysis.

Source and Purity of Materials:

(1) Fluka reagent, purified by distillation before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. H. Lincoff and J. M. Gossett, in *Gas Transfer at Water Surfaces*, edited by W. Brutsaert and G. H. Jirka (Reidel, Dordrecht, 1984), pp. 17–25.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

EPICS method

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	1.32×10^{-2}	0.1313	1.775

$\log_e H=10.21-4262/(T/\mathrm{K})$

Batch air stripping method

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	1.34×10^{-2}	0.1293	1.748

$\log_e H=9.975-4186/(T/\mathrm{K})$

Auxiliary Information

Method/Apparatus/Procedure:

Henry's law constants were measured by EPICS and Batch Air Stripping Methods. The Equilibrium Partitioning in the Closed Systems technique compares the GC peak heights upon direct injection of headspace samples. In the Batch Air Stripping Method, equal volume samples were placed in serum battles and the equilibrated headspaces contained concentrations proportional to original concentrations in the aqueous samples. Full equilibrium was achieved in a few hours.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5%–10%.
Temperature: ±0.1 K.

Components:	Original Measurements:
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
Variables:	**Prepared By:**
T/K=303	A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
30	0.4798	4.816×10^{-2}	6.506

Auxiliary Information

Method/Apparatus/Procedure:

Standard 1,1,1-trichloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA, USA., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges before use.

Estimated Errors:

Solubility: ±5.17% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:	Original Measurements:
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Water; H_2O; [7732-18-5]	C. D. Munz, Ph. D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/dimensionless	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
10	0.355	1.30	0.1300	1.758
20	0.559	1.29	0.1290	1.744
30	0.855	1.27	0.1270	1.717

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Matheson Coleman & Bell, OH, greater than 99.5% purity.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±3.8%.
Temperature: ±0.5 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. S. Barr and D. M. T. Newsham, Fluid Phase Equilib. **35**, 189 (1987).

Variables:

T/K=293–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^4\ x_1$	100 w_1 (compiler)	$10^3\ x_2$	100 w_2 (compiler)
20	1.77	0.131	2.64	3.57×10^{-2}
35	1.61	0.119	3.10	4.20×10^{-2}
50	1.71	0.126	4.35	5.90×10^{-2}

Mole fraction of 1,1,1-trichloroethane (x_1) was calculated from the activity coefficients at infinite dilution (γ_1^∞) using the relation $x_1=1/\gamma_1^\infty$.

Auxiliary Information

Method/Apparatus/Procedure:

The water-rich mixture was studied using gas–liquid chromatography in which a mixture of methane and 1,1,1-trichloroethane vapor passed through the sampling loop. The eluted 1,1,1-trichloroethane was determined with a flame ionization detector. The organic-rich mixture was studied using an isopiestic method in which $CaCl_2$ solution controlled the partial pressure of water. The water concentration of the organic phase was determined by using a Karl Fischer titration apparatus.

Source and Purity of Materials:

(1) Koch Light Laboratory Limited, redistilled in a glass sieve tray column before use.
(2) Double distilled tap water.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:

T/K=283–308

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	CV[a] %	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
9.6	7.61×10^{-3}	2.10	0.1402	1.896
17.5	1.20×10^{-2}	0.67	0.1284	1.736
24.8	1.72×10^{-2}	3.81	0.1266	1.712
34.6	2.49×10^{-2}	3.48	0.1345	1.818

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of 1,1,1-trichloroethane was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Fisher Scientific, further purified before use.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
24.85	4.92×10^{-3}	0.4568	6.193

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants, as described by Mackay, *et al.*,[1] was used. The general procedure was to add an excess quantity of 1,1,1-trichloroethane to distilled deionized water, place the sample in a thermostat bath, and mix overnight. A portion of this solution was returned to the stripping vessel. The 1,1,1-trichloroethane was stripped isothermally from the solution mixture at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used without further purification, stated purity greater than 99%.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6.0% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

Variables:

T/K=283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6 g_1/g_2$	100 w_1 (compiler)	10^4 x_1 (compiler)
10	1.399×10^3	0.1399	1.8915
20	1.559×10^3	0.1559	2.1081
30	1.420×10^3	0.1420	1.9199

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled, de-ionized water and sealed. Measured volumes of 1,1,1-trichloroethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about three weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC responses were compared with calibration plots to establish concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% pure. Used without further purification.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–313

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^4\ x_1$	$100\ w_1$ (compiler)
20	5880±75	1.70	0.126
30	5480±60	1.82	0.135
40	5410±80	1.85	0.137

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,1,1-trichloroethane (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. The 1,1,1-trichloroethane was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered, and de-ionized.

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:

(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6]
(2) MQ-Water

Original Measurements:

C. D. Munz, Ph. D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.

Variables:

T/K=293

Prepared By:

A. L. Horvath

44. 1,1,1-Trichloroethane with MQ-Water

Experimental Data

t/°C	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	0.617	0.1164	1.573

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Matheson Coleman & Bell, OH, greater than 99.5% pure.
(2) Milli-Q water; 0.25 mg total organic carbon/dm^3 and 0.75 mg COD/dm^3.

Estimated Errors:

Solubility: ±0.017 std. dev.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Municipal tap water (PASE)	C. D. Munz, Ph. D. thesis, Stanford University, Stanford, CA, 1985, 306 pp.
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

45. 1,1,1-Trichloroethane with Municipal Tap Water (PASE)

Experimental Data

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
20	0.686	0.1049	1.418

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were preconcentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:

(1) Matheson Coleman & Bell, OH, greater than 99.5% pure.
(2) 10 mg total organic carbon/dm^3 and 40 mg COD/dm^3.

Estimated Errors:

Solubility: ±0.028 std. dev.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 1,1,1-trichloroethane; $C_2H_3Cl_3$; [71-55-6] (2) Seawater	R. J. Hunter-Smith, P. W. Balls, and P. S. Liss, Tellus **35B**, 170 (1983).
Variables:	**Prepared By:**
T/K=278–298	A. L. Horvath

46. 1,1,1-Trichloroethane with Seawater

Experimental Data

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
5	0.3682	1.002×10^{-1}	1.354
10	0.4718	9.92×10^{-2}	1.341
15	0.5993	9.79×10^{-2}	1.324
20	0.7552	9.66×10^{-2}	1.305
25	0.9442	9.50×10^{-2}	1.284

The Henry's law constant (H, dimensionless) was derived from a van't Hoff plot best-fit equation: $\log_e H=13.04-3905/(T/\mathrm{K})$.

Auxiliary Information

Method/Apparatus/Procedure:

The multiple equilibration technique was used to measure the Henry's law constant as described by McAuliffe.[1] A known volume of pure 1,1,1-trichloroethane in a syringe was shaken with a known volume of pure water. After equilibration, the headspace was separated and analyzed for the compound of interest. A gas chromatograph fitted with an electron capture detector was used for the analysis.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Atlantic ocean samples, 48 °N to 65 °S latitudes, in late 1981.

Estimated Errors:

Solubility: ±5.5% std. dev.
Temperature: ±0.2 K.

References:

[1] C. D. McAuliffe, Chem. Techn. **1**, 46 (1971).

Components:	**Evaluator:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

47. 1,1,2-Trichloroethane with Water

Critical Evaluation

The 1,1,2-trichloroethane (1) and water (2) binary system is treated in two parts; part 1 is 1,1,2-trichloroethane (1) in water (2) and part 2 is water (2) in 1,1,2-trichloroethane (1).

Part 1. The solubility of 1,1,2-trichloroethane (1) in water (2) has been studied by 16 groups of workers in the temperature range from 273.15 to 328.15 K. The results of only two groups were not used in the data smoothing procedure. The solubility data of Wright and Schaffer[1] and Veight *et al.*[2] are significantly lower than other results and are therefore rejected. Even though there appears to be some inconsistency in the reported solubility data of Leighton and Calo[3] and Howe *et al.*,[4] that is, the former does not give a minimum and the latter shows a maximum in solubility, the combined results of 14 laboratories have been used for the smoothing equation. The data of van Arkel and Vles,[5] McGovern,[6] Treybal *et al.*,[7] Newman *et al.*,[8] Walraevens *et al.*,[9] Sato and Nakijima,[10] Coca and Diaz,[11] Coca *et al.*,[12] Newsham,[13] Leighton and Calo,[3] McNally and Grob,[14] Barr and Newsham,[15] Howe *et al.*,[4] and Wright *et al.*[16] were included to obtain the following mass percent (1) equation:

$$\text{Solubility } [100\ w_1] = 2.89796 - 1.8585\times10^{-2}\ (T/\text{K}) + 3.48961\times10^{-5}\ (T/\text{K})^2,$$

which shows a standard deviation of 3.41×10^{-2} in the temperature range from 273.15 to 328.15 K. The above equation represents the combined data with maximum deviation of 15%, usually less, and may be considered tentative for solubility if 1,1,2-trichloroethane in water.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 15. A solubility minimum does not appear in the temperature range involved. Additional details concerning the presence of a solubility minimum for aqueous hydrocarbon systems are provided in the Preface.

The tentative values for this system are given in Table 1 as smoothed values at 5 K intervals.

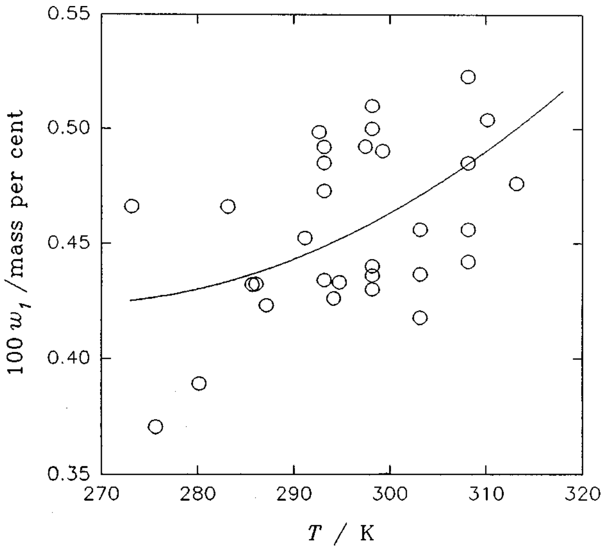

FIG. 15. Solubility of 1,1,2-trichloroethane (1) in water (2).

TABLE 1. Tentative solubility of 1,1,2-trichloroethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^4\ x_1$
0	273.15	0.425	5.76
5	278.15	0.428	5.80
10	283.15	0.433	5.87
15	288.15	0.440	5.96
20	293.15	0.449	6.09
25	298.15	0.459	6.22
30	303.15	0.471	6.39
35	308.15	0.485	6.58
40	313.15	0.500	6.78
45	318.15	0.517	7.01
50	328.15	0.536	7.27
55	328.15	0.557	7.56

Part 2. The solubility of water (2) in 1,1,2-trichloroethane (1) has been studied by six groups of workers in the temperature range from 264.15 to 323.15 K. The data of Coca and Diaz[11] and Coca *et al.*[12] are several percent lower than the smoothed solubility values and are therefore rejected. Both results seem to be reported from the same laboratory with some discrepancy between the two data values.

The remaining data of Staverman,[17] McGovern,[6] Treybal *et al.*,[7] and Barr and Nesham[15] were compiled or used for the smoothing equation. The fitting equation used was:

$$\log_{10} x_2 = 2.48799 - 1356.67/(T/\text{K}).$$

This equation yielded a standard deviation of 6.99×10^{-2} in the temperature range from 264 to 323 K. The recommended solubilities at 5 K intervals for water in 1,1,2-trichloroethane are presented in Table 2.

TABLE 2. Recommended solubility of water (2) in 1,1,2-trichloroethane (1)

Temperature		Solubility	
°C	K	100 w_2	$10^3\ x_2$
−5	268.15	0.0489	2.68
0	273.15	0.0606	3.32
5	278.15	0.0745	4.08
10	283.15	0.0908	4.97
15	288.15	0.1101	6.02
20	293.15	0.1328	7.25
25	298.15	0.1588	8.66
30	303.15	0.1891	10.30
35	308.15	0.2238	12.17
40	313.15	0.2636	14.31
45	318.15	0.3090	16.74
50	328.15	0.3606	19.49
55	328.15	0.4188	22.58

Measured values and the curve obtained from the smoothing equation for solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature are shown in Fig. 16.

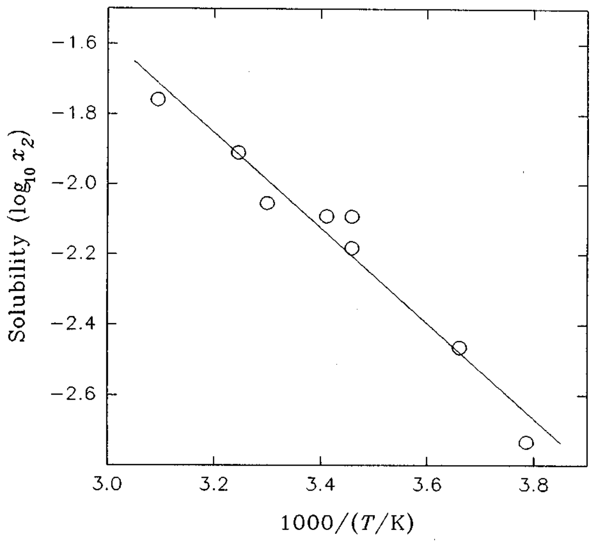

FIG. 16. Solubility of water (1) in 1,1,2-trichloroethane; log x_2 vs 1000/(T/K).

References:

[1] W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).
[2] G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. **707**, Philadelphia, 1980, pp. 116–29.
[3] D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).
[4] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).
[5] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
[6] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).
[7] R. E. Treybal, L. D. Weber, and J. F. Daley, Ind. Eng. Chem. **38**, 817 (1946).
[8] M. Newman, C. B. Hayworth, and R. E. Treybal, Ind. Eng. Chem. **41**, 2039 (1949).
[9] R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).
[10] A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
[11] J. Coca and R. Diaz, J. Chem. Eng. Data **25**, 80 (1980).
[12] J. Coca, R. M. Diaz, and C. Pazos, Fluid Phase Equilibr. **4**, 125 (1980).
[13] D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).
[14] M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
[15] R. S. Barr and D. M. T. Newsham, Fluid Phase Equilibr. **35**, 189 (1987).
[16] D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).
[17] A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

W. H. Wright and J. M. Schaffer, Amer. J. Hyg. **16**, 325 (1932).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$V_2 g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	2.70×10^2	0.370	5.01

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,1,2-trichloroethane with a large volume of water and measuring the volume of the undissolved 1,1,2-trichloroethane.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with a $NaHCO_3$ solution and then redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=273–328

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	0.466	0.464	6.29
20	0.436	0.434	5.88
35	0.458	0.456	6.18
55	0.532	0.529	7.18

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]

Original Measurements:

A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	6.18×10^{-2}	4.60×10^{2}	3.43×10^{-3}
25	1.185×10^{-1}	8.79×10^{2}	6.58×10^{-3}
30	1.59×10^{-1}	1.180×10^{3}	8.82×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Water was shaken with 1,1,2-trichloroethane for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. The result is an average of two measurements. A full description of the method used is given in a thesis.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±5 K (compiler).

References:

[1] A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K=264–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
−9	—	—	2.5×10^{-2}	1.85
25	4.4×10^{-1}	5.96	—	—

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial grade, source not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. E. Treybal, L. D. Weber, and J. F. Daley, Ind. Eng. Chem. **38**, 817 (1946).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25.0	0.44	5.96	0.11	8.09

Auxiliary Information

Method/Apparatus/Procedure:

1,1,2-trichloroethane, while held in a water-bath thermostat, was titrated with water until the appearance of a slight turbidity, which indicated the limiting solubility concentration. At the same time, the refractive index and density of the solutions were determined. Similar measurements were made by titration of water with 1,1,2-trichloroethane.

Source and Purity of Materials:

(1) Carbide and Carbon Chemicals Co., redistilled before use, b.p.=113.3 °C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K.

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. Newman, C. B. Hayworth, and R. E. Treybal, Ind. Eng. Chem. **41**, 2039 (1949).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.44	5.96	3.3×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium between 1,1,2-trichloroethane and water was established in a water-bath thermostat and maintained through vigorous agitation. The usual procedures were followed as described elsewhere[1] with specific gravity used as the means of analysis.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.3 K (compiler).

References:

[1] J. C. Smith, Ind. Eng. Chem. **34**, 234 (1942).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).

Variables:

T/K=283–353

Prepared By:

A. L. Horvath

Experimental Data

The temperature dependence of the solubility of 1,1,2-trichloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/\text{mol dm}^{-3}) = \frac{2070}{(T/\text{K})} - 15.285 + 0.0230(T/\text{K}),$$

where S=solubility, and T=absolute temperature. For example, the calculated solubility derived from the above equation is $4.36\times10^{-1}[100\ w_1]$ at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1,2-trichloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated and the equilibrium was maintained by vigorous stirring. The concentration of 1,1,2-trichloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Fluka, rectified before use, 99.9% pure by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:

T/K = 310

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Partition coefficient[a], K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	17.1	0.504	6.836

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A 1,1,2-trichloroethane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height on the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±1.3 std. dev.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Coca and R. M. Diaz, J. Chem. Eng. Data **25**, 80 (1980).

Variables:

T/K = 298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	0.51	6.92	8.0×10^{-2}	5.89

Auxiliary Information

Method/Apparatus/Procedure:

A titration was performed in an Erlenmeyer flask by adding 1,1,2-trichloroethane to water until a permanent turbidity was observed. The flask was immersed in a water-bath thermostat while maintaining a constant agitation using a magnetic stirrer.

Source and Purity of Materials:

(1) Laboratory grade Fluka reagent, further purified by distillation, only middle fraction was used.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. Coca, R. M. Diaz, and C. Pazos, Fluid Phase Equilib. **4**, 125 (1980).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
25	0.50	6.78	8.5×10^{-2}	6.26

Auxiliary Information

Method/Apparatus/Procedure:

The mutual solubility data were determined by a method described by Othmer, *et al.*[1] A 10 cm^3 1,1,2-trichloroethane sample was added to water from a buret and agitated until the solution became turbid. The appearance of the turbidity indicated the formation of a second phase. The solubility was calculated using the known densities and volumes.

Source and Purity of Materials:

(1) Fluka reagent, further purified by distillation in a heli-packing column.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] D. F. Othmer, R. E. White, and E. Trueges, Ind. Eng. Chem. **33**, 1240 (1941).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 707, Philadelphia, PA, 1980, pp. 116–29.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	1.12×10^{-2}	0.149	2.02

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,1,2-trichloroethane was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:	**Original Measurements:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).
Variables:	**Prepared By:**
T/K=286–323	A. L. Horvath

Experimental Data

t/°C	$10^4\ x_1$	$100\ w_1$ (compiler)	$100\ w_1M_1^{-1}$/mol g^{-1} (compiler)
12.5	5.86	0.432	3.24×10^{-3}
14.0	5.73	0.423	3.17×10^{-3}
21.0	5.77	0.426	3.19×10^{-3}
21.6	5.87	0.433	3.25×10^{-3}
25.0	5.83	0.430	3.22×10^{-3}
30.0	6.19	0.456	3.42×10^{-3}
35.0	6.00	0.442	3.31×10^{-3}
40.0	6.46	0.476	3.57×10^{-3}
50.0	7.58	0.558	4.18×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in water-bath thermostat. The concentration of 1,1,2-trichloroethane in water was determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator. A helium carrier gas and a Poropack QS column were used for the chromatographic analyses.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).
Variables:	**Prepared By:**
T/K=293; pH=2–9	A. L. Horvath

Experimental Data

t/°C	pH	$10^4\ x_1$	$100\ w_1$ (compiler)	$100\ w_1M_1^{-1}$/mol g^{-1} (compiler)
20	2.0	5.60 ± 0.06	0.413	3.10×10^{-3}
20	7.3	5.67 ± 0.06	0.416	3.12×10^{-3}
20	8.8	5.53 ± 0.10	0.408	3.06×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water-bath thermostat. The pH of the samples was adjusted by addition of either hydrochloric acid or sodium hydroxide. The concentration of 1,1,2-trichloroethane was determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled (compiler).

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).

Variables:	**Prepared By:**
T/K=321; P/mm Hg=6–48	A. L. Horvath

Experimental Data

t/°C	p_1 /mm Hg	$10^4\ x_1$	100 w_1 (compiler)
48.2	6.03	0.39	2.88×10^{-2}
48.2	12.2	0.86	6.36×10^{-2}
48.2	14.5	1.10	8.14×10^{-2}
48.2	18.0	1.24	9.18×10^{-2}
48.2	31.4	2.77	2.05×10^{-1}
48.2	47.6	4.49	3.31×10^{-1}

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water-bath thermostat. The concentration of 1,1,2-trichloroethane in water was determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator. A helium carrier gas and a Poropack QS column were used for the chromatographic analyses.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:	**Prepared By:**
T/K=276–299	A. L. Horvath

Experimental Data

t/°C	Distribution coefficient[a], D_L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
2.5	16.67	0.3705	5.0191
7.0	20.96	0.3891	5.2719
12.9	26.91	0.4323	5.8595
18.0	34.14	0.4523	6.1327
19.5	33.64	0.4985	6.7619
24.3	44.61	0.4922	6.6761
26.1	48.47	0.4902	6.6486

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,1,2-trichloroethane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,1,2-trichloroethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±10%.
Temperature: ±0.5 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]

Original Measurements:

K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.30	9.0×10^{-2}	6.63

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 1,1,2-trichloroethane in a flask and it was lowered into a thermostatic bath. The flask was then shaken vigorously until the first cloud (turbidity) appeared. The water content in the sample was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial JIS extra pure reagent, further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	4.3653	0.4365	5.917

Auxiliary Information

Method/Apparatus/Procedure:

Standard 1,1,2-trichloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±7.8% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:	**Original Measurements:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	R. S. Barr and D. M. T. Newsham, Fluid Phase Equilib. **35**, 189 (1987).
Variables:	**Prepared By:**
T/K=293–323	A. L. Horvath

Experimental Data

t/°C	10^4 x_1	100 w_1 (compiler)	10^3 x_2	100 w_2 (compiler)
20	6.67	0.492	8.11	0.110
35	6.58	0.485	12.3	0.168
50	6.99	0.515	17.5	0.240

Mole fraction of 1,1,2-trichloroethane (x_1) was calculated from the activity coefficient at infinite dilution (γ_1^∞) using the relation $x_1 = 1/\gamma_1^\infty$.

Auxiliary Information

Method/Apparatus/Procedure:

The water-rich mixture was studied using gas–liquid chromatography in which a mixture of methane and 1,1,2-trichloroethane vapor passed through the sampling loop. The eluted 1,1,2-trichloroethane was determined with a flame ionization detector. The organic-rich mixture was studied using an isopiestic method in which $CaCl_2$ solution controlled the partial pressure of water. The water concentration of the organic phase was determined by using a Karl Fischer titration apparatus.

Source and Purity of Materials:

(1) Aldrich Chemical Co. Ltd., redistilled in a glass sieve tray column before use.
(2) Double distilled tap water.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:	**Original Measurements:**
(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	10^6 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
10	4.659×10^3	0.4659	6.3168
20	4.727×10^3	0.4727	6.4094
30	4.177×10^3	0.4177	5.6610

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled, de-ionized water and sealed. Measured volumes of 1,1,2-trichloroethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about three weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC responses were compared with calibration plots to establish concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^4\ x_1$	100 w_1 (compiler)
20	1520±10	6.58	0.485
35	1410±125	7.09	0.523
50	1220±20	8.20	0.604

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,1,2-trichloroethane (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. The 1,1,2-trichloroethane was injected into the mixture cells and a magnetic stirrer was turned on. Then, the cells were allowed to equilibrate. The stirrer was then turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered and deionized

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:

(1) 1-bromo-2-chloroethane; C_2H_4BrCl; [107-04-0]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., May 1993.

48. 1-Bromo-2-Chloroethane with Water

Critical Evaluation

All the available data for the solubility of 1-bromo-2-chloroethane (1) in water are summarized in Table 1.

With only a narrow temperature difference between the solubility data of Gross *et al.*[1] and Chitwood,[2] the agreement is very good. In the absence of other independent studies, it is not possible to judge the temperature dependence of the solubility between 298.15 and 303.15 K. Further studies are required to establish the solubility versus temperature behavior.

TABLE 1. Tentative solubility of 1-bromo-2-chloroethane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	$10^4\ x_1$	References
25	298.15	0.69	8.72	2
30	303.15	0.683	8.63	1

References:

[1] P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).
[2] B. G. Chitwood, Adv. in Chem. Ser., Am. Chem. Soc., Washington, 1952, No. 7, pp. 91–9.

Components:

(1) 1-bromo-2-chloroethane; C_2H_4BrCl; [107-04-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, J. H. Saylor, and M. A. Gorman, J. Am. Chem. Soc. **55**, 650 (1933).

Variables:

$T/K=303$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	6.88	8.63	0.683

Auxiliary Information

Method/Apparatus/Procedure:

The saturated solution was prepared in a flask and placed in a water bath thermostat. The samples were analyzed using a Zeiss combination liquid and gas interferometer described elsewhere.[1] A detailed description of the complete procedure is given in a M. A. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Co., distilled fractionally before use, b.p. $=106.62-106.71$ °C.
(2) Distilled.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

[2] M. A. Gorman, M. A. thesis, Duke University, Durham, 1932.

Components:

(1) 1-bromo-2-chloroethane; C_2H_4BrCl; [107-04-0]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, Adv. Chem. Ser. **7**, 91 (1952).

Variables:

$T/K=298$

Prepared By:

A. L. Horvath

Experimental Data

$t/°C$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_1M_1^{-1}/\text{mol g}^{-1}$ (compiler)
25	0.69	8.72	4.81×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Evaluator:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., June 1993.

49. 1,2-Dibromoethane with Water

Critical Evaluation

The 1,2-dibromoethane (1) and water (2) binary system is treated in two parts; part 1 is 1,2-dibromoethane (1) in water (2) and part 2 is water (2) in 1,2-dibromoethane (1).

Part 1. The solubility of 1,2-dibromoethane (1) in water (2) has been studied by 14 groups of workers in the temperature range from 273.15 to 348.15 K. The datum of Booth and Everson[1] is noticeably higher than the likely solubility and is rejected. Similar conclusions were found for the poor reliability of other solubility data (see e.g., CCl_4 , $CHBr_3$, $CHCl_3$, CH_2Cl_2 , and CH_2Br_2), which justifies the rejection of these data. The measurements of Wade[2] and Dreisbach[3] are significantly lower than the solubility values calculated from the smoothing equation and are also rejected. The temperature dependence of the solubility data of Howe *et al.*[4] contradicts that of all other measured data and therefore the datum at 303.15 K is rejected.

The remaining data from the other ten laboratories were compiled or used for the smoothing equation. The combined data values of Gross and Saylor,[5] van Arkel and Vles,[6] Shostakovsky and Druzhinin,[7] Druzhinin and Shostakovsky,[8] Chitwood,[9] Call,[10] O'Connell,[11] Chiou and Freed,[12] Mackay *et al.*,[13] and Tokoro *et al.*[14] were used to obtain the following mass percent (1) equation:

$$\text{Solubility }[100\ w_1] = 3.8651 - 2.7921\times10^{-2}(T/\text{K}) + 5.45647\times10^{-5}(T/\text{K})^2,$$

which shows a standard deviation of 3.72×10^{-2} in the temperature range from 273 to 348 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 17. The curve obtained from the smoothing equation shows no minimum over the temperature interval under examination. Additional details concerning the appearance of a solubility minimum in most aqueous halogenated hydrocarbon systems within the temperature interval of 270–320 K are provided in the Preface.

The tentative values of solubility at 5 K intervals for 1,2-dibromoethane (1) in water (2) are presented in Table 1.

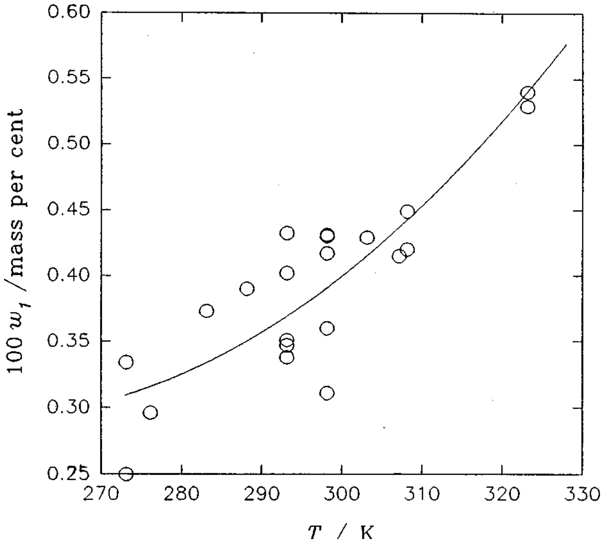

FIG. 17. Solubility of 1,2-dibromoethane (1) in water (2).

TABLE 1. Tentative solubility of 1,2-dibromoethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
0	273.15	0.309	2.971
5	278.15	0.320	3.077
10	283.15	0.334	3.212
15	288.15	0.350	3.367
20	293.15	0.369	3.550
25	298.15	0.391	3.763
30	303.15	0.415	3.994
35	308.15	0.442	4.255
40	313.15	0.472	4.546
45	318.15	0.505	4.865
50	323.15	0.540	5.203
55	328.15	0.578	5.572
60	333.15	0.619	5.969
65	338.15	0.663	6.396
70	343.15	0.709	6.843
75	348.15	0.758	7.319

Part 2. The solubility of water (2) in 1,2-dibromoethane (1) has been reported by six groups of workers in the temperature range from 288 to 348 K with partially consistent results. The solubility data of Shostakovsky and Druzlinin[7] are significantly higher than all other measurements and are therefore rejected. These data are an order of magnitude too high. The datum of Mackay *et al.*[13] is several percent lower than other results and is also rejected.

The remaining data of Bell,[15] Staverman,[16] Hutchison and Lyon,[17] and O'Connell[11] were used for data smoothing. The fitting equation used was:

$$\log_{10} x_2 = 0.75213 - 868.78/(T/\text{K}),$$

which gave a standard deviation of 5.19×10^{-2} in the narrow temperature range from 288 to 303 K. The tentative solubility values at 5 K intervals for water (2) in 1,2-dibromoethane (1) are presented in Table 2.

TABLE 2. Tentative solubility of water (2) in 1,2-dibromoethane (1)

Temperature		Solubility	
°C	K	100 w_2	10^3 x_2
15	288.15	0.0526	5.459
20	293.15	0.0593	6.145
25	298.15	0.0665	6.890
30	303.15	0.0743	7.697

Measured values and the linear relationship between the solubility expressed as $\log_{10} x_2$ versus $1/(T/\text{K})$ are plotted in Fig. 18. This linear relationship is a characteristic of water solubility in halogenated hydrocarbons. The phenomenon is discussed in some detail in the Preface.

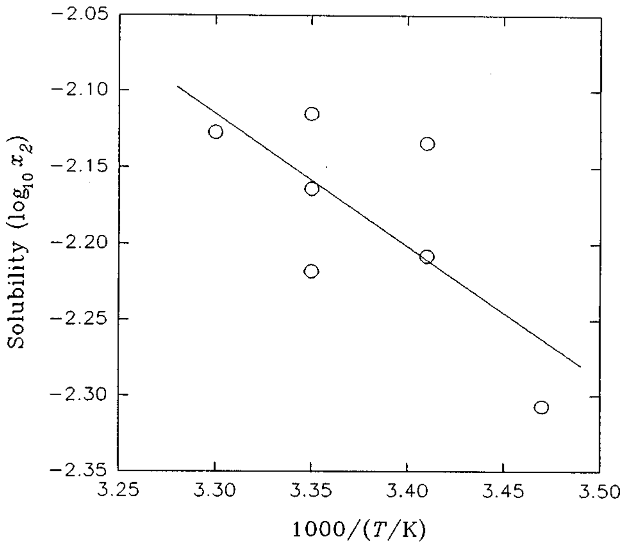

FIG. 18. Solubility of water (2) in 1,2-dibromoethane (1); log x_2 vs 1000/(T/K).

References:

[1] H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

[2] P. Wade, J. Sci. Food Agric. **5**, 184 (1954).

[3] R. R. Dreisbach, ''Physical Properties of Chemical Compounds,'' Adv. in Chem. Ser. No. 22, Am. Chem. Soc., Washington, D.C., 1959, p. 208.

[4] G. B. Howe, M. E. Mullins, and T. N. Rogers, AFESC Tyndall Air Force Base, Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

[5] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

[6] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

[7] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

[8] I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

[9] B. G. Chitwood, Adv. in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

[10] F. Call, J. Sci. Food Agric. **8**, 630 (1957).

[11] W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

[12] C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U.S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).

[13] D. Mackay *et al.* ''Volatilization of Organic Pollutants from Water,'' U.S. EPA Report 600/3-82-019, Athens, Georgia (1982) (PB-82-230939).

[14] R. Tokoro, R. Bilewicz, and J. Osteryoung, Anal. Chem. **58**, 1964 (1986).

[15] R. P. Bell, J. Chem. Soc. 2905 (1932).

[16] A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

[17] C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
Variables:	**Prepared By:**
T/K=288–303	A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
15	3.92	0.390	3.75
30	4.31	0.429	4.13

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,2-dibromoethane in 500 g water was shaken for 12 h in a water bath thermostat. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss.[1] A detailed description of the complete procedure is given in a Ph.D. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Co., purified by fractional freezing five times before use.

(2) Distilled.

Estimated Errors:

Solubility: ±1%.

Temperature: ±0.02 K.

References:

[1] P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).

[2] J. H. Saylor, Ph.D. thesis, Duke University, Durham, 1930.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]	R. P. Bell, J. Chem. Soc. 2905 (1932).
Variables:	**Prepared By:**
T/K=288–298	A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
15	1.04	4.75×10^{-2}	4.93
20	1.30	5.97×10^{-2}	6.19
25	1.61	7.42×10^{-2}	7.68

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of water and 1,2-dibromoethane of about 1 to 5 volume ratio was placed in a sample vessel and rotated in a thermostat for 12 h. After the equilibrium was attained, samples were taken and filtered through cotton-wool. The determination of the water content was based upon the reaction with α-napht-hoxydichlorophosphine. The evolved HCl gas was absorbed in water and titrated with NaOH solution.[1] Two to three successive determinations were carried out with the samples.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Merck reagent, analytical grade, redistilled before use.

Estimated Errors:

Solubility: ±1.5% mean dev.
Temperature: ±0.02 K.

References:

[1] R. P. Bell, J. Chem. Soc. 2903 (1932).

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
Variables:	**Prepared By:**
T/K=273–323	A. L. Horvath

Experimental Data

t/°C	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
0	0.335	0.334	3.21
20	0.404	0.402	3.87
35	0.451	0.449	4.32
50	0.532	0.529	5.10

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]

Original Measurements:

A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:

T/K=298–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	6.565×10^{-2}	6.85×10^2	0.00364
30	7.145×10^{-2}	7.46×10^2	0.00397

Auxiliary Information

Method/Apparatus/Procedure:

Water was shaken with 1,2-dibromoethane for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. The result is an average of two measurements. A full description of the method used is given in a thesis.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Variables:

T/K=273–348

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
0	0.25	2.40	—	—
25	0.36	3.46	0.54	5.36
35	0.42	4.04	0.63	6.20
50	0.54	5.20	1.18	11.07
75	0.77	7.43	1.83	16.27

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 water in a flask fitted with a thermostat jacket and a powerful stirrer. After the samples were stirred for 2–3 days, portions were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic-rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. J. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).
Variables:	**Prepared By:**
T/K=308	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
35.0	0.42	4.04	2.23×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 water in a flask fitted with a thermostat jacket and a powerful stirrer. After the samples were stirred for 2–3 days, portions were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic-rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. J. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dibromoethane; $C_2H_4Br_2$; [106-934]	C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	3.24×10^{-3}	5.84×10^{-2}	6.06

Auxiliary Information

Method/Apparatus/Procedure:

A 1 to 15 volume ratio mixture of water and 1,2-dibromoethane was introduced into an equilibration flask and then lowered into the water bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. The description of procedure was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given. Purified and dried before use.

Estimated Errors:

Solubility: $\pm1.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

Production of Heavy Water, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, N. Y., 1955), p. 129.

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-934]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

H. S. Booth and H. E. Everson, Ind. Eng. Chem. **40**, 1491 (1948).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 V_1 /V_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25.0	0.40	0.86	8.3

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium was established through repeated shaking and centrifuging of a 1,2-dibromoethane and water mixture in a stoppered Goetz tube and returned the tube to a constant temperature water bath. The difference between the total amount of 1,2-dibromoethane which was added and the amount which remained in excess was the amount of solute dissolved in the known volume of water. The determination of the excess amount of solute added is described in the Ph. D. thesis of Hanslick.[1]

Source and Purity of Materials:

(1) Commercial reagent, G. P. grade, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] R. S. Hanslick, Ph. D. thesis, Columbia University, New York, N.Y., 1935.

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

B. G. Chitwood, ''Advances in Chem. Ser.,'' Am. Chem. Soc. **7**, 91 (1952).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.43	4.14	2.29×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	P. Wade, J. Sci. Food Agric. **5**, 184 (1954).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	0.431	4.31×10^{-2}	4.13

Auxiliary Information

Method/Apparatus/Procedure:

The equilibration between 1,2-dibromoethane and water was established in a constant temperature room maintained at 20 °C for 24 h. At the end of the time period, two samples were withdrawn from each unit and 1,2-dibromoethane was determined by the catalytic thermal decomposition procedure. The decomposition products were absorbed in a solution of NaOH containing H_2O_2 . The generated bromide was titrated with $AgNO_3$ solution.[1]

Source and Purity of Materials:

(1) Laboratory sample, washed with $NaHCO_3$ solution, dried over Na_2SO_4 and redistilled twice.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

References:

[1] P. Wade, Ph. D. Thesis, University of London, London, U. K., 1953.

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	F. Call, J. Sci. Food Agric. **8**, 630 (1957).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	3.37×10^{-2}	0.338	3.25

Auxiliary Information

Method/Apparatus/Procedure:

100 cm^3 distilled water and a known amount of 1,2-dibromoethane were placed in a sorption flask. The equilibrium was attained by placing the flask on a mechanical shaker for one hour. The experiment was performed in a constant temperature room. The results were obtained from two separate experiments.[1]

Source and Purity of Materials:

(1) Source and purity not specified.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] F. Call, Ph. D. thesis, University of London, London, U. K., 1956.

Components:
(1) Water; H_2O; [7732-18-5]
(2) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]

Original Measurements:
R. R. Dreisbach, ''Physical Properties of Chemical Compounds,'' Adv. in Chem. Ser. No. 22, Am. Chem. Soc., Washington, D. C. (1959), p. 208.

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	7.1×10^{-2}	7.35	3.94×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Distilled.

(2) Dow Chemical Co., 99.91% pure, purified by distillation before use.

Estimated Errors:
Solubility: not specified.
Temperature: ±1 K (compiler).

Components:
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:
T/K=293–298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	$10^4\ x_1$ (compiler)	100 g_2/g_1	$10^3\ x_2$ (compiler)
20	—	—	7.1×10^{-2}	7.35
25	4.17×10^{-1}	4.00	—	—

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Dow Chemical Co., used as received.

(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U. S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).

Variables:

T/K=276–307

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
3	2.97	0.296	2.85
20	3.52	0.351	3.38
34	4.14	0.415	3.99

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5–10 g 1,2-dibromoethane was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on determination and evaluation of the procedure have been reported by Chiou and Schmedding.[1]

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou and D. W. Schmedding, ''Test. Protec. Environ. Fate Mov. Toxicants,'' Proc. Symp., 1980, pp. 28–42 (Publ. 1981).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Mackay *et al.*, ''Volatilization of Organic Pollutants from Water,'' U. S. EPA Report 600/3-82-019, Athens, Georgia (1982) (PB 82-230939).

Variables:

T/K=293–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	c_1 /mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)	100 w_2 (compiler)	10^3 x_2
20	23.0	0.432	4.16	—	—
25	22.94	0.431	4.15	3.85×10^{-2}	4.00

Auxiliary Information

Method/Apparatus/Procedure:

An aqueous solution with an excess amount of 1,2-dibromoethane was stirred for 1 day before being introduced into a 1 L glass vessel. Nitrogen entered at the bottom of the vessel through a sintered glass disk. The exit gas flow rate was measured by a soap bubble flow meter. The concentration of 1,2-dibromoethane in water was determined by gas chromatography. The GC was equipped with both a dual flame ionization detector and an electron

Source and Purity of Materials:

(1) Source and purity not given.
(2) Doubly distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1.0 K.

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	R. Tokoro, R. Bilewicz, and J. Osteryoung, Anal. Chem. **58**, 1964 (1986).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	3.12	0.311	2.99

Auxiliary Information

Method/Apparatus/Procedure:

A saturated aqueous solution of 1,2-dibromoethane was filtered and samples of 50, 100, and 200 μL were diluted in a 0.1 M tetraethylammonium perchlorate aqueous solution. A cathodic voltammogram on the HMDE was recorded. Quantization was done by standard addition using 0.01 M solute in ethanol as the standard.

Source and Purity of Materials:

(1) Fisher Scientific Co., E173 certified, 99.5% pure. Used as received.
(2) Distilled and further purified using a Millipore Milliq system.

Estimated Errors:

Solubility: $\pm 4.0\times10^{-5}\ g_1/g_2$.
Temperature: ±0.2 K.

Components:	**Original Measurements:**
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, ''AFESC Tyndall Air Force Base,'' Report ESL-TR-86-66, Vol. 1, Florida (September, 1987), 86 pp. (AD-A188 571).
Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
10	3.731×10^3	0.3731	3.590
20	3.471×10^3	0.3471	3.339
30	2.397×10^3	0.2400	2.304

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled, de-ionized water and sealed. Measured volumes of 1,2-dibromoethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC responses were compared with calibration plots to obtain concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent, at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Magnesium chloride; $MgCl_2$; [7786-30-3]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:

T/K=308 and Concentration

Prepared By:

A. L. Horvath

50. 1,2-Dibromoethane with Magnesium Chloride and Water

Experimental Data

t/°C	100 w_2	100 w_1	10^4 x_1 (compiler)
35.0	12.28	1.9×10^{-1}	2.36
	21.57	4.3×10^{-2}	0.567

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Magnesium chloride; $MgCl_2$; [7786-30-3]
(3) Magnesium sulfate; $MgSO_4$; [7487-88-9]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:

T/K=308 and Concentration

Prepared By:

A. L. Horvath

51. 1,2-Dibromoethane with Magnesium Chloride, Magnesium Sulfate, and Water

Experimental Data

t/°C	100 w_2	100 w_3	100 w_1
35.0	8.46	6.58	8.46×10^{-2}
	12.80	4.63	6.51×10^{-2}
	19.31	2.17	6.14×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Source and purity not given.
(4) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. G. Druzlinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Magnesium sulfate; $MgSO_4$; [7487-88-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:
T/K=308 and Concentration

Prepared By:
A. L. Horvath

52. 1,2-Dibromoethane with Magnesium Sulfate and Water

Experimental Data

t/°C	100 w_2	100 w_1	$10^4\ x_1$ (compiler)
35.0	2.13	2.6×10^{-1}	2.89
	9.96	1.9×10^{-1}	2.27
	15.74	9.0×10^{-2}	1.14

Auxiliary Information

Method/Apparatus/Procedure:
A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:
(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:
[1] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:
(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:
I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:
T/K=308 and Concentration

Prepared By:
A. L. Horvath

53. 1,2-Dibromoethane with Sodium Chloride and Water

Experimental Data

t/°C	100 w_2	100 w_1	$10^4\ x_1$ (compiler)
35.0	3.68	3.9×10^{-1}	4.36
	11.24	2.7×10^{-1}	3.19
	26.42	9.0×10^{-2}	1.20

Auxiliary Information

Method/Apparatus/Procedure:
A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:
(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:
[1] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1972).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Magnesium chloride; $MgCl_2$; [7786-30-3]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:

T/K=308 and Concentration

Prepared By:

A. L. Horvath

54. 1,2-Dibromoethane with Sodium Chloride, Magnesium Chloride, and Water

Experimental Data

t/°C	100 w_2	100 w_3	100 w_1
35.0	10.20	13.07	1.6×10^{-2}
	17.93	6.36	1.2×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Source and purity not given.
(4) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Sodium sulfate; Na_2SO_4 ; [7757-82-6]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:

T/K=308 and Concentration

Prepared By:

A. L. Horvath

55. 1,2-Dibromoethane with Sodium Chloride, Sodium Sulfate, and Water

Experimental Data

t/°C	100 w_2	100 w_3	100 w_1
35.0	19.61	12.24	1.5×10^{-2}
	16.40	16.82	1.0×10^{-2}
	10.08	24.18	1.1×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Source and purity not given.
(4) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. G. Druzhinin, Zr. Obshch. Khim. **12**, 42 (1942).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Sodium sulfate; Na_2SO_4; [7757-82-6]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:

T/K=308 and Concentration

Prepared By:

A. L. Horvath

56. 1,2-Dibromoethane with Sodium Sulfate and Water

Experimental Data

$t/°C$	$100\ w_2$	$100\ w_1$	$10^4\ x_1$ (compiler)
35.0	5.47	7.8×10^{-1}	8.96
	17.09	1.1×10^{-1}	1.42
	24.13	6.0×10^{-2}	0.868
	32.96	1.2×10^{-2}	0.185

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:

(1) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]
(2) Sodium sulfate; Na_2SO_4; [7757-82-6]
(3) Magnesium sulfate; $MgSO_4$; [7487-88-9]
(4) Water; H_2O; [7732-18-5]

Original Measurements:

I. G. Druzhinin and M. F. Shostakovskii, J. Gen. Chem. USSR **12**, 48 (1942).

Variables:

T/K=308 and Concentration

Prepared By:

A. L. Horvath

57. 1,2-Dibromoethane with Sodium Sulfate, Magnesium Sulfate, and Water

Experimental data

$t/°C$	$100\ w_2$	$100\ w_3$	$100\ w_1$
35.0	10.42	12.76	6.0×10^{-2}
	18.07	9.81	8.2×10^{-2}
	23.79	4.35	1.0×10^{-1}
	28.10	1.54	5.2×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A 20 cm^3 1,2-dibromoethane sample was mixed with 40 cm^3 aqueous electrolyte solution in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 2–3 days, samples were taken from both phases for analysis. The bromine concentration was determined by adding HNO_3 to the solution and the free bromine was titrated with $AgNO_3$ solution. The water content of the organic rich phase was calculated by the method of Kariusu.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Source and purity not given.
(4) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] M. F. Shostakovskii and I. G. Druzhinin, Zh. Obshch. Khim. **12**, 42 (1942).

Components:

(1) Water-d_2 ; D_2O; [7789-20-0]
(2) 1,2-dibromoethane; $C_2H_4Br_2$; [106-93-4]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

58. 1,2-Dibromoethane with Water-d_2

Experimental Data

t/°C	$100\ w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	2.79×10^{-3}	5.59×10^{-2}	5.22

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 to 15 volume ratio of heavy water and 1,2-dibromoethane was introduced into an equilibration flask and then lowered into a water bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure description was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Probably a commercial reagent, further purified and dried before use.

Estimated Errors:

Solubility: $\pm1.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by, M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) 1-chloro-2-fluoroethane; C_2H_4ClF; [762-50-5]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. V. Razumovskii and A. E. Fridenberg, J. Gen. Chem. USSR **19**, 83 (1949).

Variables:

T/K=298

Prepared By:

A. L. Horvath

59. 1-Chloro-2-Fluoroethane with Water

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	25	2.44	5.43

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Prepared by the authors.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:	**Evaluator:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., June 1993.

60. 1,1-Dichloroethane with Water

Critical Evaluation

The 1,1-dichloroethane (1) and water (2) binary system is treated in two parts; part 1 is 1,1-dichloroethane (1) in water (2) and part 2 is water (2) in 1,1-dichloroethane (1).

Part 1. The solubility of 1,1-dichloroethane (1) in water (2) has been studied by 15 groups of investigators in the temperature interval from 273 to 323 K with reasonably good agreement. However, some reported measurements have been rejected. The datum of Ley *et al.*[1] is significantly lower than all other measurements and is therefore rejected. The solubility values of Howe *et al.*[2] are several per cent higher than those calculated from the smoothing equation and are also rejected.

The remaining data of Rex,[3] Gross,[4] Wright and Schaffer,[5] van Arkel and Vles,[6] Walraevens *et al.*,[7] Sato and Nakijima,[8] Newsham,[9] McNally and Grob,[10,11] Barr and Newsham,[12] Gossett,[13] Warner *et al.*,[14] and Wright *et al.*[15] were used to obtain the following mass percent (1) equation:

$$\text{Solubility } [100\ w_1] = 9.4136 - 5.7249\times10^{-2}\ (T/\text{K}) + 9.17839\times10^{-5}\ (T/\text{K})^2,$$

which shows a standard deviation of 3.70×10^{-2} in the temperature range from 273 to 323 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 19. A solubility minimum calculated from the above regression equation is 0.487 [100 w_1] at 311.87 K. Additional details concerning the solubility minimum for aqueous hydrocarbon systems are discussed in the Preface.

The recommended solubility values at 5 K intervals for 1,1-dichloroethane (1) in water (2) are presented in Table 1.

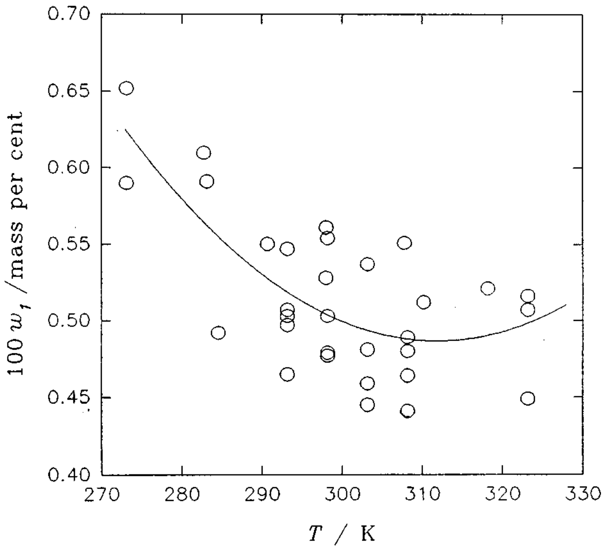

FIG. 19. Solubility of 1,1-dichloroethane (1) in water (2).

TABLE 1. Recommended solubility of 1,1,1-dichloroethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^3\ x_1$
0	273.15	0.624	1.142
5	278.15	0.591	1.081
10	283.15	0.562	1.028
15	288.15	0.538	0.984
20	293.15	0.519	0.949
25	298.15	0.504	0.921
30	303.15	0.493	0.901
35	308.15	0.488	0.892
40	313.15	0.487	0.890
45	318.15	0.490	0.896
50	323.15	0.498	0.910

Part 2. The solubility of water (2) in 1,1,-dichloroethane (1) has been reported in 3 works only. The agreement is quite good in general, however, some discrepancy is apparent at 20 °C between the investigators at the same laboratory.[9,12] The combined data of Staverman,[16] Newsham,[9] and Barr and Newsham[12] were used for the smoothing equation:

$$\log_{10} x_2 = 1.2719 - 1049.07/(T/\text{K}).$$

This equation represents the combined data with a standard deviation of 4.13×10^{-2} in the temperature range from 273 to 323 K. The recommended solubility values at 5 K intervals for water (2) in 1,1-dichloroethane (1) are presented in Table 2.

TABLE 2. Recommended solubility of water (2) in 1,1-dichloroethane (1)

Temperature		Solubility	
°C	K	100 w_2	$10^3\ x_2$
0	273.15	0.0493	2.70
5	278.15	0.0577	3.16
10	283.15	0.0674	3.69
15	288.15	0.0782	4.28
20	293.15	0.0903	4.94
25	298.15	0.1030	5.67
30	303.15	0.1184	6.47
35	308.15	0.1350	7.37
40	313.15	0.1532	8.36
45	318.15	0.1730	9.43
50	323.15	0.1947	10.60

Measured values and the curve obtained from the smoothing equation for solubility expressed as $\log_{10} x_2$ versus the reciprocal of absolute temperature are shown in Fig. 20. The figure illustrates the linear relation between the solubility expressed as $\log_{10} x_2$ versus $1/T(\text{K})$. Such straight line plots are characteristic for water solubility in halogenated hydrocarbons. The reader should consult the Preface for further details.

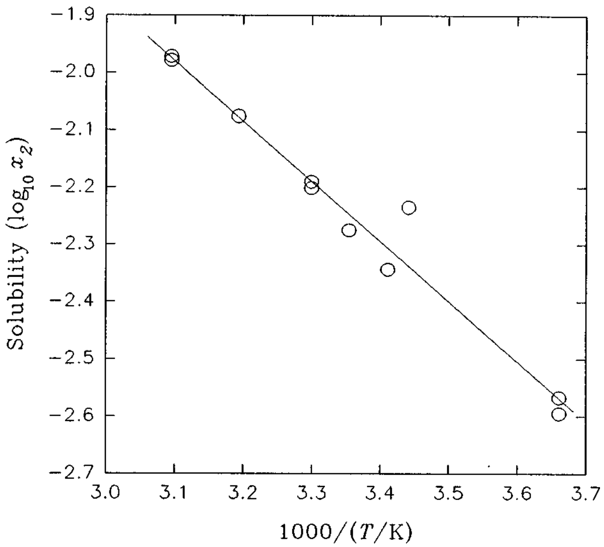

FIG. 20. Solubility of water (2) in 1,1-dichloroethane (1); log x_2 vs 1000/(T/K).

References:

[1]G. J. M. Ley, D. O. Hummel, and C. Schneider, Adv. in Chem. Ser. No. **66**, Am. Chem. Soc., Washington, D. C. (1967), pp. 184–202.

[2]G. B. Howe, M. E. Mullins, and T. N. Rogers, ''AFESC Tyndall Air Force Base,'' Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

[3]A. Rex, Z. Phys. Chem. **55**, 355 (1906).

[5]P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).

[5]W. H. Wright and J. M. Schaffer, Am. J. Hygiene **16**, 325 (1932).

[6]A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

[7]R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).

[8]A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

[9]D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, January 1981).

[10]M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

[11]M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

[12]R. S. Barr and D. M. T. Newsham, Fluid Phase Equilibr. **35**, 189 (1987).

[13]J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

[14]H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' EPA Technical Report, PB87-212 684, Cincinnati, OH (July 1987).

[15]D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

[16]A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Rex, Z. Phys. Chem. **55**, 355 (1906).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	0.656	0.652	1.19
10	0.595	0.591	1.08
20	0.550	0.547	1.00
30	0.540	0.537	0.982

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,1-dichloroethane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostatic bath, their volumes and weights were determined and the solubility was calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use, b.p.=57 °C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
25	0.506	0.503	9.19

Auxiliary Information

Method/Apparatus/Procedure:

A weighted amount of 1,1-dichloroethane was mixed with 1000 g water in a bottle and immersed in a water-bath thermostat. The bottle was placed on a shaker and shaken until no more droplets of the liquid remained undissolved. The concentration of 1,1-dichloroethane in water was determined using a Zeiss water interferometer. One or more samples were syphoned out for the determination of the solubility. The German translation of the article is also published.[1]

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Distilled.

Estimated Errors:

Solubility: ±2.0%.
Temperature: ±0.01 K.

References:

[1] P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	W. H. Wright and J. M. Schaffer, Am. J. Hyg. **16**, 325 (1932).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	$V_2g_1^{-1}$/cm^3 g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.80×10^2	0.554	1.01

Auxiliary Information

Method/Apparatus/Procedure:

The solubility was determined by mixing definite quantities of 1,1-dichloroethane with a large volume of water and measuring the volume of the undissolved portion.

Source and Purity of Materials:

(1) Commercial grade, further purified by washing with a $NaHCO_3$ solution and redistilled.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=273–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	0.594	0.590	10.79
20	0.506	0.503	9.20
35	0.482	0.480	8.77
50	0.519	0.516	9.43

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]

Original Measurements:

A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	4.60×10^{-2}	2.54	2.55×10^{-3}
25	9.66×10^{-2}	5.31	5.36×10^{-3}
30	1.145×10^{-1}	6.30	6.36×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Water was shaken with 1,1-dichloroethane for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. The result is an average of two measurements. A full description of the method used is given in a thesis.[1]

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. J. M. Ley, D. O. Hummel, and C. Schneider, Advances in Chem. Ser., Am. Chem. Soc. **66**, 184 (1967).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	1.0×10^{-2}	1.86	1.03×10^{-4}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source not given. High grade, purified by distillation and checked GC analysis.

(2) Triple distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).

Variables:

T/K=283–353

Prepared By:

A. L. Horvath

Experimental Data

The temperature dependence of the solubility of 1,1-dichloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/\mathrm{mol\ dm^{-3}}) = \frac{2070}{(T/\mathrm{K})} - 15.116 + 0.0230(T/\mathrm{K}),$$

where S=solubility, and T=absolute temperature.

For example, the calculated solubility derived from the above equation is 4.77×10^{-1} [100 w_1] at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,1-dichloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated. An equilibrium was maintained by vigorous stirring. The concentration of 1,1-dichloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Solvay, rectified before use. Purity was 99.9% by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).
Variables:	**Prepared By:**
T/K=310	A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
37	2.7	0.512	9.36

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:

A 1,1-dichloroethane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height on the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±0.6 std. dev.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).
Variables:	**Prepared By:**
T/K=273–323	A. L. Horvath

Experimental Data

t/°C	10^4 x_1	100 w_1 (compiler)	10^3 x_2	100 w_2 (compiler)
0.0	—	—	2.71	4.94×10^{-2}
11.4	8.99	0.492	—	—
20.0	8.50	0.465	4.53	8.28×10^{-2}
25.0	8.75	0.479	—	—
30.0	8.13	0.445	6.45	1.18×10^{-1}
35.0	8.49	0.464	—	—
40.0	—	—	8.39	1.54×10^{-1}
50.0	8.21	0.449	10.67	1.96×10^{-1}

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water bath thermostat. Water analysis was performed with an automatic Karl Fischer titration apparatus. The concentration of 1,1-dichloroethane in water was determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator. A helium carrier gas and a Poropack QS column were used for the chromatographic analyses.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).

Variables:

T/K = 293–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	pH	$10^4\ x_1$	$100\ w_1$ (compiler)
20	2.9	8.30±0.14	0.454
	5.6	8.63±0.23	0.472
	10.6	8.66±0.16	0.474
50	2.2	8.00±0.27	0.438
	7.7	8.20±0.23	0.449
	10.0	8.30±0.20	0.454

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 14 days in a water-bath thermostat. The pH was adjusted by addition of either hydrochloric acid or sodium hydroxide. The concentration of 1,1-dichloroethane was determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled (compiler).

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).

Variables:

T/K = 298–321

Prepared By:

A. L. Horvath

Experimental Data

t/°C	p_1 /mm Hg	$10^4\ x_1$	$100\ w_1$ (compiler)
24.5	7.10×10^1	2.06	0.113
	1.050×10^2	3.36	0.184
	1.499×10^2	5.08	0.278
	1.922×10^2	6.74	0.369
47.5	1.817×10^2	2.19	0.120
	2.270×10^2	2.66	0.146
	2.821×10^2	3.68	0.202
	4.123×10^2	5.64	0.309

p_1 = partial pressure of (1).

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water bath thermostat. The concentration of 1,1-dichloroethane was determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator. A helium carrier gas and a Poropack QS column were used for the chromatographic analyses.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	4.8344×10^3	0.4811	8.793

Auxiliary Information

Method/Apparatus/Procedure:

Standard solutions were prepared in 100 cm^3 flask. They were shaken for 5 min and then allowed to equilibrate in a constant temperature bath held at 30 °C for 24 h. Samples were pipetted in headspace vials, sealed, thermostated and then examined by the gas chromatographic head space analysis technique. An F&M model 402 gas chromatograph, equipped with dual columns and dual flame ionization detectors, was used.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA. Purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: 3.13% R. E.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	4.589	0.4588	8.384

Auxiliary Information

Method/Apparatus/Procedure:

Standard 1,1-dichloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA., USA. Purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±4.53% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

R. S. Barr and D. M. T. Newsham, Fluid Phase Equilib. **35**, 189 (1987).

Variables:

T/K=293–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^4\ x_1$	$100\ w_1$ (compiler)	$10^3\ x_2$	$100\ w_2$ (compiler)
20	9.26	0.507	5.82	0.106
35	8.93	0.489	—	—
50	9.26	0.507	10.5	0.193

Mole fraction of 1,1-dichloroethane (x_1) was calculated from the activity coefficient at infinite dilution (γ_1^∞) using the relation $x_1 = 1/\gamma_1^\infty$.

Auxiliary Information

Method/Apparatus/Procedure:

The water-rich mixture was studied using gas–liquid chromatography in which a mixture of methane and 1,1-dichloroethane vapor passed through the sampling loop. The eluted 1,1-dichloroethane was determined with a flame ionization detector. The organic-rich mixture was studied using an isopiestic method in which $CaCl_2$ solution controlled the partial pressure of water. The water concentration of the sample was determined using a Karl Fischer titration apparatus.

Source and Purity of Materials:

(1) Fluochem Limited. Redistilled in a glass sieve tray column.
(2) Double distilled tap water.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:

T/K=283–308

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3/atm mol^{-1}	CV[a] %	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
9.6	2.48×10^{-3}	3.40	0.6099	1.116
17.5	3.89×10^{-3}	1.15	0.5501	1.006
24.8	5.62×10^{-3}	4.13	0.5280	0.9654
34.6	8.10×10^{-3}	3.54	0.5509	1.0075

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:

A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of 1,1-dichloroethane was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:

(1) Fluka AG Chemicals Fab., greater than 98% pure by GC analysis.
(2) Distilled.

Estimated Errors:

Solubility: see above.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).

Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
24.85	5.45×10^{-3}	0.561	1.026

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants, as described by Mackay *et al.*,[1] was used. The general procedure was to add an excess quantity of 1,1-dichloroethane to distilled de-ionized water, place the sample in a water bath thermostat, and mix over night. A portion of this solution was returned to the stripping vessel. 1,1-dichloroethane was stripped isothermally from the solution mixture at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used without further purification, stated purity greater than 99%.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) Water; H_2O; [7732-18-5]	G. B. Howe, M. E. Mullins, and T. N. Rogers, ''AFESC Tyndall Air Force Base,'' Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

Variables:	**Prepared By:**
T/K=283–303	A. L. Horvath

Experimental Data

t/°C	10^6 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
10	7.435×10^3	0.7435	1.3613
20	7.137×10^3	0.7137	1.3069
30	6.130×10^3	0.6130	1.1216

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled de-ionized water and sealed. Measured volumes of 1,1-dichloroethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC responses were compared with calibration plots to establish concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% pure, used as received.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–318

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^4\ x_1$	100 w_1 (compiler)
20	1100±15	9.09	0.497
35	1240±20	8.06	0.441
45	1050±25	9.52	0.521

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,1-dichloroethane (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. 1,1-Dichloroethane was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered and de-ionized

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) 1,1,2-trichloroethane; $C_2H_3Cl_3$; [79-00-5]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).

Variables:

T/K=285–304

Prepared By:

A. L. Horvath

Experimental Data

61. 1,1-Dichloroethane with 1,1,2-Trichloroethane and Water

t/°C	$10^4\ x_1$	100 w_1 (compiler)	$10^4\ x_2$	100 w_2 (compiler)
11.8	3.83	0.2096	3.34	0.2464
25.0	3.92	0.2145	3.40	0.2508
30.8	3.89	0.2129	3.34	0.2464

Solubility of equimolar mixtures of 1,1-dichloroethane and 1,1,2-trichloroethane in water.

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water bath thermostat. The chlorinated hydrocarbons were determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator. A helium carrier gas and a Poropack QS column were used for the chromatographic analyses.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Source not given, contained less than 0.1% dissolved material.
(3) Distilled (compiler).

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3] (2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (3) Water; H_2O; [7732-18-5]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U. K., January 1981).
Variables: T/K=298	**Prepared By:** A. L. Horvath

62. 1,1-Dichloroethane with 1,2-Dichloroethane and Water

Experimental Data

Mixture of solutes ($x_1=0.30+x_2=0.70$):

t/°C	$10^4\ x_1$	100 w_1 (compiler)	$10^4\ x_2$	100 w_2 (compiler)
24.5	2.12	1.16×10^{-1}	3.92	0.215

Mixture of solutes ($x_1=0.216+x_2=0.784$):

t/°C	$10^4\ x_1$	100 w_1 (compiler)	$10^4\ x_2$	100 w_2 (compiler)
24.5	1.75	9.59×10^{-2}	4.37	0.239

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water bath thermostat. The chlorinated hydrocarbons were determined using a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digital integrator. A helium carrier gas and a Poropack QS column were used for the chromatographic analyses.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Source not given, contained less than 0.1% dissolved material.
(3) Distilled (compiler).

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Calcium chloride; $CaCl_2$; [10043-52-4] (3) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U. K., January 1981).
Variables: T/K=298–323	**Prepared By:** A. L. Horvath

63. 1,1-Dichloroethane with Calcium Chloride and Water

Experimental Data

100 w_2	t/°C	a_1	p_1/mm Hg	$10^3\ x_1$
45.54	25	0.280	6.65	1.96
	50	0.330	30.5	3.65
39.69	25	0.399	9.48	2.42
	50	0.434	40.1	4.85
35.77	25	0.498	11.83	2.91
	50	0.522	48.3	5.84
31.86	25	0.597	14.18	3.54
27.44	25	0.700	16.63	4.11
	50	0.710	65.7	7.70
18.96	25	0.850	20.19	4.74
	50	0.850	78.6	9.15
0.0	25	1.000	23.76	5.30
	50	1.000	92.51	10.67

a_1=water activity ($=p_1/p°$).
p_1=partial pressure of water in solution.
$p°$=vapor pressure of pure water.

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water thermostat. Water analysis was done using an automatic Karl Fischer titration apparatus. The instrument accuracy was specified to be 1%. All samples were handled with a hypodermic syringe which was weighted before and after each addition. The instrument was calibrated using a synthetic mixture of 1% water in methanol.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.
(3) Source not given, contained less than 0.1% dissolved material.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) Calcium chloride; $CaCl_2$; [10043-52-4]
(3) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(4) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U. K., January 1981).

Variables:

$T/\mathrm{K}=298-323$

Prepared By:

A. L. Horvath

64. 1,1-Dichloroethane with 1,2-Dichloroethane, Calcium Chloride, and Water

Experimental Data

Equivalent mixture of (3) and (4)

$100\ w_2$	$t/°\mathrm{C}$	a_1	p_1 /mm Hg	$10^5\ x_1$
45.54	25	0.280	6.65	2.09
45.04	50	0.330	30.5	5.21
39.69	25	0.399	9.48	2.99
	50	0.434	40.1	6.80
35.77	25	0.498	11.83	3.72
	50	0.522	48.3	8.30
31.86	25	0.597	14.18	4.63
	50	0.615	56.9	9.56
27.44	25	0.700	16.63	5.44
	50	0.710	65.7	10.75
18.96	25	0.850	20.19	6.57
	50	0.850	78.6	12.94
0.0	25	1.000	23.76	7.70
	50	1.000	92.51	15.41

a_1 = water activity ($=p_1/p°$).
p_1 = partial pressure of water in solution.
$p°$ = vapor pressure of pure water.

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water thermostat. Water analysis was done using an automatic Karl Fischer titration apparatus. The instrument accuracy was specified to be 1%. All samples were handled with a hypodermic syringe which was weighted before and after each addition. The instrument was calibrated using a synthetic mixture of 1% water in methanol.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.
(3) Source not given, contained less than 0.1% dissolved material.
(4) Source not given, contained less than 0.1% dissolved material.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) Calcium chloride; $CaCl_2$; [10043-52-4]
(3) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(4) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U. K., January 1981).

Variables:

$T/\mathrm{K}=298-323$

Prepared By:

A. L. Horvath

Experimental Data

Equivalent mixture of (3) and (4)

$100\ w_2$	$t/°\mathrm{C}$	a_1	p_1 /mm Hg	$10^3\ x_1$
53.2	25	7.03×10^{-2}	1.67	0.713
59.2	50	2.3×10^{-2}	2.1	1.21
0.0	25	1.000	23.76	7.70
0.0	50	1.000	92.51	15.41

a_1 = water activity ($=p_1/p°$).
p_1 = partial pressure of water in solution.
$p°$ = vapor pressure of pure water.

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water thermostat. Water analysis was done using an automatic Karl Fischer titration apparatus. The instrument accuracy was specified to be 1%. All samples were handled with a hypodermic syringe which weighted before and after each addition. The instrument was calibrated using a synthetic mixture of 1% water in methanol.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.
(3) Source not given. Contained less than 0.1% dissolved material.
(4) Source not given. Contained less than 0.1% dissolved material.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Magnesium sulfate; $MgSO_4$; [9487-38-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

T/K=298

Prepared By:

A. L. Horvath

65. 1,1-Dichloroethane with Magnesium Sulfate and Water

Experimental Data

t/°C	$10^{-3}\ c_2$ /mol dm^{-3}	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	0.5	0.316	0.315	6.06

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10 to 20 cm^3 1,1-dichloroethane in 500 cm^3 of an aqueous $MgSO_4$ solution in a bottle was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of the 1,1-dichloroethane was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaun chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.01 K.

Components:

(1) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]
(2) Potassium chloride; KCl; [7447-40-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

T/K=298

Prepared By:

A. L. Horvath

66. 1,1-Dichloroethane with Potassium Chloride and Water

Experimental Data

t/°C	$10^{-3}\ c_2$ /mol dm^{-3}	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	0.5	0.443	0.441	8.29

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10 to 20 cm^3 1,1-dichloroethane in 500 cm^3 of an aqueous KCl solution in a bottle was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of the 1,1-dichloroethane was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaun chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.01 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) Sodium hydroxide; NaOH; [1310-73-2]
(3) 1,1-dichloroethane; $C_2H_4Cl_2$; [75-34-3]

Original Measurements:

D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U. K., January 1981).

Variables:

$T/K = 298-323$

Prepared By:

A. L. Horvath

67. 1,1-Dichloroethane with Sodium Hydroxide and Water

Experimental Data

$100\ w_2$	$t/°C$	a_1	p_1 /mm Hg	$10^3\ x_1$
53.2	25	7.03×10^{-2}	1.67	0.558
59.2	50	2.3×10^{-2}	2.1	1.04
0.0	25	1.000	23.76	5.30
0.0	50	1.000	92.51	10.67

a_1 = water activity ($= p_1/p°$).
p_1 = partial pressure of water in solution.
$p°$ = vapor pressure of pure water.

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in a water thermostat. Water analysis was done using an automatic Karl Fischer titration apparatus. The instrument accuracy was specified to be 1%. All samples were handled with a hypodermic syringe which was weighted before and after each addition. The instrument was calibrated using a synthetic mixture of 1% water in methanol.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.
(3) Source not given, contained less than 0.1% dissolved material.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., June 1993.

68. 1,2-Dichloroethane with Water

Critical Evaluation

The 1,2-dichloroethane (1) and water (2) binary system is treated in two parts; part 1 is 1,2-dichloroethane (1) in water (2) and part 2 is water (2) in 1,2-dichloroethane (1).

Part 1. The solubility of 1,2-dichloroethane (1) in water (2) has been studied by 38 groups of workers with reasonably consistent results. However, the experimental work of several investigators was not used for a variety of reasons. The measured solubility of Salkowski,[1] Palatnik *et al.*,[2] Ababi *et al.*,[3] Coca and Diaz,[4] Coca *et al.*,[5] and Warner *et al.*[6] are markedly higher than the solubility values calculated from the smoothing equation and are therefore rejected. Similarly, the data of Chiou *et al.*[7] at 35°C and Howe *et al.*[8] at 30 °C are excluded. The data of Sato and Nakijima,[9] Leighton and Calo,[10] McNally and Grob,[11] and Prosyanov *et al.*[12] are several percent lower than the smoothed solubility values and are rejected. Also not used are the data of Baranaev *et al.*,[24] measured at 1 atm total pressure. (The decreasing solubility between 345 and 371 K indicates that the data were determined at a constant pressure.) The temperature for the separation factors of Bakin[53] was not stated so his reported data are also excluded from the regression analysis.

The remaining data from 27 laboratories were compiled or used for the smoothing equation. The data analysis was conducted using all the measurements of Rex,[13] Gross,[14] Gross and Saylor,[15] Doolittle,[16] Lichascherstov *et al.*,[17] van Arkel and Vles,[18] McClure,[19] McGovern,[20] Chitwood,[21] Udovenko and Fatkulina,[22] Kudryavtseva and Krutikova,[23] O'Connell,[25] Johnson,[26] Svetlanov *et al.*,[27] Antropov *et al.*,[28] Walraevens *et al.*,[29] McConnell *et al.*,[30] Pearson and McConnell,[31] Chiou *et al.*,[7] Earhart *et al.*,[32] Veith *et al.*,[33] Banerjee *et al.*,[34] Takano *et al.*,[35] Barr and Newsham,[36] Howe *et al.*,[8] Bobok *et al.*,[37] and Wright *et al.*,[38] all values within the temperature interval from 273 to 372 K, to obtain the following mass percent (1) equation:

$$\text{Solubility}\ [100\ w_1] = 17.9147 - 0.11684\ (T/K) + 2.0003\times10^{-4}(T/K)^2,$$

which yielded a standard deviation of 4.62×10^{-2}. The recommended solubility values at 5 K intervals for 1,2-dichloroethane (1) in water (2) are listed in Table 1.

TABLE 1. Recommended solubility of 1,2-dichloroethane (1) in water (2).

Temperature		Solubility	
°C	K	$100\ w_1$	$10^3\ x_1$
0	273.15	0.924	1.69
5	278.15	0.891	1.63
10	283.15	0.868	1.59
15	288.15	0.855	1.57
20	293.15	0.852	1.56
25	298.15	0.860	1.58
30	303.15	0.877	1.61
35	308.15	0.904	1.66
40	313.15	0.941	1.73
45	318.15	0.989	1.82
50	323.15	1.046	1.92
55	328.15	1.113	2.04
60	333.15	1.190	2.19
65	338.15	1.278	2.35
70	343.15	1.375	2.53
75	348.15	1.482	2.73
80	353.15	1.599	2.95
85	358.15	1.727	3.19
90	363.15	1.864	3.45
95	368.15	2.011	3.72
100	373.15	2.168	4.02

The measurements and the curve obtained from the smoothing equation are shown in Fig. 21. A solubility minimum calculated from the above regression equation is 0.853 [100 w_1] at 292.06 K. Additional details concerning the solubility minimum for aqueous hydrocarbon systems are discussed in the Preface.

Part 2. The solubility of water (2) in 1,2-dichloroethane (1) has been studied by 27 groups of workers in the temperature interval from 253 to 381 K.

Although all the measurements show a general increase in solubility with temperature, the extent of the increase is variable. The data of McClure,[19] Ababi *et al.*,[3] and Ödberg and Högfeldt[52] are substantially higher than all other studies and are rejected. The data of Udovenko and Fatkulina,[22] Zielinski,[39] Chistyakov and Shapurova,[40] Sellers,[41] and Antropov *et al.*[28] are markedly lower than the smoothed solubility values and are also rejected. The solubility calculated from the distribution coefficients of Prosyanov *et al.*[42] are in very poor agreement, providing no confidence in their values which are regarded as dubious.

The remaining data, mainly due to Doolittle,[16] Staverman,[43] McGovern,[20] Davies *et al.*,[44] Kudryavtseva and Krutikova,[23] O'Connell,[25] Johnson,[26] Johnson *et al.*,[45] Masterton and Gendrano,[46] Christian *et al.*,[47] Coca and Diaz,[4] Coca *et al.*,[5] Czapkiewicz *et al.*,[48] Newsham,[49] Ohtsuka and Kazama,[50] Barr and Newsham,[36] Bobok *et al.*,[37] and Avet'yan *et al.*[51] were compiled or used for the smoothing equation:

$$\log_{10} x_2 = 1.7624 - 1118.41/(T/\mathrm{K}).$$

This equation represents the combined data values which gives a standard deviation of 3.34×10^{-2} in the temperature range from 253 to 381 K.

The recommended solubility values at 5 K intervals for water (2) in 1,2-dichloroethane (1) are presented in Table 2.

TABLE 2. Recommended solubility of water (2) in 1,2-dichloroethane (1)

Temperature		Solubility	
°C	K	100 w_2	$10^3\ x_2$
−20	253.15	0.0403	2.21
−15	258.15	0.0436	2.69
−10	263.15	0.0593	3.25
−5	268.15	0.0712	3.90
0	273.15	0.0850	4.65
5	278.15	0.1008	5.51
10	283.15	0.1188	6.49
15	288.15	0.1392	7.60
20	293.15	0.1624	8.86
25	298.15	0.1884	10.26
30	303.15	0.2175	11.83
35	308.15	0.2500	13.58
40	313.15	0.2862	15.52
45	318.15	0.3262	17.66
50	323.15	0.3705	20.02
55	328.15	0.4192	22.60
60	333.15	0.4728	25.43
65	338.15	0.5314	28.51
70	343.15	0.5953	31.85
75	348.15	0.6652	35.48
80	353.15	0.7411	39.40
85	358.15	0.8235	43.62
90	363.15	0.9127	48.16
95	368.15	1.0090	53.02
100	373.15	1.1131	58.02
105	378.15	1.2254	63.80
110	383.15	1.3462	69.73

Measured values and the linear relationship between the solubility expressed as $\log_{10} x_2$ versus $1/(T/\mathrm{K})$ are plotted in Fig. 22. This linear relationship is a characteristic of water solubility in halogenated hydrocarbons. The phenomenon is discussed in some detail in the Preface.

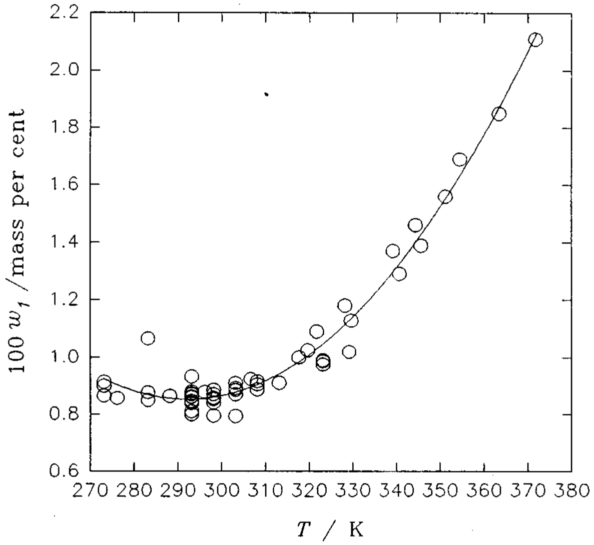

FIG. 21. Solubility of 1,2-dichloroethane (1) in water (2).

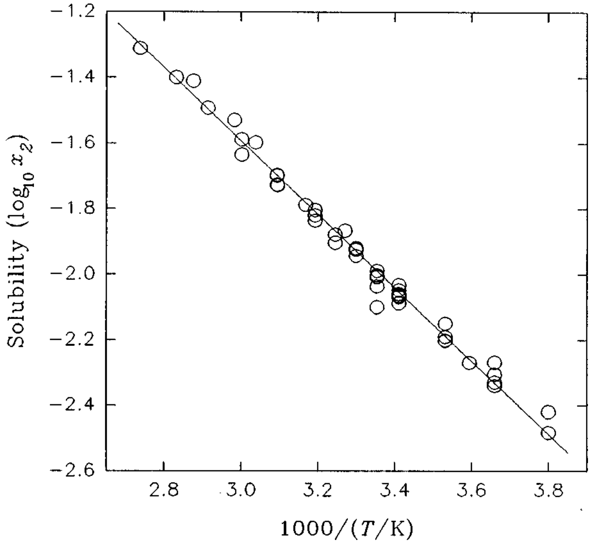

FIG. 22. Solubility of water (2) in 1,2-dichloroethane (1); log x_2 vs 1000/(T/K).

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Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. Rex, Z. Phys. Chem. **55**, 355 (1906).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	0.922	0.914	1.68
10	0.885	0.877	1.61
20	0.869	0.861	1.58
30	0.894	0.885	1.62

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,2-dichloroethane in water was determined in specially designed flasks with calibrated capillary cylinders. After equilibration in a thermostat bath, the volume and the weight of the samples were measured and the solubility calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use, b.p.=83.7–84.3 °C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. Salkowski, Biochem. Z. **107**, 191 (1920).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	1000 V_1 /V_2	100 w_1 (compiler)	10^3 x_1 (compiler)
20	8.0	0.99	1.82

Auxiliary Information

Method/Apparatus/Procedure:

A volumetric method similar to that introduced by Alexejew was used. 1,2-dichloroethane was gradually added to water from a pipet under constant agitation. The appearance of clouding was the indication of saturation.

Source and Purity of Materials:

(1) Schuchard, Görlitz, used as received.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±2 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
25	0.865	0.858	1.58

Auxiliary Information

Method/Apparatus/Procedure:

A weighted amount of 1,2-dichloroethane was mixed with 1000 g water in a bottle and immersed in a water bath thermostat. The bottle was placed on a shaker and shaken until no more droplets of the liquid remained undissolved. The concentration of 1,2-dichloroethane in water was determined using a Zeiss water interferometer. One or more samples were syphoned out for the determination of the solubility. The German translation of the article is also published.[1]

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Distilled.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.01 K.

References:

[1] P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

Variables:

T/K=288–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^3\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
15	8.72	0.864	1.58
30	9.00	0.892	1.64

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,2-dichloroethane in 500 g water was shaken for 12 h in a water bath thermostat. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss.[1] A detailed description of the complete procedure is given in a Ph.D. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Co., purified by fractional distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: ±0.5%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).

[2] J. H. Saylor, Ph.D. thesis, Duke University, Durham, 1930.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. K. Doolittle, Ind. Eng. Chem. **27**, 1169 (1935).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
20	0.87	1.60	0.16	8.73

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial reagent, 99% pure.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. Lichascherstov, S. Aleksejev, and T. Schalajewa, Nitrocellulose **6**, 226 (1935).

Variables:

T/K=273–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	0.922	0.914	1.676
20	0.869	0.862	1.580
30	0.894	0.886	1.625

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=273–329

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	0.873	0.865	1.58
20	0.849	0.842	1.54
35	0.895	0.887	1.63
56	1.030	1.019	1.87

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. B. McClure, Ind. Eng. Chem. News Ed. **17**, 149 (1939).

Variables:
T/K=293

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 w_2	10^2 x_2 (compiler)
20	0.86	1.58	0.5	2.69

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:
A. J. Staverman, Recl. Trav. Chim. Pays-Bas **60**, 836 (1941).

Variables:
T/K=273–303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	100 x_1	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
0	900×10^{-2}	0.495	4.99×10^{-3}
25	1.865×10^{-1}	1.025	1.03×10^{-2}
30	2.165×10^{-1}	1.190	1.20×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of 1,2-dichloroethane and water was shaken for about 12 h in a paraffin liquid bath thermostat. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicate. A full description of the method used is given in a thesis.[1]

Source and Purity of Materials:
(1) Distilled.
(2) Source and purity not given.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] A. J. Staverman, Ph.D. thesis, University of Leiden, Leiden, Belgium, 1938.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:

T/K=273–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
0	0.90	1.65	—	—
10	0.85	1.56	—	—
20	0.84	1.54	0.16	8.73
25	0.84	1.54	—	—
30	0.87	1.59	—	—
40	0.91	1.67	—	—
50	0.99	1.82	—	—

Solubility data as a function of temperature are presented in graphical form except for the tabulated data at 20 and 25 °C.

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Commercial grade, source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

W. Davies, J. B. Jagger, and H. K. Whalley, J. Soc. Chem. Ind. (London) **68**, 26 (1949).

Variables:

T/K=253–353

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^3\ w_1$	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
−20	0.5	2.7	2.8×10^{-3}
−10	0.7	3.8	3.9×10^{-3}
0	1.0	5.4	5.6×10^{-3}
10	1.3	7.1	7.2×10^{-3}
20	1.7	9.3	9.4×10^{-3}
30	2.2	12.0	1.22×10^{-2}
40	2.9	15.7	1.6×10^{-2}
50	3.7	20.0	2.1×10^{-2}
60	4.8	25.8	2.7×10^{-2}
70	6.0	32.1	3.3×10^{-2}
80	7.5	39.8	4.2×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of water and 1,2-dichloroethane was agitated in a flask until equilibrium was established. The apparatus was assembled in a water bath thermostat. The equilibrium was established after 30 min. The pipette used for withdrawing samples from the mixture was fitted with a cotton wool filter at the tip to prevent ice particles from being withdrawn at low temperatures. The solvent layer was titrated with Karl Fischer reagent.

Source and Purity of Materials:

(1) Commercial quaility, source not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5%.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
B. G. Chitwood, Adv. in Chem. Ser., Am. Chem. Soc. **7**, 91 (1952).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.87	1.60	8.79×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
V. V. Udovenko and L. G. Fatkulina, Zh. Fiz. Khim. **26**, 892 (1952).

Variables:
T/K=292–346

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^2\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
19.0	—	—	0.0857	0.47
23.0	0.8774	0.163	—	—
25.5	—	—	0.1136	0.62
30.0	0.9098	0.167	—	—
33.5	0.9239	0.169	0.1509	0.82
42.0	—	—	0.2079	1.13
44.5	1.0001	0.184	—	—
46.5	1.0242	0.190	—	—
47.5	—	—	0.2448	1.33
53.0	—	—	0.2994	1.62
56.5	1.1278	0.207	—	—
57.0	—	—	0.3494	1.90
58.0	—	—	0.3689	1.99
67.5	1.2906	0.238	—	—
69.0	—	—	0.5148	2.76
72.5	1.3886	0.255	—	—

Auxiliary Information

Method/Apparatus/Procedure:
The mutual solubility between 1,2-dichloroethane and water was determined by the method described by Alexejew.[1]

Source and Purity of Materials:
(1) Technical grade, further purified by distillation, b.p.=82.5 °C.
(2) Double distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. T. Kudryavtseva and A. D. Krutikova, J. Appl. Chem. USSR **26**, 1129 (1953).

Variables:

T/K=293

Prepared By:

Z. Maczynska

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
20	0.86	1.58	0.15	8.18

Auxiliary Information

Method/Apparatus/Procedure:

The mutual solubility between water and 1,2-dichloroethane was determined by titration from a microburet until turbidity appeared. The end point of the titration, when turbidity first appeared, was determined with an accuracy of 0.3%–0.5%. The titration of the solution took place in a thermostat bath at 20°C. The caprolactam–water–dichloroethane ternary system was also reported. The original paper was published in Russian.[1]

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:

[1] G. T. Kudryavtseva and A. D. Krutikova, Zh. Prikl. Khim. **26**, 1190 (1953).

Components:

(1) Dichloroethane; $C_2H_4Cl_2$; [1300-21-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

M. K. Baranaev, I. S. Gilman, L. M. Kogan, and N. P. Rodinova, J. Appl. Chem. USSR **27**, 1031 (1954).

Variables:

T/K=345–371

Prepared By:

A. L. Horvath

69. Dichloroethane with Water

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
72.0	0.87	1.59	8.79×10^{-3}
89.3	0.59	1.08	5.96×10^{-3}
92.3	0.43	0.786	4.35×10^{-3}
94.0	0.33	0.602	3.33×10^{-3}
98.0	0.13	0.237	1.31×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

After being cooled to −70 °C, the solutions of various 1,2-dichloroethane concentrations were immersed in a thermostat bath. The condensate from several distillations was analyzed by measuring its weight and volume. From these data and the density of 1,2-dichloroethane, the solubility was calculated.

Source and Purity of Materials:

(1) Source not given, b. p.=83.2 °C. d_4=1.2559 and n_D=1.4443 at 20 °C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.2 K (compiler).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]	A. Z. Zielinski, Chem. Stosow. **3**, 377 (1959).
Variables: T/K=298	**Prepared By:** A. L. Horvath

70. 1,2-Dichloroethane with Water

Experimental Data

t/°C	c_1 /kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.5	0.120	6.56

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of water in the organic phase was determined by the Karl Fischer titration method as described elsewhere.[1]

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Gliwice Chemical, washed and redistilled before use.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] J. Mitchell and D. M. Smith, *Aquametry: A Treatise on Methods for the Determination of Water* (Wiley, New York, 1952), pp. 73, 260.

Components:	**Original Measurements:**
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	L. S. Palatnik, G. R. Vinogorov, M. B. Kagan, and V. B. Kuropiatnik, Zh. Fiz. Khim. **33**, 1933 (1959).
Variables: T/K=291	**Prepared By:** Z. Maczynska

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
18	1.3	2.4	1.31×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

The titration method was used. The data for the 1,2-dichloroethane–water–methanol ternary system was also reported.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: less than $\pm2.0\times10^{-3}$ g_1 /g_t .
Temperature: ±0.5 K.

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
W. L. O'Connell, Trans. Am. Inst. Mech. Eng. **226**, 126 (1963).

Variables:
T/K=293

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
20	0.87	1.58	0.15	8.18

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Dow Chemical Co., used as received.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
V. Ababi, A. Popa, and Gh. Mihaila, Analele Stiint. Univ. Al. I. Cuza Iasi. Sect. IC. Chem. **10**, 71 (1964).

Variables:
T/K=294

Prepared By:
Z. Maczynska

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
20.45	1.2	2.2	0.5	2.7

Auxiliary Information

Method/Apparatus/Procedure:
The isothermic titration method as described by Ababi *et al.*[1,2] was used. The data for the 1,2-dichloroethane–water–allyl alcohol ternary system was also reported.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±0.1 K.

References:
[1] V. Ababi and A. Popa, Analele Stiint. Univ. AI. I. Cusa Iasi. Sect. I. **VI**, 929 (1960).
[2] V. Ababi and A. Popa, Analele Stiint. Univ. AI. I. Cusa Iasi. Sect. I. **VIII**, 233 (1960).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

V. M. Chistyakov and V. V. Shapurova, Izv. Vyssh. Uchebn. Zaved., Khim. Khim. Tekhnol. **7**, 349 (1964).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	9.0×10^{-2}	4.92	5.0×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

J. R. Johnson, Ph.D. thesis, University of Oklahoma, Norman, Oklahoma, 1966.

Variables:

T/K=283–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	100 $w_2M_2^{-1}$	100 w_2 (compiler)
10	—	—	8.12×10^{-2}	0.115
25	0.0895	0.886	1.262×10^{-1}	0.182

Auxiliary Information

Method/Apparatus/Procedure:

The equilibrium between 1,2-dichloroethane and water took place in a well-stirred water bath. The experimental samples were allowed to equilibrate for 2 or more days. Water analyses were made with a Beckman Aquameter using a Karl Fischer reagent. The solubility of 1,2-dichloroethane in water was obtained by using a vapor pressure measuring device. Full details are available in the thesis.

Source and Purity of Materials:

(1) Allied Chemical Corp., purified by distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: ±2%.
Temperature: ±0.1 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

J. R. Johnson, S. D. Cristian, and H. E. Affsprung, J. Chem. Soc. A 77 (1966).

Variables:

T/K=283–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
10	8.12×10^{-2}	0.115	6.28
25	1.262×10^{-1}	0.182	9.92

Auxiliary Information

Method/Apparatus/Procedure:

Samples of the organic-water solutions were equilibrated in water bath isotherms. The description of the solute isopiestic apparatus has been reported elsewhere.[1] Water solubility was determined using the Beckman Model KF-3 Aquameter.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source not given. Reagent grade, distilled in an Oldershaw column before use.

Estimated Errors:

Solubility: $\pm1.2\times10^{-3}$.
Temperature: ±0.1 K.

References:

[1] S. D. Christian, H. E. Affsprung, J. R. Johnson, and J. D. Worley, J. Chem. Educ. **40**, 419 (1963).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

W. L. Masterton and M. C. Gendrano, J. Phys. Chem. **70**, 2895 (1966).

Variables:

T/K=278–298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
5	6.96×10^{-2}	9.83×10^{-2}	5.38
25	1.264×10^{-1}	1.828×10^{-1}	9.96

Auxiliary Information

Method/Apparatus/Procedure:

1,2-dichloroethane was equilibrated with water in an apparatus which has been described elsewhere.[1] The equilibration occurred over a two day time period with the entire apparatus immersed in a water bath thermostat. The organic phase was analyzed for water by the Karl Fischer titration method (dead-stop end point). The microburet used for the titration was read to ±0.01 cm^3. All titrations were carried out in an atmosphere of dry nitrogen.

Source and Purity of Materials:

(1) Distilled.
(2) Source not given, redistilled before use, $n_D=1.444$ at 20 °C.

Estimated Errors:

Solubility: $\pm2.0\times10^{-4}$.
Temperature: ±0.05 K.

References:

[1] S. D. Christian, H. E. Affsprung, and J. R. Johnson, J. Chem. Soc. 1896 (1963).

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]	S. D. Christian, H. E. Affsprung, W. J. A. Hunter, W. S. Gillam, and W. H. McCoy, ‘‘Solute Properties of Water,’’ U.S. Office of Saline Water Research and Development Program, Report No. 301 (1968), pp. 71 and 76.
Variables:	**Prepared By:**
T/K=283–308	A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
10	0.0812±0.0010	0.115	6.30
25	0.1262±0.0014	0.182	9.94
35	0.1570±0.0016	0.230	12.49

Auxiliary Information

Method/Apparatus/Procedure:

The solute isopiestic method was used without modification. The apparatus employed consisted of a closed vessel divided into two compartments, one for water and the other for the organic solvent. Equilibrium was attained after a period of 6–8 h. Samples of the solution were analyzed for water with the Beckman KF-Aquameter. The Karl Fischer reagent was standardized against crystalline sodium tartarate dihydrate.

Source and Purity of Materials:

(1) Distilled.

(2) Certified or regant grade, distilled through a 30 plate Oldershaw column before use.

Estimated Errors:

Solubility: see above.

Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]	L. Ödberg and E. Högfeldt, Acta Chem. Scand. **23**, 1330 (1969).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^2 x_1 (compiler)
25	1.230×10^2	0.221	1.20

Auxiliary Information

Method/Apparatus/Procedure:

Samples were prepared and analyzed as described elsewhere.[1] Several samples of 1,2-dichloroethane were shaken in bottles with water solutions of $CaCl_2$ and LiCl at room temperature overnight. The bottles were centrifuged and samples were taken from the organic-rich phase. The water determinations were carried out according to a modified Karl Fischer titration method. At least two samples were taken. Correction was made for the water content of air.

Source and Purity of Materials:

(1) Distilled.

(2) Prepared by the authors, 99.9% pure by VPC analysis.

Estimated Errors:

Solubility: not specified.

Temperature: ±1 K.

References:

[1] E. Högfeldt and B. Bolander, Arkiv för Kemie **21**, 161 (1963).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

E. B. Svetlanov, S. M. Velichko, M. I. Levinskii, Yu. A. Treger, and R. M. Flid, Russ. J. Phys. Chem. **45**, 488 (1971).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
30	8.00	0.794	1.45

Auxiliary Information

Method/Apparatus/Procedure:

The dynamic method used for the solubility determination consisted of the saturation of nitrogen with 1,2-dichloroethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of water. After 2–3 h, the solution became saturated and samples were taken periodically.[1] The concentration of 1,2-dichloroethane in water was determined by GLC. Some 3–5 measurements were taken at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±15%.
Temperature: ±0.05 K

References:

[1] Yu. A. Treger, R. M. Flid, and S. S. Spektor, Russ. J. Phys. Chem. **38**, 253 (1964).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

P. Sellers, Acta Chem. Scand. **25**, 2295 (1971).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

	GLC method:		CaH_2 method:	
t/°C	100 V_1/V_t	10^3 x_1 (compiler)	100 V_1/V_t	10^3 x_1 (compiler)
25	0.124±0.004	6.77	0.120±0.005	7.04

Auxiliary Information

Method/Apparatus/Procedure:

Samples of 1,2-dichloroethane saturated with water were analyzed by two different methods: a gas chromatographic method and a calcium hydride reaction method. The gas chromatographic method used a Varian Aerograph fitted with a thermal conductor and the column packed with Poropak P and Q. The calcium hydride reaction method consisted of mixing the sample with CaH_2 and determining the amount of hydrogen evolved from the reaction between the hydride and water present in the samples.

Source and Purity of Materials:

(1) Distilled.
(2) British Drug House, dried on molecular sieves before use.

Estimated Errors:

Solubility: see above.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

V. M. Bakin, Russ. J. Phys. Chem. **45**, 1870 (1971) (VINITI No. 2878-71).

Variables:

T/K=Not given and P/mmHg=530–760

Prepared By:

A. L. Horvath

Experimental Data

p/mm Hg	α[a]	100 w_1 (compiler)	10^3 x_1 (compiler)
5.30×10^2	6.60×10^2	0.580	1.06
6.40×10^2	4.70×10^2	0.975	1.79
7.60×10^2	3.50×10^2	1.551	2.86

[a] Separation factor, $(\alpha)=[\text{solute/water}]_{\text{vapor phase}}/[\text{solute/water}]_{\text{liquid phase}}$.

Auxiliary Information

Method/Apparatus/Procedure:

1,2-dichloroethane was labeled with ^{36}Cl β-active isotope. The concentration of 1,2-dichloroethane in the aqueous phase was determined from the radioactivities of the samples as measured by the tracer atom method.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±10%.
Temperature: not specified.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. I. Antropov, V. E. Pogulyai, V. D. Simonov, and T. M. Shamsutdinov, Russ. J. Phys. Chem. **46**, 311 (1972) (VINITI No. 3739-71).

Variables:

T/K=291–299

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
18	—	—	0.082	4.49
20	0.811	1.49	—	—
26	—	—	0.114	6.23

Auxiliary Information

Method/Apparatus/Procedure:

The Alexejew's synthetic method of solubility determination was used.[1] A fixed weight of 1,2-dichloroethane and water was sealed in a tube and subjected to gradually increasing temperature with constant agitation. The appearance of an opalescence or clouding was an indication of saturation temperature. The temperature was then allowed to fall and an observation made, while the tube was constantly agitated, to establish the temperature of the first appearance of opalescence. The observation was repeated several times.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] W. Alexejew, Ann. Phys. Chem. **28**, 305 (1886).

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 100 (1973).

Variables:

T/K=296–352

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
23	24.9	2.07×10^{-2}	1.14
25	24.7	2.31×10^{-2}	1.27
50	16.7	1.34×10^{-1}	7.30
65	14.6	3.12×10^{-1}	16.92
79.2	12.0	7.33×10^{-1}	38.96

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

The concentration of water in the organic-rich phase was determined radiometrically using tritium labeled water. A full description of the apparatus and method used is given in the paper.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

N. N. Prosyanov, V. A. Shalygin, and Ya. D. Zel'venskii, Tr. Mosk. Khim.-Tekhnol. Inst. 183 (1973).

Variables:

T/K=288–373

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient,[a] D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
14	2.58×10^3	0.0128	0.2333
32	1.62×10^3	0.0488	0.8889
41	1.40×10^3	0.0835	1.521
50	1.12×10^3	0.1505	2.744
60	9.00×10^2	0.2735	4.991
70	7.80×10^2	0.449	8.204
80	6.50×10^2	0.748	13.705
90	5.50×10^2	1.201	22.076
95.7	4.90×10^2	1.648	30.408
100	4.30×10^2	2.040	37.770

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

The distribution coefficient was determined by distillation of the sample in a stream of inert carrier gas used to provide sampling of the equilibrium vapor phase. The concentrations of 1,2-dichloroethane in both phases were determined using ^{36}Cl labeled compound.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	R. Walraevens, P. Trouillet, and A. Devos, Int. J. Chem. Kinet. **6**, 777 (1974).
Variables:	**Prepared By:**
T/K=283–353	A. L. Horvath

Experimental Data

The temperature dependence of the solubility of 1,2-dichloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/\text{mol dm}^{-3}) = \frac{2070}{(T/\text{K})} - 15.369 + 0.0247(T/\text{K}),$$

where S=solubility and T=absolute temperature.

For example, the calculated solubility derived from the above equation is 8.53×10^{-1} [100 w_1] at 298.15 K (compiler).

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1,2-dichloroethane and water was preheated to the desired temperature before rapid mixing. The resulting mixture was thermostated and the equilibrium was maintained by vigorous stirring. The concentration of 1,2-dichloroethane in water was determined by gas chromatography.

Source and Purity of Materials:

(1) Solvay, rectified before use, 99.9% pure by GLC analysis.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

Components:	**Original Measurements:**
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	G. McConnell, D. M. Ferguson, and C. R. Pearson, Endeavour **34**, 13 (1975).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	8.80×10^3	0.872	1.60

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of 1,2-dichloroethane in water was determined by gas–liquid chromatography (GLC) using an electron capture detector. Where possible, identification was confirmed by a linked mass spectrometer (MS).

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. R. Pearson and G. McConnell, Proc. Roy. Soc. London Ser. B **189**, 305 (1975).

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	8.80×10^3	0.880	1.61

Auxiliary Information

Method/Apparatus/Procedure:

Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with n-pentane and an aliquot of the extract taken for GLC analysis. The gas chromatograph was fitted with a ^{63}Ni electron capture detector.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

C. T. Chiou and V. H. Freed, ''Chemodynamic Studies on Bench Mark Industrial Chemicals,'' U.S. Dept. of Comm., Natl. Tech. Inf. Ser., PB-274 263 (1977).

Variables:

T/K=276–307

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/kg m^{-3}	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
3	8.64	0.857	1.57
20	8.45	0.839	1.54
34	10.3	1.025	1.88

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 5–10 g 1,2-dichloroethane was equilibrated with 100 cm^3 of distilled water for 24 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ^{63}Ni electron capture detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on the determination and evaluation of the procedure are found elsewhere.[1]

Source and Purity of Materials:

(1) Commercial reagent, used as received.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K.

References:

[1] C. T. Chiou and D. W. Schmedding, Test. Protec. Environ. Fate Mov. Toxicants, Proc. Symp., 1980, pp. 28–42 (Publ. 1981).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. P. Erhart, K. W. Won, H. V. Wong, J. M. Prausnitz, and C. J. King, Chem. Eng. Progr. **73**, 67 (1977).

Variables:
T/K=293

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^1 (compiler)
20	8.1×10^{-1}	1.48	8.19×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Union Carbide Corp., purity not given, used as received.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Sato and T. Nakijima, Arch. Environ. Health **34**, 69 (1979).

Variables:
T/K=310

Prepared By:
A. L. Horvath

Experimental Data

t/°C	Partition coefficient,[a] K_L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
37	11.3	0.794	1.455

[a] Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:
A 1,1-dichloroethane vapor sample was equilibrated in an airtight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airtight syringe and then injected into a gas chromatograph and analyzed. The signal peak height on the chromatogram was used to calculate the partition coefficient.

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled.

Estimated Errors:
Solubility: ±0.4 std. dev.
Temperature: ±0.5 K (compiler).

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Coca and R. Diaz, J. Chem. Eng. Data **25**, 80 (1980).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	1.06	1.95	0.18	9.81

Auxiliary Information

Method/Apparatus/Procedure:
A titration was performed in an Erlenmeyer flask by adding 1,2-dichloroethane to water until a permanent turbidity was observed. The flask was immersed in a water bath thermostat while maintaining a constant agitation using a magnetic stirrer.

Source and Purity of Materials:
(1) Probus Chemicals, laboratory grade reagent, further purified by distillation; middle fraction was used.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.05 K.

Components:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. Coca, R. M. Diaz, and C. Pazos, Fluid Phase Equilib. **4**, 125 (1980).

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	1.10	2.02	0.18	9.81

Auxiliary Information

Method/Apparatus/Procedure:
The mutual solubility data were determined by a method described by Othmer *et al.*[1] A 10 cm^3 1,2-dichloroethane sample was added to water from a buret and agitated until the solution became turbid. The appearance of the turbidity indicated the formation of a second phase. The solubility was calculated using the known densities and volumes.

Source and Purity of Materials:
(1) Probus Chemicals reagent, further purified by distillation in a heli-packing column.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).

References:
[1] D. F. Othmer, R. E. White, and E. Trueger, Ind. Eng. Chem. **33**, 1240 (1941).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. D. Veith, K. J. Macek, S. R. Petrocelli, and J. Carroll, Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 707, Philadelphia, PA, 1980 pp. 116–29.

Variables:

T/K=293

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$n_1V_2^{-1}$/mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	8.13×10^{-2}	8.00×10^{-1}	1.47

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,2-dichloroethane was added to 10 cm^3 distilled water in a 50 cm^3 flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ^{14}C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

J. Czapkiewicz and B. Czapkiewicz-Tulaj, J. Chem. Soc. Faraday Trans. I **76**, 1663 (1976).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	0.126	0.182	9.92

Auxiliary Information

Method/Apparatus/Procedure:

The water content of the saturated 1,2-dichloroethane solution was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled.
(2) Source and purity not given.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K.

Components:	**Original Measurements:**
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	S. Banerjee, S. H. Yalkowsky, and S. C. Valvani, Environ. Sci. Technol. **14**, 1227 (1980).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	10^{-3} c_1 /mol dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	8.07×10^{-2}	0.795	1.46

Auxiliary Information

Method/Apparatus/Procedure:

An excess of 1,2-dichloroethane was added to a stainless steel tube containing water and then the tube was sealed. The equilibration occurred during shaking for 1 week at 25 °C. After centrifugation, the concentration was obtained from a measurement of radioactivity through liquid scintillation counting. The solubility procedure was carried out at least twice for each sample and the analysis was done in duplicate.

Source and Purity of Materials:

(1) New England Nuclear, used as received.
(2) Distilled.

Estimated Errors:

Solubility: ±3.5% std. dev.
Temperature: ±0.3 K.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]	D. M. T. Newsham, *Measurement and Correlation of Thermodynamic Data for Chlorinated Hydrocarbons* (UMIST Press, Manchester, U.K., January 1981).
Variables:	**Prepared By:**
T/K=273–323	A. L. Horvath

Experimental Data

t/°C	10^2 x_1	100 w_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	0.457	8.35×10^{-2}	4.63×10^{-3}
20	0.895	1.64×10^{-1}	9.10×10^{-3}
30	1.205	2.22×10^{-1}	1.23×10^{-2}
40	1.515	2.79×10^{-1}	1.55×10^{-2}
50	2.015	3.73×10^{-1}	2.07×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

Samples were equilibrated for at least 10 days in water thermostat. Water analysis was done using an automatic Karl Fischer titration apparatus. The accuracy of the instrument was specified to be 1%. All samples were handled with a hypodermic syringe which was weighted before and after each addition. The instrument was calibrated using a synthetic mixture of 1% water in methanol.

Source and Purity of Materials:

(1) Source not given, contained less than 0.1% dissolved material.
(2) Distilled (compiler).

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. T. Leighton and J. M. Calo, J. Chem. Eng. Data **26**, 382 (1981).

Variables:

T/K=274–300

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Distribution coefficient[a], D_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
1.0	30.62	0.5256	9.610
1.3	30.89	0.5363	9.807
11.0	46.56	0.6032	11.035
21.0	68.89	0.6801	12.451
22.0	76.59	0.6426	11.761
27.2	95.46	0.6548	11.985

[a] Gas–liquid system analysis parameter, from calibration measurements.

Auxiliary Information

Method/Apparatus/Procedure:

A 5 μL 1,2-dichloroethane sample was injected into a 2.3 dm^3 equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 min, the homogeneity of the liquid sample was maintained with a magnetic stirrer. Compressed air was passed through the cell and the gas flow was measured with a soap film flowmeter. The 1,2-dichloroethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: ±5.0%.
Temperature: ±0.5 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

K. Ohtsuka and K. Kazama, Sen'i Seihin Shohi Kagaku Kaishi **22**, 197 (1982).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.80	0.146	7.97

Auxiliary Information

Method/Apparatus/Procedure:

Water was added gradually to 50 cm^3 1,2-dichloroethane in a flask which was then lowered into a thermostat bath. The flask was shaken vigorously until the first cloud (turbidity) appeared. The sample water content was determined by the Karl Fischer titration method.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Commercial JTS extra pure reagent. Further purified by conventional methods.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	Original Measurements:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	M. E. McNally and R. L. Grob, J. Chromatogr. **284**, 105 (1984).
Variables:	**Prepared By:**
T/K=303	A. L. Horvath

Experimental Data

$t/°C$	$g_1V_2^{-1}$/g dm^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	3.506	0.3509	6.406

Auxiliary Information

Method/Apparatus/Procedure:

Standard 1,2-dichloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere.[1] The aqueous organic liquid phase was 25 cm^3 and the vapor phase above the mixture was 35 cm^3. The system was allowed to reach equilibrium in a constant temperature bath and then a sample was injected into the gas chromatograph. Values reported are an average of at least five measurements.

Source and Purity of Materials:

(1) Chemical Service, West Chester, PA, USA, purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:

Solubility: ±4.91% std. dev.
Temperature: ±0.5 K (compiler).

References:

[1] M. E. McNally and R. L. Grob, J. Chromatogr. **260**, 23 (1983).

Components:	Original Measurements:
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	J. Takano, Y. Ishihara, T. Yasuoka, and S. Mitsuzawa, Nippon Kagaku Kaishi 2116 (1985).
Variables:	**Prepared By:**
T/K=293	A. L. Horvath

Experimental Data

$t/°C$	10^3 ρ_1 /μg cm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	8.490×10^3	0.8490	1.556
	9.170×10^3	0.9170	1.682
	8.420×10^3	0.8420	1.544
	8.830×10^3	0.8830	1.619

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 1 cm^3 1,2-dichloroethane and 30 cm^3 water was introduced into a centrifuge tube which was then shaken for 60 min in a shaker at room temperature. After standing for 48 h, the samples were filtered through four types of filter papers in order to free the solutions from emulsions. The concentrations of the aqueous solutions were determined by the TOC (total organic carbon) method. Nine measurements were performed for each solution.

Source and Purity of Materials:

(1) Nakai Chemical Co., analytical grade reagent, redistilled before use.
(2) Double distilled.

Estimated Errors:

Solubility: ±0%–2.3% coef. of var.
Temperature: ±1.0 K.

Components:	**Original Measurements:**
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	R. S. Barr and D. M. T. Newsham, Fluid Phase Equilib. **35**, 189 (1987).
Variables:	**Prepared By:**
T/K=293–323	A. L. Horvath

Experimental Data

t/°C	$10^3\ x_1$	100 w_1 (compiler)	$10^3\ x_2$	100 w_2 (compiler)
20	1.60	0.873	8.55	0.157
35	1.66	0.905	13.2	0.243
50	1.81	0.986	18.8	0.348

Mole fraction of 1,2-dichloroethane (x_1) was calculated from the activity coefficients at infinite dilution (γ_1^∞) using the relation $x_1 = 1/\gamma_1^\infty$.

Auxiliary Information

Method/Apparatus/Procedure:

The water-rich mixture was studied using gas–liquid chromatography in which a mixture of methane and 1,2-dichloroethane vapor passed through the sampling loop. The eluted 1,2-dichloroethane was determined with a flame ionization detector. The organic-rich mixture was studied using an isopiestic method in which $CaCl_2$ solution controlled the partial pressure of water. The water concentration of the sample was determined using a Karl Fischer titration apparatus.

Source and Purity of Materials:

(1) Fisons Scientific Equipment Ltd., used as received.
(2) Double distilled tap water.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.05 K.

Components:	**Original Measurements:**
(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2] (2) Water; H_2O; [7732-18-5]	H. P. Warner, J. M. Cohen, and J. C. Ireland, ''Determination of Henry's Law Constants of Selected Priority Pollutants,'' U.S. EPA Technical Report, PB87-212684, Cincinnati, OH (July 1987).
Variables:	**Prepared By:**
T/K=298	A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
24.85	1.10×10^{-3}	1.020	1.872

Auxiliary Information

Method/Apparatus/Procedure:

The original method and apparatus for the determination of Henry's law constants, as described by Mackay *et al.*,[1] was used. The general procedure was to add an excess quantity of 1,2-dichloroethane to distilled de-ionized water, place the sample in a thermostat bath, and mix overnight. A portion of this solution was returned to the stripping vessel. The 1,2-dichloroethane was stripped isothermally from the solution mixture at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

Source and Purity of Materials:

(1) Purest quality available, used as received, stated purity greater than 99%.
(2) Distilled and de-ionized.

Estimated Errors:

Solubility: ±6% std. dev.
Temperature: ±0.05 K.

References:

[1] D. Mackay, W. Y. Shiu, and R. D. Sutherland, Environ. Sci. Technol. **13**, 333 (1979).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

G. B. Howe, M. E. Mullins, and T. N. Rogers, ''AFESC Tyndall Air Force Base,'' Report ESL-TR-86-66, Vol. 1, Florida (September 1987), 86 pp. (AD-A188 571).

Variables:

T/K = 283–303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
10	1.0654×10^4	1.0654	1.9566
20	8.467×10^3	0.8467	1.5521
30	1.0467×10^4	1.0467	1.9219

Auxiliary Information

Method/Apparatus/Procedure:

250 cm^3 bottles were filled with distilled de-ionized water and sealed. Measured volumes of 1,2-dichloroethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shaker and allowed to equilibrate for about three weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack column and a FID detector. The GC responses were compared with calibration plots to establish concentrations.

Source and Purity of Materials:

(1) Probably a commercial reagent at least 99% pure. Used as received.
(2) Distilled de-ionized.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. Bobok, E. Kossaczky, and J. Surovy, Coll. Czech. Chem. Commun. **54**, 2848 (1989).

Variables:

T/K = 306–381

Prepared By:

A. L. Horvath

Experimental Data

t/°C	$100\ w_1$	$10^2\ x_1$ (compiler)	$100\ w_2$	$10^2\ x_2$ (compiler)
32.55	—	—	0.25	1.36
42.55	—	—	0.30	1.63
48.55	1.09	0.200	—	—
55.05	1.18	0.217	—	—
56.05	—	—	0.47	2.53
62.05	—	—	0.55	2.95
66.05	1.37	0.252	—	—
71.25	1.46	0.269	—	—
74.55	—	—	0.73	3.88
78.05	1.56	0.288	—	—
81.35	1.69	0.312	—	—
90.25	1.85	0.342	—	—
92.05	—	—	1.08	4.89
98.55	2.11	0.391	1.24	6.45
107.55	—	—	1.54	7.91

Auxiliary Information

Method/Apparatus/Procedure:

Samples were prepared of different composition by mixing the determined amount of pure components in sealed glass ampoules. A homologous liquid phase was achieved by heating the sample sufficiently. Upon cooling, the temperature was found when the turbidity of the solution appeared at a given composition.

Source and Purity of Materials:

(1) Supplied by Lachema, Brno, designated by ''Import.'' Redistilled before use, 99.9% pure.
(2) Double distilled.

Estimated Errors:

Solubility: ±0.0251 std. dev.(1).
$\pm6.2\times10^{-5}$ std. dev.(2).

Temperature: ±0.1 K.

Components:

(1) Water; H_2O; [7732-18-5]
(2) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]

Original Measurements:

M. G. Avet'yan, E. V. Sonin, and I. F. Pimenov, Sov. Chem. Ind. **23**, 18 (1991).

Variables:

T/K=263–333

Prepared By:

A. L. Horvath

Experimental Data

t/°C	n_1/n_2	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
−10	3.3×10^{-3}	6.00×10^{-2}	3.29
0	4.7×10^{-3}	8.55×10^{-2}	4.68
10	6.5×10^{-3}	1.18×10^{-1}	6.46
20	8.7×10^{-3}	1.58×10^{-1}	8.62
30	1.15×10^{-2}	2.09×10^{-1}	11.4
40	1.48×10^{-2}	2.69×10^{-1}	14.6
50	1.91×10^{-2}	3.47×10^{-1}	18.7
60	2.37×10^{-2}	4.30×10^{-1}	23.2

Auxiliary Information

Method/Apparatus/Procedure:

Equilibrium was established between water and 1,2-dichloroethane after 2–3 hours in a thermostat. The amount of water was determined by potentiometric titration using a Karl Fischer apparatus.

Source and Purity of Materials:

(1) Distilled (compiler).
(2) Source and purity not given.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.1 K.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. A. Wright, S. I. Sandler, and D. DeVoll, Environ. Sci. Technol. **26**, 1828 (1992).

Variables:

T/K=293–323

Prepared By:

A. L. Horvath

Experimental Data

t/°C	γ_1^∞	$10^3\ x_1$	100 w_1 (compiler)
20	585±6	1.71	0.932
35	597±12	1.68	0.916
50	559±6	1.79	0.975

Auxiliary Information

Method/Apparatus/Procedure:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,2-dichloroethane (γ_1^∞) in water. Cells containing degassed water were submerged in a thermostat water bath. The 1,2-dichloroethane was injected into the mixture cells and a magnetic stirrer was turned on. Next, the cells were allowed to equilibrate. Then, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled, filtered and de-ionized

Estimated Errors:

Solubility: see above.
Temperature: ±0.05 K.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Hydrogen chloride; HCl ; [7647-01-0]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

E. B. Svetlanov, S. M. Velichko, M. I. Levinskii, Yu. A. Treger, and R. M. Flid, Russ. J. Phys. Chem. **45**, 488 (1971).

Variables:

T/K=303–333

Prepared By:

A. L. Horvath

71. 1,2-Dichloroethane with Hydrogen Chloride and Water

Experimental Data

1. Solubility of 1,2-dichloroethane in 10 wt % HCl solution

t/°C	1000 w_1	100 w_1 (compiler)	10^5 x_1 (compiler)
30	8.20	0.820	15.84
45	5.26	0.526	10.13
60	3.04	0.304	5.844

2. Solubility of 1,2-dichloroethane in 20 wt % HCl solution

t/°C	1000 w_1	100 w_1 (compiler)	10^5 x_1 (compiler)
30	8.04	0.804	16.41
45	5.68	0.568	11.56
60	3.00	0.300	6.093

Auxiliary Information

Method/Apparatus/Procedure:

The dynamic method used for the solubility determination consisted of the saturation of nitrogen with 1,2-dichloroethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of water. After 2–3 h, the solution became saturated and samples were taken periodically.[1] The concentration of the 1,2-dichloroethane in the solution was determined by GLC. Some 3–5 measurements were taken at each temperature.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled (compiler).

Estimated Errors:

Solubility: ±15%.
Temperature: ±0.05 K.

References:

[1] Yu. A. Treger, R. M. Flid, and S. S. Spektor, Russ. J. Phys. Chem. **38**, 253 (1964).

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Magnesium sulfate; $MgSO_4$; [7487-88-9]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

T/K=298

Prepared By:

A. L. Horvath

72. 1,2-Dichloroethane with Magnesium Sulfate and Water

Experimental Data

t/°C	10^{-3} c_2 /mol dm^{-3}	100 g_1 /g_2	100 w_2 (compiler)	10^3 x_2 (compiler)
25	0.5	0.552	0.549	1.06

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10 to 20 cm^3 1,2-dichloroethane in 500 cm^3 of an aqueous solution of $MgSO_4$ was placed in a bottle and immersed in a water bath thermostat. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the 1,2-dichloroethane concentration was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.01 K.

Components:

(1) 1,2-dichloroethane; $C_2H_4Cl_2$; [107-06-2]
(2) Potassium chloride; KCl; [7447-40-7]
(3) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross, Z. Phys. Chem. **6B**, 215 (1929).

Variables:

$T/K=298$

Prepared By:

A. L. Horvath

73. 1,2-Dichloroethane with Potassium Chloride and Water

Experimental Data

$t/°C$	$10^{-3}\ c_2$ /mol dm^3	$100\ g_1/g_2$	$100\ w_2$ (compiler)	$10^3\ x_2$ (compiler)
25	0.5	0.752	0.746	1.406

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of 10 to 20 cm^3 1,2-dichloroethane in 500 cm^3 of an aqueous solution of KCl was placed in a bottle and immersed in a water bath thermostat. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the 1,2-dichloroethane concentration was determined using a Zeiss water interferometer.

Source and Purity of Materials:

(1) Commercial reagent, fractionally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

Estimated Errors:

Solubility: ±1%.
Temperature: ±0.01 K.

Components:

(1) Bromoethane; C_2H_5Br; [74-96-4]
(2) Water; H_2O; [7732-18-5]

Evaluator:

A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., June 1993.

74. Bromoethane with Water

Critical Evaluation

The bromoethane (1) and water (2) binary system is treated in two parts; part 1 is bromoethane (1) in water (2) and part 2 is water (2) in bromoethane (1).

Part 1. The solubility of bromoethane (1) in water (2) has been studied at ambient temperature by four groups of workers with reasonably good agreement. A temperature dependence of the solubility was reported in only one paper,[1] between 273 and 303 K.

The available solubility data of Rex,[1] Führer,[2] van Arkel and Vles,[3] and Donahue and Bartell[4] were used to obtain the following mass percent (1) equation:

$$\text{Solubility}\ [100\ w_1]=13.2481-8.0012\times10^{-2}(T/\text{K})+1.29448\times10^{-4}(T/\text{K})^2.$$

This equation, which represents the combined data points, shows a standard deviation of 1.53×10^{-2} in the narrow temperature interval from 273 to 303 K. The tentative solubility at 5 K intervals for bromoethane (1) in water (2) is listed in Table 1.

While it is most likely that a solubility minimum exists above 303 K, as yet no measurements have been reported for this temperature range.

TABLE 1. Tentative solubility of bromoethane (1) in water (2)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^3\ x_1$
0	273.15	1.051	1.753
5	278.15	1.008	1.681
10	283.15	0.971	1.618
15	288.15	0.941	1.568
20	293.15	0.917	1.528
25	298.15	0.900	1.499
30	303.15	0.889	1.481

Part 2. The solubility of water (2) in bromoethane (1) has been reported by two workers at 298 K only. The two measurements of Hutchison and Lyon[5] and Donahue and Bartell[4] compares favorably with the likely solubility. It is not possible to say which of the two measurements is more reliable; therefore, the average of the two determinations is probably the most reliable value, that is, 0.0774 [$100\ w_2$] at 298.15 K. This value is classified as tentative. More accurate solubility determinations are required, most certainly at the higher temperatures.

References:

[1] A. Rex, Z. Phys. Chem. **55**, 355 (1906).
[2] H. Führer, Ber. **57**, 510 (1925).
[3] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).
[4] D. J. Donahue and F. E. Bartell, J. Phys. Chem. **56**, 480 (1952).
[5] C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1943).

Components:	**Original Measurements:**
(1) Bromoethane; C_2H_5Br; [74-96-4] (2) Water; H_2O; [7732-18-5]	A. Rex, Z. Phys. Chem. **55**, 355 (1906).
Variables:	**Prepared By:**
T/K=273–303	A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	1.067	1.055	1.76
10	0.965	0.956	1.59
20	0.914	0.906	1.51
30	0.896	0.888	1.48

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of bromoethane in water was determined using specially designed flasks with calibrated capillary cylinders. After the samples were equilibrated in a thermostatic bath at the desired temperature, the volume and the weight of the samples were determined and the solubility calculated.

Source and Purity of Materials:

(1) Merck, redistilled and washed before use, b. p.=37.7°C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components: 439	**Original Measurements:**
(1) Bromoethane; C_2H_5Br; [74-96-4] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. **57**, 510 (1924).
Variables:	**Prepared By:**
T/K=291	A. L. Horvath

Experimental Data

t/°C	ρ_1 /kg m^{-3}	10^3 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
17.5	9.52	1.59	8.74×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Bromoethane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the bromoethane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Bromoethane; C_2H_5Br; [74-96-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $n_1 g_2^{-1}$/mol g^{-1}	$10^2\ x_1$	100 w_1 (compiler)
30.0	8.2×10^{-3}	0.148	0.888

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Water; H_2O; [7732-18-5]
(2) Bromoethane; C_2H_5Br; [74-96-4]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $w_1 M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	4.17×10^{-3}	7.51×10^{-2}	4.52

Auxiliary Information

Method/Apparatus/Procedure:

A 1 to 15 volume ratio mixture of water and bromoethane was introduced into an equilibration flask and then lowered into the water bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. The description of procedure was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Distilled.
(2) Probably a commercial reagent, purified and dried before use.

Estimated Errors:

Solubility: $\pm4.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey (McGraw-Hill, New York, 1955), p. 129.

Components:

(1) Bromoethane; C_2H_5Br; [74-96-4]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

D. J. Donahue and F. E. Bartell, J. Phys. Chem. **56**, 480 (1952).

Variables:

T/K=298

Prepared By:

A. L. Horvath

Experimental Data

t/°C	x_1	100 w_1 (compiler)	x_2	100 w_2 (compiler)
25	1.5×10^{-3}	0.900	4.8×10^{-3}	7.97×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

A mixture of water and bromoethane was placed in a glass stoppered flask and was shaken intermittently for at least 3 days in a water bath held at constant temperature. The organic phase was analyzed for water content by the Karl Fischer titration method and the aqueous phase was analyzed interferometrically.

Source and Purity of Materials:

(1) Reagent grade, purified by fractional distillation.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.1 K.

Components:

(1) Water-d_2 ; D_2O; [7789-20-0]
(2) Bromoethane; C_2H_5Br; [74-96-4]

Original Measurements:

C. A. Hutchison and A. M. Lyon, Columbia University Report A-745 (July 1, 1943).

Variables:

T/K=298

Prepared By:

A. L. Horvath

75. Bromoethane with Water-d_2

Experimental Data

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	3.52×10^{-3}	7.05×10^{-2}	3.82

Auxiliary Information

Method/Apparatus/Procedure:

A 1 to 15 volume ratio mixture of heavy water and bromoethane was introduced into an equilibration flask and then lowered into the water bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration. The determination was done in triplicate. The description of the procedure was taken from a secondary source.[1] The original university report is no longer available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Source not given, purified and dried before use.

Estimated Errors:

Solubility: $\pm5.0\times10^{-5}$ av. dev.
Temperature: ±0.05 K.

References:

[1] *Production of Heavy Water*, edited by M. L. Eidinoff, G. G. Joris, H. S. Taylor, and H. C. Urey, (McGraw-Hill, New York, 1955), p. 129.

Components:	**Evaluator:**
(1) Chloroethane; C_2H_5Cl; [75-00-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., June 1993.

76. Chloroethane with Water

Critical Evaluation

The chloroethane (1) and water (2) binary system is treated in two parts; part 1 is chloroethane (1) in water (2) and part 2 is water (2) in chloroethane (1).

Part 1. The solubility of chloroethane (1) in water (2) has been studied by seven groups of workers over the temperature range from 273 to 313 K. The data are in very poor agreement and in the absence of other independent studies it is not possible to determine which values are more reliable. Further studies will be necessary before even tentative values can be nominated. All the available data for the solubility of chloroethane (1) in water (2) are summarized in Table 1.

TABLE 1. Reported solubility of chloroethane (1) in water (2)

Temperature		Solubility		
°C	K	100 w_1	10^3 x_1	References
0	273.15	0.445	1.25	1
		0.45	1.26	2
10.3	283.45	0.9087	2.554	3
12.5	285.65	0.570	1.60	4
17.5	290.65	0.9256	2.602	3
20	293.15	0.749	2.10	5
		0.57	1.60	6
24.8	297.95	0.9195	2.585	3
25	298.15	0.671	1.88	5
30	303.15	0.661	1.85	5
		0.632	1.77	7
34.6	307.75	0.9176	2.580	3
40	313.15	0.573	1.61	5

Part 2. Only the datum of Jenkin and Shorthose[8] is available for the solubility of water (2) in chloroethane (1) at 284.15 K; therefore, no critical evaluation is possible. Further studies are required before any value can be recommended.

References

[1] A. E. van Arkel and S. E. Vles, Recl. Trans. Chim. Pays-Bas **55**, 407 (1936).

[2] E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

[3] J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

[4] H. Fühner, Ber. **57**, 510 (1924).

[5] M. Nicloux and L. Scotti-Foglieni, Ann. Physiol. Physicochem. Biol. **5**, 434 (1929).

[6] du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon Compounds,'' Tech. Bull. B-7, Wilmington, Del. (1966), 16 pp.

[7] L. Scotti-Foglieni, C. R. Soc. Biol. **105**, 959 (1930).

[8] C. F. Jenkin and D. N. Shorthose, ''The Thermal Properties of Ethyl Chloride,'' Food Investigation Board, Spec. Rept. No. 14, HMSO, London (1923), 35 pp.

Components:	**Original Measurements:**
(1) Water; H_2O; [7732-18-5] (2) Chloroethane; C_2H_5Cl; [75-00-3]	C. F. Jenkin and D. N. Shorthose, ''The Thermal Properties of Ethyl Chloride,'' Food Investigation Board, Spec. Rept. No. 14, HMSO, London (1923), 35 pp.
Variables:	**Prepared By:**
T/K=284	A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
11	0.2	7.12	1.1×10^{-2}

Auxiliary Information

Method/Apparatus/Procedure:

Chloroethane was saturated with water by evaporating it and mixing its vapor with steam and condensing the mixture. The condensate in a closed vessel was mixed and allowed to stand until the two layers became quite clear. Samples were taken from the saturated chloroethane layer and a weighed amount distilled through tubes containing $CaCl_2$ and P_2O_5 . The amount of water trapped in the drying tubes gave the water solubility in chloroethane.

Source and Purity of Materials:

(1) Distilled (compiler).

(2) Prepared at the National Physical Laboratory; purity not given.

Estimated Errors:

Solubility: Not specified.

Temperature: ±1 K (compiler).

Components:	**Original Measurements:**
(1) Chloroethane; C_2H_5Cl; [75-00-3] (2) Water; H_2O; [7732-18-5]	H. Fühner, Ber. **57**, 510 (1924).
Variables:	**Prepared By:**
T/K=286	A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
12.5	0.570	1.60	8.83×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Chloroethane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the chloroethane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:	**Original Measurements:**
(1) Chloroethane; C_2H_5Cl; [75-00-3] (2) Water; H_2O; [7732-18-5]	M. Nicloux and L. Scotti-Foglieni, Ann. Physiol. Physicochim. Biol. **5**, 434 (1929).
Variables:	**Prepared By:**
T/K=293–313	A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	2.12	0.749	2.10
25	1.62	0.671	1.88
30	1.37	0.661	1.85
40	0.89	0.573	1.61

Auxiliary Information

Method/Apparatus/Procedure:

An all glass apparatus which consisted of a liquid container with a mechanical stirrer and a gas storage tube was used for measurements. Water was saturated with gaseous chloroethane at a pressure of 750 mm Hg. The absorbed gas volume was calculated from the initial dry gas and final solvent vapor saturated gas volume. The amount of solvent was determined by measuring the displacement of a mercury mass.

Source and Purity of Materials:

(1) Laboratory reagent, source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Chloroethane; C_2H_5Cl; [75-00-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

L. Scotti-Foglieni, CR Soc. Biol. **105**, 959 (1930).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
30	1.31	0.632	1.77

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±1 K.

Components:

(1) Chloroethane; C_2H_5Cl; [75-00-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=273

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	0.447	0.445	1.25

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) Chloroethane; C_2H_5Cl; [75-00-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
E. W. McGovern, Ind. Eng. Chem. **35**, 1230 (1943).

Variables:
T/K=273

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	0.45	1.26	6.97×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available.

Source and Purity of Materials:
(1) Commercial grade, source not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±1 K (compiler).

Components:
(1) Chloroethane; C_2H_5Cl; [75-00-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
du Pont de Nemours & Company, ''Solubility Relationship of the Freon Fluorocarbon Compounds,'' Tech. Bull. B-7, Wilmington, Del. (1966), 16 pp.

Variables:
T/K=293

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	0.57	1.60	8.83×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:
Details are not available. The original report is not obtainable; therefore, the solubility data were taken from a secondary source.[1]

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ±1 K (compiler).

References:

[1] P. A. Sanders, *Handbook of Aerosol Technology*, 2nd ed. (Van Nostrand Reinhold, New York, 1979), p. 42.

Components:
(1) Chloroethane; C_2H_5Cl; [75-00-3]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
J. M. Gossett, Environ. Sci. Technol. **21**, 202 (1987).

Variables:
T/K=283–308

Prepared By:
A. L. Horvath

Experimental Data

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	CV[a] %	100 w_1 (compiler)	10^3 x_1 (compiler)
10.3	6.51×10^{-3}	3.90	0.9087	2.554
17.5	8.46×10^{-3}	3.62	0.9256	2.602
24.8	1.11×10^{-2}	5.84	0.9195	2.585
34.6	1.55×10^{-2}	4.44	0.9176	2.580

[a] CV=coefficient of variation (=100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:
A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of chloroethane was injected into serum bottles which contained distilled water. The bottles were incubated for 18–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.3%.

Source and Purity of Materials:
(1) Supelco Inc., GC standard reagent, 0.2 mg/cm^3 in methanol.
(2) Distilled.

Estimated Errors:
Solubility: See above.
Temperature: ±0.1 K.

Components:
(1) Iodoethane; C_2H_5I; [75-03-6]
(2) Water; H_2O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K., June 1993.

77. Iodoethane with Water

Critical Evaluation

The solubility of iodoethane (1) in water (2) has been studied by four groups of workers; however, the solubility of water (2) in iodoethane (1) has not yet been investigated.

All the experimental data of Rex,[1] Fühner,[2] Gross and Saylor,[3] and van Arkel and Vles[4] are in reasonable agreement at 303.15 K. However, the temperature dependence of the solubility in the temperature range from 273 to 303 K was studied only by Rex.[1] There are no comparable data for the solubility of iodoethane in water above and below 303 K. In the absence of other independent measurements, no critical evaluation is possible.

The reported solubilities[1–4] were smoothed by least squares analysis to obtain the following mass percent (1) equation:

$$\text{Solubility}\ [100\ w_1]=8.5757-5.5568\times10^{-2}\ (T/\text{K})+9.43918\times10^{-5}(T/\text{K})^2,$$

which shows a standard deviation of 6.048×10^{-3} over the range of temperatures involved. The tentative values for this system are given in Table 1 as smoothed weight percent at 5 K intervals. Additional measurements are required to produce more reliable solubility data.

TABLE 1. Tentative solubility of iodoethane (1) in water (2)

Temperature		Solubility	
°C	K	100 w_1	10^4 x_1
0	273.15	0.440	5.10
5	278.15	0.422	4.89
10	283.15	0.409	4.74
15	288.15	0.401	4.65
20	293.15	0.398	4.61
25	298.15	0.400	4.64
30	303.15	0.405	4.70

References:

[1] A. Rex, Z. Phys. Chem. **55**, 355 (1906).
[2] H. Fühner, Ber. **57**, 510 (1926).
[3] P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).
[4] A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Components:
(1) Iodoethane; C_2H_5I; [75-03-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
A. Rex, Z. Phys. Chem. **55**, 355 (1906).

Variables:
T/K=273–303

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	0.441	0.439	5.09
10	0.414	0.412	4.78
20	0.403	0.401	4.65
30	0.415	0.413	4.79

Auxiliary Information

Method/Apparatus/Procedure:

The solubility of iodoethane in water was determined using specially designed flasks with calibrated capillary cylinders. After the samples were equilibrated in a thermostatic bath at the desired temperature, their volumes and the weights were determined and the solubility calculated.

Source and Purity of Materials:

(1) Kahlbaum, redistilled and washed before use, b.p.=72.3 °C.
(2) Distilled.

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:
(1) Iodoethane; C_2H_5I; [75-03-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:
H. Führer, Ber. **57**, 510 (1924).

Variables:
T/K=296

Prepared By:
A. L. Horvath

Experimental Data

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
22.5	0.391	4.53	2.51×10^{-3}

Auxiliary Information

Method/Apparatus/Procedure:

Iodoethane was added gradually from a pipette to 100 cm^3 water in a sample container with continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of the iodoethane added to a known quantity of water present.

Source and Purity of Materials:

(1) E. Merck, Darmstadt, further pruified before use.
(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

Components:

(1) Iodoethane; C_2H_5I; [75-03-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

P. M. Gross and J. H. Saylor, J. Am. Chem. Soc. **53**, 1744 (1931).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 g_1 /g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
30	4.04	0.402	4.66

Auxiliary Information

Method/Apparatus/Procedure:

An excess of iodoethane in 500 g water was shaken for 12 h in a water bath thermostat. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss.[1] A detailed description of the complete procedure is given in a Ph. D. thesis.[2]

Source and Purity of Materials:

(1) Eastman Kodak Co., purified by fractional distillation before use.
(2) Distilled.

Estimated Errors:

Solubility: ±0.5%.
Temperature: ±0.02 K.

References:

[1] P. M. Gross, J. Am. Chem. Soc. **51**, 2362 (1929).

[2] J. H. Saylor, Ph. D. thesis, Duke University, Durham, 1930.

Components:

(1) Iodoethane; C_2H_5I; [75-03-6]
(2) Water; H_2O; [7732-18-5]

Original Measurements:

A. E. van Arkel and S. E. Vles, Recl. Trav. Chim. Pays-Bas **55**, 407 (1936).

Variables:

T/K=303

Prepared By:

A. L. Horvath

Experimental Data

t/°C	100 $n_1 g_2^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	2.59×10^{-3}	0.402	4.66

Auxiliary Information

Method/Apparatus/Procedure:

Details are not available.

Source and Purity of Materials:

(1) Source and purity not given.

(2) Distilled (compiler).

Estimated Errors:

Solubility: not specified.
Temperature: ±0.5 K (compiler).

78. System Index

Page numbers preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables. Substances are listed as in the Chemical Abstracts.

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Acetylene tetrabromide (see ethane, 1,1,2,2-tetrabromo-)
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sym-Dichloroethylene (see ethene, cis-1,2-dichloro-)
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