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
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. © 1999 American Institute of Physics and American Chemical Society.

Key words: aqueous solutions; halogenated ethanes; halogenated ethenes; solubility.

Contents

1. Preface .................................................. 397
1.1. References to the Preface .............................. 400

2. Introduction to the Solubility Data Series.
   Solubility of Liquids in Liquids ...................... 401
   2.1. The Nature of the Project ........................... 401
   2.2. Compilations and Evaluations ..................... 401

2.2.1. Compilations ...................................... 401
2.2.2. Evaluations ...................................... 402

2.3. Quantities and Units Used in Compilations
   and Evaluation of Solubility Data .................... 403
   2.3.1. Mixtures, Solutions and Solubilities .......... 403
   2.3.2. Physicochemical Quantities and
          Units ............................................ 403
   2.4. References for the Introduction ................ 402

3. Halogenated Ethanes and Ethenes Solubilities ...... 406
   4. 1,2-Dibromo-1,1,2,2-Tetrafluoroethane with
       Water .............................................. 406
   5. 1,1,2-Trichloro-1,2,2-Trifluoroethane with
       Water .............................................. 406

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邮寄地址：getzen@chemdept.chem.ncsu.edu

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0047-2669/99/28(2)/395233/$10.00 395

| 6. | 1,1,2-Trichloro-1,2,2-Trifluoroethane with Sodium Chloride and Water. | 410 |
| 7. | Tetrachloroethene with Water*. | 411 |
| 8. | Tetrachloroethene with MQ-Water. | 427 |
| 9. | Tetrachloroethene with Municipal Tap Water (PASE). | 428 |
| 10. | Tetrachloroethene with Ammonium Carbonate and Water. | 428 |
| 11. | Tetrachloroethene with Hydrogen Chloride and Water. | 429 |
| 12. | Tetrachloroethene with Hydrogen Chloride, Sodium Chloride, and Water. | 429 |
| 13. | Tetrachloroethene with Nitric Acid, Ammonium Nitrate, and Water. | 430 |
| 14. | Tetrachloroethene with Phosphoric Acid, Sulfuric Acid, and Water. | 430 |
| 15. | Tetrachloroethene with Sodium Chloride and Water. | 431 |
| 16. | Tetrachloroethene with Sulfuric Acid and Water. | 431 |
| 17. | Tetrachloroethene with Sulfuric Acid, Ammonium Sulfate and Water. | 432 |
| 18. | 1,1,2,2,2-Tetrachloro-1,2-Difluoroethane and Water. | 432 |
| 19. | Hexachloroethane and Water*. | 433 |
| 20. | 2-Bromo-2-Chloro-1,1,1-Trifluoroethane with Water. | 437 |
| 21. | 2,2-Dichloro-1,1,1-Trifluoroethane with Water*. | 446 |
| 22. | Trichloroethene with Water*. | 448 |
| 23. | Trichloroethene with MQ-Water. | 470 |
| 24. | Trichloroethene with Municipal Tap Water (PASE). | 471 |
| 25. | Trichloroethene with Water-d₂. | 471 |
| 26. | Pentachloroethene with Water*. | 472 |
| 27. | Pentachloroethene with Water-d₂. | 477 |
| 28. | 1,2-Dibromo-1,2-Dichloroethane with Water. | 478 |
| 29. | 1,1,2,2-Tetrabromoethane with Water*. | 478 |
| 30. | 1,1,2,2-Tetrabromoethane with Water-d₂. | 482 |
| 31. | 1,1-Dichloroethene with Water*. | 482 |
| 32. | cis-1,2-Dichloroethene with Water*. | 490 |
| 33. | trans-1,2-Dichloroethene with Water*. | 494 |
| 34. | 1,2-Dichloro-1,1-Difluoroethane with Water. | 498 |
| 35. | 1,1,1,1,2,2-Tetrachloroethane with Water*. | 498 |
| 36. | 1,1,2,2-Tetrachloroethene with Water*. | 502 |
| 37. | 1,1,2,2-Tetrachloroethene with Water-d₂. | 518 |
| 38. | cis 1,2 Diiodoethene with Water. | 518 |
| 39. | trans-1,2-Diiodoethene with Water. | 519 |
| 40. | 1,2-Dibromo-1-Chloroethane with Water. | 519 |
| 41. | 1,1,2,2-Trichloroethene with Water. | 520 |
| 42. | 1,1-Dichloro-1-Fluoroethene with Water. | 520 |
| 43. | 1,1-Trichloroethene with Water*. | 521 |
| 44. | 1,1,1-Trichloroethene with MQ-Water. | 536 |
| 45. | 1,1,1-Trichloroethene with Municipal Tap Water (PASE). | 537 |
| 46. | 1,1,1-Trichloroethene with Seawater. | 537 |
| 47. | 1,1,2-Trichloroethene with Water*. | 538 |
| 48. | 1-Bromo-2-Chloroethene with Water*. | 549 |
| 49. | 1,2-Dibromoethene with Water*. | 551 |

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**List of Figures**

1. Logarithm of saturated molarity vs solute molar volume at 25 °C for halogenated methanes in water.  
2. Solubility of tetrachloroethene (1) in water (2).

*Note: an asterisk (*) indicates presence of a Critical Evaluation*
3. Solubility of water (2) in tetrachloroethene (1)...
4. Solubility of 2-bromo-2-chloro-1,1,1-
   trifluoroethane (1) in water (2)...
5. Solubility of trichloroethene (1) in water (2)...
6. Solubility of water (2) in trichloroethene (1)...
7. Solubility of 1,1-dichloroethene (1) in water (2)...
8. Solubility of cis-1,2-dichloroethene (1) in water (2)...
9. Solubility of trans-1,2-dichloroethene (1) in water (2)...
10. Solubility of 1,1,2-tetrachloroethene (1) in water (2)...
11. Solubility of 1,1,2,2-tetrachloroethane (1) in water (2)...
12. Solubility of water (2) in 1,1,2,2-tetrachloroethane (1); log $x_2$ vs 1000/(TK)
13. Solubility of 1,1,1-trichloroethane (1) in water (2)...
14. Solubility of water (2) in 1,1,1-trichloroethane (1); log $x_2$ vs 1000/(TK)
15. Solubility of 1,1,1-trichloroethane (1) in water (2)...
16. Solubility of water (1) in 1,1,2-trichloroethane; log $x_2$ vs 1000/(TK)
17. Solubility of 1,2-dibromoethane (1) in water (2)...
18. Solubility of water (2) in 1,2-dibromoethane (1); log $x_2$ vs 1000/(TK)
19. Solubility of 1,1-dichloroethane (1) in water (2)...
20. Solubility of water (2) in 1,1-dichloroethane (1); log $x_2$ vs 1000/(TK)
21. Solubility of 1,2-dichloroethane (1) in water (2)...
22. Solubility of water (2) in 1,2-dichloroethane (1); log $x_2$ vs 1000/(TK)

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;
(b) Secondary sources (books, reviews);
(c) Databases (computer softwares);
(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 TRC\(^2\) 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.

The solubility of carbon tetrachloride (CCl₄) in water (H₂O) is 0.10 cm³/100 cm³ water at 25 °C. The solubility in mass percent (g CCl₄/100 g soln.) is required. The density of pure carbon tetrachloride is 1.5834 g CCl₄/cm³ 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

\[ g \text{ CCl}_4/100 \text{ g H}_2\text{O} \approx g \text{ CCl}_4/100 \text{ g soln}. \]

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 (CH₂Cl₂) is 2.363 g/100 g water at 0 °C. The solubility in g CH₂Cl₂/100 g soln. at the same temperature is required. If 100 g water dissolves 2.363 g CH₂Cl₂, then the total mass of the solution becomes 102.363 g. This means that 100 g aqueous solution will dissolve less CH₂Cl₂ than 100 g pure water, that is

\[ 2.363 \text{ g CH}_2\text{Cl}_2 \text{/102.363 g soln.} = 2.3084 \text{ g CH}_2\text{Cl}_2/100 \text{ g soln.}. \]

The result is 2.3084 g CH₂Cl₂/100 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 CCl₄ in 100 g water or 100 g aqueous solution at 25 °C.

All critical evaluations of the solubility data are presented in 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 weight-
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 ($\Delta_{\text{solute}}H^\circ$). 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 ($\Delta_{\text{solute}}C_p^\circ$) is required for the calculation of the minimum solubility temperature ($T_{\text{min}}$):

$$T_{\text{min}} = 298.15 \text{ K} - \frac{\Delta_{\text{solute}}H^\circ}{\Delta_{\text{solute}}C_p^\circ} \times 298.15 \text{ K}.$$

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 relationship 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:

$$\log(S/\text{mole/dm}^3) = 1.8995 - 4.3707 \times 10^{-2}(V_m/\text{cm}^3/\text{mole})^1.$$

1.1. References for the Preface

2. TRCVP, Thermodynamic Research Center, Texas A & M University System, College Station, TX (1989).
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 of 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 or 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 system and the choice of formula is governed by what is usual for most current users: i.e., IUPAC for inorganic compounds, and Hill system for organic compounds. Components are ordered on a given compilation sheet according to:

(a) saturating components;
(b) non-saturating components in alphabetical order;
(c) solvents in alphabetical order.

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

- 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:

(d) 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:

- \( \text{C}_2\text{H}_8 \): cyclopentane
- 2-methyl-1,3-butadiene
- 1,4-pentadiene
- 1-pentyne

- \( \text{C}_3\text{H}_{10} \): cyclohexane
- 3-methyl-1-butene
- 2-methyl-2-butene
- 1-pentene
- 2-pentene

- \( \text{C}_4\text{H}_{12} \): 2,2-dimethylpropane
- 2-methylbutane
- pentane

- \( \text{C}_5\text{H}_{12} \): 2,2-dimethyl-1-propanol
- 2-methyl-1-butanol
- 2-methyl-2-butanol
- 3-methyl-1-butanol
- 3-methyl-2-butanol
- 1-pentanol
- 2-pentanol
- 3-pentanol

- \( \text{C}_6\text{H}_{12} \): cyclohexanol
- 4-methyl-1-penten-3-ol
- 1-hexen-3-ol
- 4-hexen-3-ol

Deuterated \(^{2}\text{H}\) compounds follow immediately the corresponding \(\text{H}\) 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 indicates the publication used for compilation of the data.

Variables

Ranges of temperature, pressure, etc., are indicated here.
Prepared by

The names of all compilers are given here.

Experimental Values

Components are described as (1), (2), etc., as defined in
the "Components" box. Data are reported in the units used
in the original publication, with the exception that modern
names for units and quantities are used; e.g., mass 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. Temperatures are expressed as °C,
°F or °K as in the original; if necessary, conversions to
°K are made, sometimes in the compilations, and always in
the critical evaluation. However, the author's units are ex-
pressed according to IUPAC recommendations 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 re-
ported 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 tem-
perature 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 de-
duced 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. Ab-
reviations 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 fol-
lowing information (in this order and an abbreviated form) is
provided if available in the original paper: source and spec-
ified 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
events 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 omit-
ted. 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 rec-
ommend "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.

Evaluatof

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, esti-
mates errors where necessary, and recommends numerical
values based on all the published data (including theses, re-
ports 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 corre-
sponding compilations may be removed.

The solubility of comparatively few systems is known
with sufficient accuracy to enable a set of recommended val-
ues to be presented. Although many systems have been stud-
ied 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 sufficiently unreliable but estimated that it should cause only minimal 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 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 solute, 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 from 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*\(^2\) 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 \(x_1\) (1 condensed phases), \(y_1\) (gases):

\[
x_1 = \frac{n_1}{\sum_{i=1}^{c} n_i}
\]

where \(n_i\) is the amount of substance of \(i\), 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 \(v_{i+}\) cations and \(v_{i-}\) anions, with \(u_i = v_{i+} + v_{i-}\) and a mixture of \(p\) nonelectrolytes \(j\), of which some may be solvent components, a generalization of the definition in Ref. 11 gives

\[
x_{i+} = \frac{u_{i+} x_{i+}}{\sum_{i=1}^{s} (u_i - 1) x_i}, \quad x_{i-} = \frac{u_{i-} x_{i-}}{u_{i+}} \quad i = 1...s
\]

\[
1 + \sum_{i=1}^{s} (u_i - 1) x_i
\]

---

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

<table>
<thead>
<tr>
<th>( x_i )</th>
<th>( w_i )</th>
<th>( m_i )</th>
<th>( c_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_i = )</td>
<td>( x_i )</td>
<td>( 1 + \frac{M_i}{M_c} \left( \frac{1}{w_i} - 1 + \sum_{j=1}^{c-1} \frac{M_j}{M_i} \right) \frac{w_i}{w_i} )</td>
<td>( 1 + \frac{1}{m_i} \sum_{j=1}^{c-1} m_j )</td>
</tr>
<tr>
<td>( w_i = )</td>
<td>( 1 + \frac{M_c}{M_i} \left( \frac{1}{w_i} - 1 - \sum_{j=1}^{c-1} \frac{M_j}{M_c} \right) \frac{x_i}{x_i} )</td>
<td>( w_i )</td>
<td>( 1 + \frac{1}{m_i} \sum_{j=1}^{c-1} m_j )</td>
</tr>
<tr>
<td>( m_i = )</td>
<td>( M_c \left( \frac{1}{w_i} - 1 - \sum_{j=1}^{c-1} \frac{w_j}{w_i} \right) )</td>
<td>( M_i \left( \frac{1}{w_i} - 1 - \sum_{j=1}^{c-1} \frac{w_j}{w_i} \right) )</td>
<td>( m_i )</td>
</tr>
<tr>
<td>( c_i = )</td>
<td>( \frac{\rho}{M_i + M_c \left( \frac{1}{w_i} - 1 - \sum_{j=1}^{c-1} \frac{w_j}{w_i} \right)} )</td>
<td>( \frac{\rho w_i}{M_i} )</td>
<td>( \frac{1}{m_i} \left( \frac{1}{\sum_{j=1}^{c-1} m_j} \right) - \frac{M_i}{M_c} )</td>
</tr>
</tbody>
</table>

5. Aquamolality, Solvomolality of substance 1 in a mixed solvent with components, 2, 3, \( m_1(3) \):

\[
m_1(3) = m_1 M_2/M_3
\]

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

\[
\bar{M} = x_2 M_2 + (1-x_2) M_3
\]

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 their mixtures.

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

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

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 \( \rho_1 \): base units: kg m\(^{-3}\).

\[
\rho_1 = g_1 / V
\]

8. Mole ratio, \( r_{AB} \) (dimensionless)\(^{10}\)

\[
r_{AB} = n_1 / n_2
\]

Mass ratio, symbol \( \xi_{AB} \), 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, \( \rho \):

\[
\rho = g / V
\]

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 the volume.

**2.4. References for the Introduction**


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


Section 2 was written by:
A. F. M. Barton
Perth, WA, Australia
P. W. Greven
Raleigh, NC, USA
G. T. Hetter
December, 1993
Perth, WA, Australia
D. G. Shaw
Fairbanks, AK, USA
3. Halogenated Ethanes and Ethenes in Water

Components:
1. 1,2-Dichloro-1,2,2-trifluoroethane, C₂ClF₃
2. Water, H₂O

Original Measurements:

Prepared By:
A. L. Borvath

4.1,2-Dibromo-1,1,2,2-Tetrafluoroethane with Water

Experimental Data

<table>
<thead>
<tr>
<th>°C</th>
<th>1000w₁ (10⁻⁵)</th>
<th>1000w₁M⁻¹mol⁻¹g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>3.0X10⁻⁴</td>
<td>4.33</td>
</tr>
</tbody>
</table>

Auxiliary Information:

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

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

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

References:

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 was 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-trifluoroethane (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 table immediately following this Critical Evaluation. The data at 298.15 K are in good agreement except that of du Pont,² which are markedly higher than other results. It may be assumed that the data in water in the same laboratories with similar methods and accuracy as at 298.15 K are also rejected. Consequently, the higher value is rejected. The remaining three values at 298.15 K show a good agreement.

Part 2. The solubility of water (2) in 1,1,2-trichloro-1,2,2-trifluoroethane (1) was reported in three references.³ It may be assumed that the data reported in the du Pont bulletin were produced in the same laboratories with similar methods and accuracy as at 298.15 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 298.15 K of du Pont² and Baquias³ compare favorably and are classified as Tentative in Table 2.

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

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>K</th>
<th>1000w₁</th>
<th>Solubility</th>
<th>10²w₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>298.15</td>
<td></td>
<td>0.017</td>
<td>1.63</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>K</th>
<th>1000w₁</th>
<th>Solubility</th>
<th>10²w₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>298.15</td>
<td></td>
<td>0.009</td>
<td>9.35</td>
<td></td>
</tr>
</tbody>
</table>

References:
### Components:
(1) 1,1,2-trichloro-1,2,2-trifluoroethane; C₃Cl₃F₃; [76-13-1]
(2) Water; H₂O; [7732-11-5]

### Original Measurements:

### Variables:

**Initial Data**

<table>
<thead>
<tr>
<th>T(°C)</th>
<th>w₁</th>
<th>10^3 x₁ (compiler)</th>
<th>10^3 x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.7×10⁻²</td>
<td>1.63</td>
<td>1.1×10⁻²</td>
</tr>
</tbody>
</table>

**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.

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

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

**References:**
### Experimental Data

<table>
<thead>
<tr>
<th>$t/{}^\circ C$</th>
<th>100$m_1$</th>
<th>100$m_2$</th>
<th>100$m_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>21.1</td>
<td>1.7×10^{-2}</td>
<td>1.63</td>
<td>9.0×10^{-3}</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
- A calibrated bottle was filled with nitrogen, 1 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-trichloro-2,2-difluoroethane was detected by means of a nitrogen-15 electron capture detector.

**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; C₂Cl₃F₆; [76-13-1]
(2) Water: H₂O; [7732-18-5]

Original Measurements:
G. W. Helmersen, E. R. Jacobs, and R. F. Boehm, Report
DGC-1549-4, University of Utah, Salt Lake City, Utah
(December, 1976), 9 pp.

Variables:
T/K = 303.15–383 and P/atm = 0.5–1.1

Prepared By:
A. L. Horvah

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>p₁/atm</th>
<th>S/ppm atm⁻¹</th>
<th>10⁶w₁ (compiler)</th>
<th>10⁹e₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.0</td>
<td>4.536</td>
<td>37.8</td>
<td>2.178×10⁻⁵</td>
<td>2.094</td>
</tr>
<tr>
<td>34.2</td>
<td>0.629</td>
<td>248.5</td>
<td>2.485×10⁻³</td>
<td>2.390</td>
</tr>
<tr>
<td>57.5</td>
<td>1.374</td>
<td>291.1</td>
<td>2.911×10⁻³</td>
<td>2.800</td>
</tr>
<tr>
<td>75.0</td>
<td>3.31</td>
<td>302.2</td>
<td>2.023×10⁻⁵</td>
<td>1.944</td>
</tr>
<tr>
<td>90.0</td>
<td>6.347</td>
<td>38.0</td>
<td>3.80×10⁻³</td>
<td>0.3654</td>
</tr>
<tr>
<td>93.2</td>
<td>1.09</td>
<td>106.8</td>
<td>1.068×10⁻²</td>
<td>1.027</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The saturation of 1,1,2-trichloro-1,2,2-trifluoroethane with
water took place in a stirred vessel during 10 days. 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 detection of the
solubility at a given condition was repeated five or six times.

Source and Purity of Materials:
(1) cu Pont samples, purity not given.
(2) Distilled.

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

References:
G. W. Helmersen, Sc. Sc. thesis, University of Utah, Salt Lake

Source and Purity of Materials:
(1) Precisely 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:
1. 1,1,2-trichloro-1,2,2-trifluoroethane; C\textsubscript{3}F\textsubscript{3}Cl \cite{76-13-1}
2. Sodium chloride; NaCl \cite{7647-14-5}
3. Water; H\textsubscript{2}O \cite{7732-18-5}

### Original Measurements:

### Variables:
T/K = 298–368 and P/atm = 0.4–1.3

### Prepared By:
A. L. Horvath

### 5. 1,1,2-Trichloro-1,2,2-Trifluoroethane with Sodium Chloride and Water

#### Experimental Data
Solubility of C\textsubscript{3}F\textsubscript{3}Cl\textsubscript{3} in 2.5 mass % NaCl solution

<table>
<thead>
<tr>
<th>T/°C</th>
<th>p\textsubscript{1} / atm</th>
<th>S/ ppm atm\textsuperscript{-1}</th>
<th>100w\textsubscript{1} (compiler)</th>
<th>10\textsuperscript{2}x\textsubscript{1} (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.0</td>
<td>0.403</td>
<td>45.5</td>
<td>1.43x10\textsuperscript{-2}</td>
<td>1.406</td>
</tr>
<tr>
<td>24.4</td>
<td>0.430</td>
<td>47.8</td>
<td>1.77x10\textsuperscript{-2}</td>
<td>1.540</td>
</tr>
<tr>
<td>59.5</td>
<td>1.100</td>
<td>70.0</td>
<td>1.70x10\textsuperscript{-2}</td>
<td>1.469</td>
</tr>
<tr>
<td>66.0</td>
<td>1.34</td>
<td>87.8</td>
<td>1.89x10\textsuperscript{-2}</td>
<td>1.554</td>
</tr>
<tr>
<td>93.5</td>
<td>1.04</td>
<td>98.7</td>
<td>1.01x10\textsuperscript{-2}</td>
<td>0.997</td>
</tr>
<tr>
<td>95.2</td>
<td>0.517</td>
<td>17.0</td>
<td>4.90x10\textsuperscript{-3}</td>
<td>0.474</td>
</tr>
</tbody>
</table>

#### 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.\textsuperscript{1}

##### Source and Purity of Materials:
1. Source and purity not given.
2. Source and purity not given.
3. Purified.

##### Estimated Errors:
Solubility: ±3.7% std. dev.
Temperature: ±0.5 K.

##### References:

### Experiment Data
Solubility of C\textsubscript{3}F\textsubscript{3}Cl\textsubscript{3} in 10 mass % NaCl solution

<table>
<thead>
<tr>
<th>T/°C</th>
<th>p\textsubscript{1} / atm</th>
<th>S/ ppm atm\textsuperscript{-1}</th>
<th>100w\textsubscript{1} (compiler)</th>
<th>10\textsuperscript{2}x\textsubscript{1} (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.3</td>
<td>0.49</td>
<td>11.3</td>
<td>1.04x10\textsuperscript{-2}</td>
<td>10.75</td>
</tr>
<tr>
<td>63.8</td>
<td>1.2</td>
<td>984</td>
<td>9.33x10\textsuperscript{-3}</td>
<td>9.658</td>
</tr>
<tr>
<td>67.1</td>
<td>1.8</td>
<td>969</td>
<td>9.21x10\textsuperscript{-3}</td>
<td>9.565</td>
</tr>
<tr>
<td>91.5</td>
<td>1.30</td>
<td>551</td>
<td>5.30x10\textsuperscript{-3}</td>
<td>5.596</td>
</tr>
<tr>
<td>94.2</td>
<td>0.763</td>
<td>354</td>
<td>3.81x10\textsuperscript{-3}</td>
<td>3.956</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

##### 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:
7. Tetrachloroethene with Water

Critical Evaluation

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

Part 1. The solubility of tetrachloroethylene (1) in water (2) has been studied by at least 24 groups of workers as recorded in the compilation. These immediately following the Critical Evaluation.

The experimental data of most investigators is the temperature interval between 273 and 373 K are in very good agreement and in the absence of other independent evidence, 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 Tronov et al.,2 Proszynov et al.,3 Linnefors and Gosney,4 Yonhika et al.,5 and Howe et al.6 are markedly lower than other results and are therefore rejected. The solubility values of Breed et al.,7 Veith et al.,8 Besezneje et al.,9 and Stiegele et al.10 appear significantly higher than the likely solubility and are also rejected.

The remaining data of Wright and Schaffner,11 McCrae,12 Chatwood,13 O’Connell,14 Simonsen et al.,15 McCronan et al.,16 Archer and Stevens,17 Houck et al.,8 Sato and Nakahara,19 Coca and Diaz,20 Leighton and Colb,16 Kratzt,21 Gosney,22 and Ramsey et al.21 covering the temperature interval from 273 to 143 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 exception those mentioned above (Refs. 1–9) from further analysis. Therefore, all the tetrachloroethene in water solubility data (Refs. 20–30), except Refs. 1–9, were combined to obtain the following mass per cent (1) equation:

\[
\text{Solubility} = (100 C_{e}) = 0.36475 - 1.5487 \times 10^{-3} (\mathbf{K}) + 2.4477 \times 10^{-6} (\mathbf{K})^2
\]

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

The curve obtained from the smoothing equation shows a distinct minimum at 316 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 useful values.

---

![Fig. 2. Solubility of tetrachloroethene (1) in water (2).](image-url)
### Table 1. Approximate solubility of tetrachloroethylene (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>$10^4 , \text{cm}^3$</th>
<th>Solubility</th>
<th>$10^5 , \text{cm}^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.2244</td>
<td>2.65</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.2324</td>
<td>2.54</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.2225</td>
<td>2.44</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.2118</td>
<td>2.37</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.2011</td>
<td>2.29</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.2026</td>
<td>2.24</td>
<td></td>
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<tr>
<td>30</td>
<td>303.15</td>
<td>0.2026</td>
<td>2.24</td>
<td></td>
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<tr>
<td>35</td>
<td>308.15</td>
<td>0.2020</td>
<td>2.19</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.1998</td>
<td>2.15</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.1998</td>
<td>2.15</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.1999</td>
<td>2.16</td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>328.15</td>
<td>0.2002</td>
<td>2.19</td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>333.15</td>
<td>0.2005</td>
<td>2.23</td>
<td></td>
</tr>
<tr>
<td>65</td>
<td>338.15</td>
<td>0.2010</td>
<td>2.28</td>
<td></td>
</tr>
<tr>
<td>70</td>
<td>343.15</td>
<td>0.2016</td>
<td>2.35</td>
<td></td>
</tr>
</tbody>
</table>

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

### Table 2. Recommended solubility of water (2) in tetrachloroethylene (1)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>$10^4 , \text{cm}^3$</th>
<th>Solubility</th>
<th>$10^5 , \text{cm}^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>280.15</td>
<td>0.005684</td>
<td>1.425</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>285.15</td>
<td>0.005726</td>
<td>1.566</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>290.15</td>
<td>0.005756</td>
<td>1.668</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>295.15</td>
<td>0.005811</td>
<td>1.775</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>300.15</td>
<td>0.005913</td>
<td>1.894</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>305.15</td>
<td>0.005913</td>
<td>1.894</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>310.15</td>
<td>0.005913</td>
<td>1.894</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>315.15</td>
<td>0.005913</td>
<td>1.894</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>320.15</td>
<td>0.005913</td>
<td>1.894</td>
<td></td>
</tr>
</tbody>
</table>

### References
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Volume (cm³)</th>
<th>100 w</th>
<th>10² x</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>6.50x10⁻³</td>
<td>3.91x10⁻³</td>
<td>3.66</td>
</tr>
<tr>
<td>20</td>
<td>8.45x10⁻³</td>
<td>5.21x10⁻³</td>
<td>5.79</td>
</tr>
<tr>
<td>25</td>
<td>1.08x10⁻²</td>
<td>6.69x10⁻³</td>
<td>5.15</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
A mixture of water and tetrachloroethylene of about 1 to 5 volume ratio was placed in a sample vessel and heated in a thermostate for 2 h. After the equilibrium attained, samples were taken and filtered through cotton wool. The determination of the water content was based upon the reaction with m-nitrophenylhydroxylamine. The evolved HCl gas was absorbed in weak and titrated with NaOH solution. Two to three successive determinations were carried out with the sample.

**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:**
**Components:**
(1) Tetrachloroethylene (tetrachloroethylene); C₂Cl₄, [127-18-4]
(2) Water; H₂O; [7732-18-5]

**Original Measurements:**
(2) Water; H₂O; [7732-18-5]

**Variables:**
T/K = 273−343

**Prepared By:**
A. L. Horvath

---

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w₁ (compiler)</th>
<th>10⁷ x₁ (compiler)</th>
<th>10⁵ x₂ (compiler)</th>
<th>10⁶ x₃ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.64 x 10⁻²</td>
<td>1.56</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>10</td>
<td>1.46 x 10⁻²</td>
<td>1.59</td>
<td>53 x 10⁻³</td>
<td>4.88</td>
</tr>
<tr>
<td>20</td>
<td>1.88 x 10⁻²</td>
<td>1.61</td>
<td>75 x 10⁻³</td>
<td>6.90</td>
</tr>
<tr>
<td>25</td>
<td>1.50 x 10⁻²</td>
<td>1.63</td>
<td>105 x 10⁻³</td>
<td>9.66</td>
</tr>
<tr>
<td>30</td>
<td>1.55 x 10⁻²</td>
<td>1.68</td>
<td>11 x 10⁻³</td>
<td>10.1</td>
</tr>
<tr>
<td>40</td>
<td>1.67 x 10⁻³</td>
<td>1.81</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>50</td>
<td>2.05 x 10⁻³</td>
<td>2.23</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>70</td>
<td>2.0 x 10⁻³</td>
<td>2.61</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

Solubility data as a function of temperature were presented is 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: ±0.5 K (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 $w_1$ (compiler)</th>
<th>$10^5 x_1$ (compiler)</th>
<th>100 $w_1M_r^{1/2}$/mol g$^{-1}$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.5 $\times$ 10$^{-2}$</td>
<td>1.63</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>1.04 $\times$ 10$^{-2}$</td>
<td>9.56</td>
<td>5.77 $\times$ 10$^{-4}$</td>
</tr>
<tr>
<td>50</td>
<td>2.82 $\times$ 10$^{-2}$</td>
<td>25.80</td>
<td>1.56 $\times$ 10$^{-4}$</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Source and Purity of Materials:**
- (1) Distilled (compiler).
- (2) Not specified.
- Temperature: ± 0.5 K (compiler).

**Estimated Errors:**
- Solubility: not specified.
- Temperature: ± 0.5 K (compiler).

**References:**
### Components:
(1) Water: H₂O; [7732-18-5]
(2) Tetrachloroethylene (tetrachlorehylene): C₂Cl₄; [127-18-4]

### Original Measurements:

### Variables:
77K= 289–302

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Aleskev</th>
<th>10⁶ w₁ Fischer</th>
<th>Spectroscopy</th>
<th>Aleskev</th>
<th>10⁶ x Fischer</th>
<th>Spectroscopy</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>5.70</td>
<td>5.73</td>
<td>5.5</td>
<td>5.244</td>
<td>5.272</td>
<td>5.060</td>
</tr>
<tr>
<td>18</td>
<td>6.35</td>
<td>—</td>
<td>6.0</td>
<td>5.842</td>
<td>—</td>
<td>5.520</td>
</tr>
<tr>
<td>21.3</td>
<td>7.17</td>
<td>—</td>
<td>7.5</td>
<td>6.396</td>
<td>—</td>
<td>6.900</td>
</tr>
<tr>
<td>23</td>
<td>7.91</td>
<td>7.95</td>
<td>7.8</td>
<td>7.296</td>
<td>7.311</td>
<td>7.175</td>
</tr>
<tr>
<td>29</td>
<td>9.37</td>
<td>9.45</td>
<td>—8.618</td>
<td>8.692</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
<th>10⁶ w₂ (compiler)</th>
<th>10⁶ x₂ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>15</td>
<td>7.5×10⁻³</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>18</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>20</td>
<td>8.74×10⁻³</td>
<td>1.50</td>
<td>5.62×10⁻³</td>
<td>5.37</td>
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<tr>
<td>22</td>
<td>—</td>
<td>—</td>
<td>6.91×10⁻³</td>
<td>6.36</td>
</tr>
<tr>
<td>26</td>
<td>1.51×10⁻²</td>
<td>8.41</td>
<td>8.51×10⁻³</td>
<td>7.82</td>
</tr>
</tbody>
</table>

### Auxiliary Information

### Method/Apparatus/Procedure:
The determination of the solubility of water in tetrachloroethylene was based on the infrared spectroscopic method. A LR-20 spectrophotometer was used with 2 cm cuvettes and the windows made of KBr. The spectra were recorded at 0.001–0.01 cm⁻¹, and the absorbance at 3702 cm⁻¹ was found by the baseline method. Standard mixtures of tetrachloroethylene and water were used for the calibration graphs. The results obtained were compared with measurements made by the method of cloud point and a Karl Fischer titration.

### Source and Parity of Materials:
(1) Distilled.
(2) "Chem" brand, treated with Na₂CO₃ solution, dried with CaCl₂ and H₂SO₄ and then distilled before use.

### Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K.

### References:
**Components:**
(1) Tetrachloroethylene \( (\text{tetrachloroethylene}) \ C_2\text{Cl}_4 \); [127-18-4]
(2) Water: \( H_2O \); [7732-18-5]

**Original Measurements:**

**Variables**
\( T/K = 298-373 \)

<table>
<thead>
<tr>
<th>( T/°C )</th>
<th>( D_{v}/\text{cm}^3 \text{g}^{-1} \text{mol} \text{cm}^{-3} \text{sec}^{-1} )</th>
<th>( 100 \times x_1 ) (compiler)</th>
<th>( 10^5 \times x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>( 3.60 \times 10^4 )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>( 1.06 \times 10^5 )</td>
<td>7.29 ( \times 10^{-4} )</td>
<td>7.92</td>
</tr>
<tr>
<td>70</td>
<td>( 4.76 \times 10^5 )</td>
<td>6.91 ( \times 10^{-3} )</td>
<td>7.527 ( \times 10^{-1} )</td>
</tr>
<tr>
<td>90</td>
<td>( 2.37 \times 10^5 )</td>
<td>3.61 ( \times 10^{-2} )</td>
<td>3.921 ( \times 10^{0} )</td>
</tr>
<tr>
<td>100</td>
<td>( 1.70 \times 10^5 )</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

*Gas–liquid system analysis parameter, from calibration measurements.*

**Experimental Data**

\( \log_{10} a = -0.581 \) \( \frac{1}{(T/K)} \)

*where \( a \) = distribution coefficient.*

At the normal boiling point of \( C_2\text{Cl}_4 \), \( a = 58 \) and the activity coefficient, \( \gamma = 273 \).

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The water concentration in tetrachloroethylene \( \text{tch} \) phase was determined by a radiometric method using trichloro 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: \( \pm 1 \) K (compiler).

**References:**
### Components:

- (1) Tetrachloroethylene (tetrachloroethylene): \( \text{C}_2\text{Cl}_4 \); [127-8-4]
- (2) Water, \( \text{H}_2\text{O} \); [7732-1-5]

### Original Measurements:


### Variables:

- \( T/K = 313 \)

### Prepared By:

- A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>( T/K )</th>
<th>( 10^5 ) ( x_1 ) (compiler)</th>
<th>( 100 ) ( w_1 )</th>
<th>( 10^5 ) ( x_2 ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>160</td>
<td>1.66x10^-2</td>
<td>1.66x10^-2</td>
</tr>
</tbody>
</table>

### Auxiliary Information

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

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

### References:

Components: (1) Tetrachloroethane (tetrachloroethylene), C₂Cl₄; [127-11-4]
(2) Water, H₂O; [7732-18-5]

Variables
T/K = 293

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^3 χ₁</th>
<th>10^3 χ₂</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>1.50×10⁻²</td>
<td>1.03</td>
</tr>
<tr>
<td>25</td>
<td>1.5×10⁻⁸</td>
<td>1.63</td>
</tr>
</tbody>
</table>

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

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

Original Measurements:

Components: (1) Tetrachloroethane (tetrachloroethylene), C₂Cl₄; [127-11-4]
(2) Water, H₂O; [7732-18-5]

Variables
T/K = 298

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^3 χ₁</th>
<th>10^3 χ₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.5×10⁻⁸</td>
<td>1.63</td>
</tr>
<tr>
<td>30</td>
<td>1.8×10⁻²</td>
<td>9.20</td>
</tr>
</tbody>
</table>

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. "Data from Dow Chemical USA (October 23, 1975)."

Method/Apparatus/Procedure:
Auxiliary Information

Method/Apparatus/Procedure:
Details are not given.

Auxiliary Information

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) Tetrachloroethylene (tetrachloroethylene); CCl₂; [127-18-4]
(2) Water; H₂O; [7732-18-5]

Variables: 77/K=293

Prepared By: A. L. Horvath

Experimental Data

\[ \begin{array}{cccc}
\theta/\degree C & p_i/\text{kg m}^{-3} & 100 w_i \text{(compiler)} & 10^3 x_i \text{(compiler)} \\
20 & 0.205 & 2.069 \times 10^{-5} & 2.25 \\
\end{array} \]

Auxiliary Information

Solute and Purity of Materials:
(1) Type "pure" (METU 6-00 No. 695-70), redistilled as checked by GLC.
(2) Distilled.

Estimated Errors:
Solubility: ± 1.74%. Temperature: ± 0.3 K.

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).
| Component: | (1) Tetrachloroethylene (tetrachloethylen); C₂Cl₄; [127-18-4] (2) Water; H₂O; [7732-18-5] |
| Preparing By: | A. L. Horvath |
| Temperature: | T/K = 298 |

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10^6 x₁ (compiler)</th>
<th>10⁵ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>400</td>
<td>4.0 × 10⁻⁴</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
A known volume of water was mixed with tetrachloroethylene in an Erlenmeyer flask. The flask was immersed in a water bath and magnetically stirred. Samples were removed for analysis 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 99.9.
(2) Distilled and run through a resin column.

**Estimated Errors:**
Solubility: ±0.5 K

---

| Component: | (1) Tetrachloroethylene (tetrachloethylen); C₂Cl₄; [127-18-4] (2) Water; H₂O; [7732-18-5] |
| Preparing By: | A. L. Horvath |
| Temperature: | T/K = 298 |

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10⁵ x₁ (compiler)</th>
<th>10⁶ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.0 × 10⁻³</td>
<td>2.17</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Sorption was determined by titration. The measurement was performed in an Erlenmeyer flask by adding tetrachloroethylene to water until a permanent turbidity was observed. The flask was immersed in a water bath thermostated 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: (1) Tetrachloromethane (tetrachloroethylene); C₂Cl₄; [127-18-4]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
77K = 293

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>n₁V₂/mól dm⁻³</th>
<th>10⁵ x₁ (compiler)</th>
<th>10⁰ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.66×10⁻³</td>
<td>4.78×10⁻¹</td>
<td>5.19</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of tetrachloromethane was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ¹⁴C activity of the water samples was measured in a liquid scintillation counter by counting 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) Tetrachloromethane (tetrachloroethylene); C₂Cl₄; [127-18-4]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
77K = 298

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10⁻³ x₂ (mól dm⁻³)</th>
<th>10⁰ w₁ (compiler)</th>
<th>10⁰ x₁ (compiler)</th>
</tr>
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<tbody>
<tr>
<td>25</td>
<td>2.92×10⁻²</td>
<td>4.85×10⁻¹</td>
<td>5.27</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of tetrachloromethane was added to a stainless steel tube containing water and then the tube was autoclaved. The equilibrium occurred during stirring 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. lev.
Temperature: ± 0.3 K.
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Distribution-coefficient, $D_2$</th>
<th>$10^3 w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>2.097 x 10³</td>
<td>2.676 x 10⁻²</td>
<td>2.908</td>
</tr>
<tr>
<td>1.2</td>
<td>2.267 x 10³</td>
<td>2.442 x 10⁻²</td>
<td>2.654</td>
</tr>
<tr>
<td>2.5</td>
<td>2.604 x 10³</td>
<td>2.339 x 10⁻²</td>
<td>2.542</td>
</tr>
<tr>
<td>7.0</td>
<td>3.141 x 10³</td>
<td>2.566 x 10⁻²</td>
<td>2.788</td>
</tr>
<tr>
<td>10.0</td>
<td>3.702 x 10³</td>
<td>2.609 x 10⁻²</td>
<td>2.835</td>
</tr>
<tr>
<td>12.0</td>
<td>4.010 x 10³</td>
<td>2.711 x 10⁻²</td>
<td>2.946</td>
</tr>
<tr>
<td>12.9</td>
<td>4.272 x 10³</td>
<td>2.486 x 10⁻²</td>
<td>2.701</td>
</tr>
<tr>
<td>14.0</td>
<td>4.592 x 10³</td>
<td>2.545 x 10⁻²</td>
<td>2.765</td>
</tr>
<tr>
<td>18.0</td>
<td>6.151 x 10³</td>
<td>2.492 x 10⁻²</td>
<td>2.708</td>
</tr>
<tr>
<td>18.0</td>
<td>6.272 x 10³</td>
<td>2.444 x 10⁻²</td>
<td>2.656</td>
</tr>
<tr>
<td>19.0</td>
<td>6.449 x 10³</td>
<td>2.443 x 10⁻²</td>
<td>2.655</td>
</tr>
<tr>
<td>19.2</td>
<td>6.339 x 10³</td>
<td>2.513 x 10⁻²</td>
<td>2.731</td>
</tr>
<tr>
<td>19.5</td>
<td>6.479 x 10³</td>
<td>2.557 x 10⁻²</td>
<td>2.779</td>
</tr>
<tr>
<td>24.3</td>
<td>8.681 x 10³</td>
<td>2.512 x 10⁻²</td>
<td>2.795</td>
</tr>
<tr>
<td>25.2</td>
<td>8.898 x 10³</td>
<td>2.518 x 10⁻²</td>
<td>2.736</td>
</tr>
<tr>
<td>25.3</td>
<td>9.054 x 10³</td>
<td>2.523 x 10⁻²</td>
<td>2.742</td>
</tr>
<tr>
<td>26.0</td>
<td>9.068 x 10³</td>
<td>2.546 x 10⁻²</td>
<td>2.767</td>
</tr>
<tr>
<td>26.0</td>
<td>9.388 x 10³</td>
<td>2.639 x 10⁻²</td>
<td>2.858</td>
</tr>
<tr>
<td>26.1</td>
<td>9.207 x 10³</td>
<td>2.521 x 10⁻²</td>
<td>2.739</td>
</tr>
</tbody>
</table>

*Gas–liquid system analysis parameter, from calibration measurements.

### Auxiliary Information

**Method/Apparatus/Procedure:**
A 5 μL tetrachloroethylene sample was injected into a 2.3 dm³ equilibrium 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 tetrachloroethylene content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

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

**Estimated Errors:**
Solubility: ± 2.3%.
Temperature: ± 0.5 K.
Components:
(1) Tetrachloroethylene (tetrachloroethylene); C₂Cl₄; [127-18-4]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 293

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>ρ₁ /kg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁷ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.400</td>
<td>4.00x10⁻²</td>
<td>4.347</td>
</tr>
</tbody>
</table>

Estimated Errors:
Solubility: not specified.
Temperature: ±1.0 K

Auxiliary Information

Method/Apparatus/Procedure:
An aqueous solution with an excess amount of tetrachloroethylene 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 tetrachloroethylene in water was determined by gas chromatography. The GC was equipped with both a dual flame ionization detector and an electron capture detector.

Henry's law constant, T/m³ atm mol⁻¹

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁ (compiler)</th>
<th>10⁷ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.30x10⁻²</td>
<td>2.37x10⁻²</td>
</tr>
</tbody>
</table>

log H = 2.12 - 5119/T/K

Batch air stripping method

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁ (compiler)</th>
<th>10⁷ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.16x10⁻²</td>
<td>2.66x10⁻²</td>
</tr>
</tbody>
</table>

log H = 2.32 - 4622/T/K

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

Estimated Errors:
Solubility: ±5% - 10%.
Temperature: ±0.1 K.
### Components:
1. Tetrachloroethene (tetrachloroethylene); C₂Cl₄ [127-18-4]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 293

### Prepared By:
- A. L. Hewath

### Experimental Data

<table>
<thead>
<tr>
<th>n°C</th>
<th>Henry's law constant, H/dimensionless</th>
<th>100 w₁ (compiler)</th>
<th>10¹¹ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.691 × 10⁻¹</td>
<td>2.020 × 10⁻²</td>
<td>2.206</td>
</tr>
<tr>
<td>20</td>
<td>5.186 × 10⁻¹</td>
<td>2.203 × 10⁻²</td>
<td>2.534</td>
</tr>
<tr>
<td>30</td>
<td>9.544 × 10⁻¹</td>
<td>2.201 × 10⁻²</td>
<td>2.392</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
- The multiple equilibrium technique with direct aqueous injection into a gas chromatograph was used to determine the solubility. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volumes was maintained constant. Wells vapor samples were injected directly into a gas chromatograph, the liquid samples were concentrated by liquid–liquid extraction before analysis. The experiments were carried out in duplicate.

**Source and Purity of Materials:**
- (1) Nelson Coleman & Bell, O.H.; greater than 99.9% pure.
- (2) Distilled.

**Estimated Errors:**
- Solubility: ± 0.005 std. dev.
- Temperature: ± 0.5 K.

### Experimental Data

<table>
<thead>
<tr>
<th>n°C</th>
<th>10⁴ P₁ (atm)</th>
<th>10⁷ w₁ (compiler)</th>
<th>10¹¹ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.8</td>
<td>1.8 × 10⁻²</td>
<td>156</td>
</tr>
</tbody>
</table>

*Note: Value in the original paper is in error (compiler).*
Experimental Data

<p>| Variables: | 7/R = 298 |</p>
<table>
<thead>
<tr>
<th>CV%</th>
<th>100 w1</th>
<th>10^3 x1</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.6</td>
<td>6.82 x 10^{-3}</td>
<td>3.75</td>
</tr>
<tr>
<td>17.5</td>
<td>1.17 x 10^{-2}</td>
<td>1.28</td>
</tr>
<tr>
<td>24.8</td>
<td>1.77 x 10^{-2}</td>
<td>4.81</td>
</tr>
<tr>
<td>34.6</td>
<td>2.82 x 10^{-2}</td>
<td>1.63</td>
</tr>
</tbody>
</table>

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 several flasks which contained distilled water. The bottles were incubated for 18-24 h at four desired temperatures in a reciprocating water bath. The headspace concentrations of the EPICS bottle 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. J/E Products, ultrapure; greater than 99% pure.
2. Distilled.

Estimated Errors:
Solubility: see above.
Temperature: ± 0.1°C.
### 8. Tetrachloroethene with MQ-Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Henry's law constant, ( H ) (dimensionless)</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10(^2 ) ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 6.04 \times 10^{-4} )</td>
<td>2.12 \times 10^{-1}</td>
<td>2.05</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Source and Purity of Materials:**

1. Methanol (99.95% purity).
2. Other solvents (99.95% purity).

**Estimated Errors:**

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

**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 was introduced into the syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into the gas chromatograph, the liquid samples were preconcentrated by liquid-liquid extraction before analysis. The experiments were carried out in duplicates.
9. Tetrachloroethylene with Municipal Tap Water (PASB)

<table>
<thead>
<tr>
<th>$n^\circ$C</th>
<th>Henry's law constant, $R$\text{dimensionless}</th>
<th>$10^3 x_1$ (compiler)</th>
<th>$10^8 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>$6.73 \times 10^{-1}$</td>
<td>1.91 $\times 10^{-2}$</td>
<td>2072</td>
</tr>
</tbody>
</table>

**Experimental Data**

**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 duplicate.

Source and Purity of Materials: (1) Matheson Coleman & Bell, OH, greater than 99.5% pure. (2) 30 mg total organic carbon/dm$^3$ and 40 mg COD/dm$^3$.

Estimated Errors: Solubility: ± 0.005 std. dev. Temperature: ± 0.5 $^\circ$C.

10. Tetrachloroethylene with Ammonium Carbonate and Water

<table>
<thead>
<tr>
<th>$n^\circ$C</th>
<th>$10^{-3} c_2$ /mol dm$^{-3}$</th>
<th>$10^3 \rho_i$ /g m$^{-3}$</th>
<th>$100 w_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.00</td>
<td>100.0 ± 5.6</td>
<td>9.6 $\times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>1.62</td>
<td>78.8 ± 1.3</td>
<td>7.5 $\times 10^{-3}$</td>
</tr>
<tr>
<td></td>
<td>2.10</td>
<td>77.2 ± 1.8</td>
<td>7.0 $\times 10^{-3}$</td>
</tr>
</tbody>
</table>

**Experimental Data**

**Auxiliary Information**

Method/Apparatus/Procedure: The aqueous electrolyte solutions were saturated with tetrachloroethylene 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 tetrachloroethylene in the aqueous phase was measured by gas chromatography.

Source and Purity of Materials: (1) Type "pure" (MBTU F-00 No. 6590-70), redissolved and checked by GC before use. (2) Type "chemically pure." (3) Distilled.

Estimated Errors: Solubility: see above. Temperature: ± 0.2 $^\circ$C.
11. Tetrachloroethene with Hydrogen Chlorides and Water

<table>
<thead>
<tr>
<th>( T/\degree C )</th>
<th>( 10^{-3} , c_2 , \text{mol dm}^{-3} )</th>
<th>( \rho_1 , /g , \text{m}^{-3} )</th>
<th>( 100 , w_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.20</td>
<td>198.5±6.8</td>
<td>1.98×10^{-2}</td>
</tr>
<tr>
<td>1.6</td>
<td>199.0±6.1</td>
<td>1.95×10^{-2}</td>
<td></td>
</tr>
<tr>
<td>1.6</td>
<td>199.1±12.9</td>
<td>1.93×10^{-2}</td>
<td></td>
</tr>
</tbody>
</table>

Auxiliary Information

**Method/Apparatus/Procedure:**
The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals 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.

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

<table>
<thead>
<tr>
<th>( T/\degree C )</th>
<th>( 10^{-3} , c_2 , \text{mol dm}^{-3} )</th>
<th>( 10^{-3} , c_1 , \text{mol dm}^{-3} )</th>
<th>( \rho_1 , /g , \text{m}^{-3} )</th>
<th>( 100 , w_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.27</td>
<td>0.17</td>
<td>89±1.3</td>
<td>8.4×10^{-3}</td>
</tr>
<tr>
<td>0.96</td>
<td>0.17</td>
<td>85.5±4.7</td>
<td>8.41×10^{-3}</td>
<td></td>
</tr>
<tr>
<td>1.64</td>
<td>0.17</td>
<td>82.5±8.0</td>
<td>8.01×10^{-3}</td>
<td></td>
</tr>
</tbody>
</table>

Auxiliary Information

**Method/Apparatus/Procedure:**
The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks fitted with stirers and a mercury seal. Stirring was continued for several days until equilibrium was established. Samples were taken at specific time intervals 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.
### 13. Tetrachloroethene with Nitric Acid, Ammonium Nitrate, and Water

<table>
<thead>
<tr>
<th>Experimental Data</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
<td>$10^{-3} c_1$/mol dm$^{-3}$</td>
<td>$10^{-3} c_2$/mol dm$^{-3}$</td>
<td>$10^4 p_1$/g m$^{-2}$</td>
<td>$T_0$ $v_1$ (compiler)</td>
</tr>
<tr>
<td>20</td>
<td>0.08</td>
<td>1.25</td>
<td>160.0±3.0</td>
<td>1.58×10$^{-2}$</td>
</tr>
<tr>
<td>2.80</td>
<td>1.25</td>
<td>132.2±8.6</td>
<td>2.26×10$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>2.80</td>
<td>1.25</td>
<td>192.0±9.4</td>
<td>2.70×10$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>3.20</td>
<td>1.25</td>
<td>197.5±6.5</td>
<td>2.68×10$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>4.00</td>
<td>1.25</td>
<td>154.0±9.4</td>
<td>2.96×10$^{-2}$</td>
<td></td>
</tr>
</tbody>
</table>

#### 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": (MRTC 6-00 No. 6990-70), 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.

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

<table>
<thead>
<tr>
<th>Experimental Data</th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
<td>$10^{-3} c_1$/mol dm$^{-3}$</td>
<td>$10^{-3} c_2$/mol dm$^{-3}$</td>
<td>$10^3 p_1$/g m$^{-2}$</td>
<td>$T_0$ $v_1$ (compiler)</td>
</tr>
<tr>
<td>20</td>
<td>0.2</td>
<td>0.2</td>
<td>160.1±4.6</td>
<td>1.53×10$^{-2}$</td>
</tr>
<tr>
<td>2.80</td>
<td>0.2</td>
<td>146.7±1.1</td>
<td>1.35×10$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>2.80</td>
<td>0.2</td>
<td>146.1±0.9</td>
<td>1.31×10$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>3.20</td>
<td>0.2</td>
<td>131.5±2.2</td>
<td>1.14×10$^{-2}$</td>
<td></td>
</tr>
<tr>
<td>4.00</td>
<td>0.2</td>
<td>129.7±2.6</td>
<td>1.12×10$^{-2}$</td>
<td></td>
</tr>
</tbody>
</table>

#### 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": (MRTC 6-00 No. 6290-70), redistilled and checked by GC before use.
  (2) Type "analytic pure." (3) Type "chemically pure." (4) Distilled.

- **Estimated Errors:**
  Solubility: see above.
  Temperature: ±0.2 K.
### 15. Tetrachloroethylene with Sodium Chloride and Water

**Components:**
- Tetrachloroethylene (tetrachloroethylene): C₂Cl₄; [127-18-4]
- Sodium chloride: NaCl; [7647-14-5]
- Water: H₂O; [7732-18-5]

**Variables:**
- \( T/K = 293 \)
- Concentration/mol dm\(^{-3}\) = 0.2 – 2

**Prepared By:** A. L. Horvah

#### Experimental Data

<table>
<thead>
<tr>
<th>( T/°C )</th>
<th>( 10^{-3} c_1 ) mol dm(^{-3} )</th>
<th>( 10^{3} \rho_1 ) g m(^{-3} )</th>
<th>( 100 \times ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.17</td>
<td>139.2±6.8</td>
<td>1.38×10(^{-2} )</td>
</tr>
<tr>
<td></td>
<td>1.70</td>
<td>73.1±1.5</td>
<td>6.84×10(^{-3} )</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Method/Apparatus/Procedure:**
   - The aqueous electrolyte solutions were saturated with tetrachloroethylene 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 tetrachloroethylene 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

### 16. Tetrachloroethylene with Sulfuric Acid and Water

**Components:**
- Tetrachloroethylene (tetrachloroethylene): C₂Cl₄; [127-18-4]
- Sulfuric acid: H₂SO₄; [76649-97]
- Water: H₂O;[7732-18-5]

**Variables:**
- \( T/K = 293 \)
- Concentration/mol dm\(^{-3}\) = 0 – 1

**Prepared By:** A. L. Horvah

#### Experimental Data

<table>
<thead>
<tr>
<th>( T/°C )</th>
<th>( 10^{-3} c_1 ) mol dm(^{-3} )</th>
<th>( 10^{3} \rho_1 ) g m(^{-3} )</th>
<th>( 100 \times ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.05</td>
<td>194.9±6.2</td>
<td>1.94×10(^{-2} )</td>
</tr>
<tr>
<td></td>
<td>1.00</td>
<td>168.6±6.8</td>
<td>1.58×10(^{-2} )</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Method/Apparatus/Procedure:**
   - The aqueous electrolyte solutions were saturated with tetrachloroethylene 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 tetrachloroethylene 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.
### 17. Tetrachloroethene with Sulfuric Acid, Ammonium Sulfate, and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$\degree\text{C}$</th>
<th>$10^{-2} x_1$/mol dm$^{-3}$</th>
<th>$10^{-3} x_2$/mol dm$^{-3}$</th>
<th>$10^3 P_1/\text{g m}^{-3}$</th>
<th>100 $w_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.10</td>
<td>0.75</td>
<td>89.2±5.7</td>
<td>8.44×10^{-3}</td>
</tr>
<tr>
<td>28</td>
<td>0.50</td>
<td>0.75</td>
<td>72.0±2.0</td>
<td>6.82×10^{-3}</td>
</tr>
<tr>
<td>1.50</td>
<td>0.75</td>
<td>92.0±2.1</td>
<td>8.39×10^{-3}</td>
<td></td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**

The aqueous electrolyte solutions were saturated with tetrachloroethene in thermostated flasks stirred with a stirrer 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.

**Estimated Errors:**

Solubility: see above
Temperature: ±0.2 K.

### 18. 1,1,2,2-Tetrachloro-1,2-Difluoromethane and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$\degree\text{C}$</th>
<th>100 $w_1$ (compiler)</th>
<th>100 $w_2$ (compiler)</th>
<th>100 $x_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>27</td>
<td>1.5×10^{-1}</td>
<td>1.40</td>
<td>—</td>
</tr>
<tr>
<td>28</td>
<td>—</td>
<td>—</td>
<td>9.9×10^{-3}</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Source and Purity of Materials:**

(1) Source not given, 0.8% CCl$_4$, CCl$_3$, CCl$_2$ content.
(2) Distilled (compiler).

**Estimated Errors:**

Solubility: not specified.
Temperature: ±1 K.
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>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w1</th>
<th>References</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>283.15</td>
<td>1</td>
</tr>
<tr>
<td>20</td>
<td>295.15</td>
<td>2</td>
</tr>
<tr>
<td>22.3</td>
<td>295.45</td>
<td>3</td>
</tr>
<tr>
<td>24.85</td>
<td>298.00</td>
<td>4</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>5</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>6</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

References:
<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 295</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

### Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 g₁/g₂</th>
<th>10⁻⁴ x₁</th>
<th>10⁵ x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>22.3</td>
<td>5.0 x 10⁻³</td>
<td>3.81</td>
<td></td>
</tr>
</tbody>
</table>

### 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).

**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. Hexachloroethane; C₂Cl₆ [107-72-1]
2. Water; H₂O [7732-18-5]

Variables:
T/K = 293

Experimental Data

<table>
<thead>
<tr>
<th>°C</th>
<th>n₁ V₅⁻¹/m³ dm⁻¹</th>
<th>100 w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.148×10⁻⁴</td>
<td>2.72×10⁻²</td>
<td>2.069</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of hexachloroethane was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The °C activity of the water sample 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.

Original Measurements:

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>°C</th>
<th>Henry's law constant, H/dimensionless</th>
<th>10⁵ p₁/g m⁻³</th>
<th>10⁵ w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>6.12×10⁻²</td>
<td>23.1</td>
<td>2.31×10⁻³</td>
<td>1798</td>
</tr>
<tr>
<td>20</td>
<td>1.73×10⁻¹</td>
<td>27.5</td>
<td>2.75×10⁻³</td>
<td>2093</td>
</tr>
<tr>
<td>30</td>
<td>2.31×10⁻¹</td>
<td>32.4</td>
<td>3.24×10⁻³</td>
<td>2465</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess amount of hexachloroethane with water was introduced into 10 cm³ 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) Stimson, Inc., PA, contained 76-78% C₂Cl₆ as a constantant.
(2) Distilled and de-ionized

Estimated Errors:
Solubility: ± 8.5×10⁻³ std. dev.
Temperature: ± 0.5 K.

Prepared By:
A. L. Horvath

Components:
1. Hexachloroethane; C₂Cl₆ [107-72-1]
2. Water; H₂O [7732-18-5]

Variables:
T/K = 283-303

Original Measurements:
### Components

(1) Hexachloroethane: C₆Cl₆ [67-72-1]
(2) Water: HO₂ [7732-18-5]

### Original Measurements


### Prepared By:

A. L. Horvath

### Variables:

\( T/K = 293 \)

### Experimental Data

<table>
<thead>
<tr>
<th>℃</th>
<th>( \delta \times 10^{-5} )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10² ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>7.7</td>
<td>7.71 × 10⁻⁴</td>
<td>5.87</td>
</tr>
</tbody>
</table>

### 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.\(^3\) Duplicate experiments were carried out for the solubility measurement.

**Source and Purity of Materials:**
(1) Supelco, Inc., A, contained about 3% C₆Cl₆ as a contaminant.
(2) Distilled and further purified to Milli-Q reagent grade system.

**Estimated Errors:**
Solubility: ±1% - 2%.
Temperature: ±0.1 K

**References:**

### Components:

(1) Hexachloroethane: C₆Cl₆ [67-72-1]
(2) Water: HO₂ [7732-18-5]

### Original Measurements:


### Variables:

\( T/K = 298 \)

### Experimental Data

<table>
<thead>
<tr>
<th>℃</th>
<th>Henry's law constant, ( H ) ( mL ) atm mol⁻¹</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10² ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>9.85 × 10⁻³</td>
<td>1.133 × 10⁻³</td>
<td>1.547</td>
</tr>
</tbody>
</table>

### 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 deionized water, since the sample in a waterbath thermostat, and mix overnight. A portion of this solution was injected 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 average of two or more replicates.

**Source and Purity of Materials:**
(1) Purif 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:**
Components:
(1) Hexachlorethane; C₆Cl₁₂; [67-72-1]
(2) Water; H₂O; [7732-18-5]

Original Measurements:
G. J. Howe, M. J. Mellins, and T. N. Reese, Report
American Association for the Advancement of Science,

Variables:
T/K = 283–303

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/C</th>
<th>10⁶ δf/δs</th>
<th>10⁶ x₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>41</td>
<td>4.1×10⁻³</td>
<td>3.12</td>
</tr>
<tr>
<td>20</td>
<td>37</td>
<td>3.7×10⁻³</td>
<td>2.82</td>
</tr>
<tr>
<td>30</td>
<td>41</td>
<td>4.1×10⁻³</td>
<td>3.12</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
250 cm³ bottles were filled with distilled and de-ionized water
and sealed. A measured volume of hexachlorethane was
injected into the bottle through each septum using a microlitre
syringe. Hexachlorethane was in excess of the anticipated
solubility limit. The bottles were shaken for 3 h with a
twist-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, as
received.
(2) Distilled and de-ionized.

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

Components:
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; C₇BrClF₃;
[151-67-7]
(2) Water; H₂O; [7732-18-5]

Evaluator:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn,

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 (2)
binary system is discussed in two parts: part 1 is 2-bromo-2-chloro-
1,1,1-trifluoroethane (1) in water (2) 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 repeated by 14 laboratories with reasonably
consistent results. The only measurement by Saseen 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
Raveno,'² Larouze et al.³ Donnan,² Bernuth,² Love,² Ohuda,' Love and
Hagler,' Lawless and Hilsley-Whyte,² Broch,¹⁰ Scollay and
Longshore,'¹¹ Balford et al.² Larus et al.,¹¹ and Horvath.¹² 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 28°C to 313 K were correlated to obtain the following mass
percent equation:

Solubility [10₆ x₁ = 22.0805-0.1412(T/K) - 2.3000×10⁻⁴(T/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.

![Graph showing solubility of 2-bromo-2-chloro-1,1,1-trifluoroethane in water](image)

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-1,1,1-trifluoroethane (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>$10^3$ m</th>
<th>Solubility</th>
<th>$10^6 a_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>293.15</td>
<td>0.521</td>
<td>4.78</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>298.15</td>
<td>0.472</td>
<td>4.33</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.434</td>
<td>3.98</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.407</td>
<td>3.75</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.392</td>
<td>3.59</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.389</td>
<td>3.56</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.397</td>
<td>3.64</td>
<td></td>
</tr>
</tbody>
</table>

Part 2. The solubility of water (2) in 2-bromo-2-chloro-1,1,1-trifluoroethane (1) has been measured by Lee and Serram, Horvath, A. L. Horvath.

### References


### Experimental Data

<table>
<thead>
<tr>
<th>$10^5$ C</th>
<th>$10^3 m$</th>
<th>100 $w_1$ (compiler)</th>
<th>100 $a_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.345</td>
<td>0.344</td>
<td>3.15</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Details are not available.

**Source and Purify of Materials:**
1. Imperial Chemical Industries Limited, Widnes, used as received.
2. Distilled.

**Estimated Error:**
Solubility: ±0.5 K (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>°C</th>
<th>100 g/L</th>
<th>100 g/L (compiler)</th>
<th>100 °C</th>
<th>100 °C (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>0.345</td>
<td>0.344</td>
<td>3.15</td>
<td>3.15</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
The solubility was determined by equilibrating water with 2-bromo-2-chloro-1,1-dichloroethane in closed flasks and analyzing the concentration in the equilibrated gas phase with an infrared analyzer. The flasks were shaken vigorously until identical readings were obtained from the Beckman infrared analyzer. All samples attained equilibrium within 2-4 hours. Eleven determinations were carried out.

**Source and Purity of Materials:**
(1) Supplied by Ayensu Laboratories, used as received.
(2) Distilled.

**Estimated Errors:**
Solubility: ± 7%.
Temperature: ± 0.5 K.
### Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>100 $n_{1}$ (complex)</th>
<th>$10^6 n_{1}$ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.0</td>
<td>0.466</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

- Details are not available.

**Source and Purity of Materials:**

1. Commercial reagent from VEB Aczetinimteerz Dresden, contained 0.01% ethylen as a stabilizer.
2. Distilled (complex).

**Estimated Errors:**

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

---

### Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>Oswald coefficient, L/dimensionalless</th>
<th>100 $n_{1}$ (compiler)</th>
<th>$10^6 n_{1}$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>29</td>
<td>1.04</td>
<td>0.566</td>
<td>5.19</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

- The conventional Schonander apparatus was used with the reaction chamber unit surrounded by a water bath. A carrier gas containing 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:**

- Source and purity not given.
- Distilled.

**Estimated Errors:**

- Solubility: ±0.21% std. dev.
- Temperature: ±0.5 K (compiler).

**References:**

### Component 1

(1) 2-bromo-1-chloro-1,1,1-trifluoroethane; C\textsubscript{3}H\textsubscript{7}Br\textsubscript{3}F\textsubscript{7}

Original Measurements:

**Variables:**

- T/K = 298–313

**Prepared By:**

A. L. Horvath

#### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Oswald coefficient, L/dimensionless</th>
<th>100 w\textsubscript{1} (compiler)</th>
<th>10\textsuperscript{6} (X) \textsubscript{1} (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1.277±0.2</td>
<td>0.491</td>
<td>4.05</td>
</tr>
<tr>
<td>20</td>
<td>1.83±0.3</td>
<td>0.484</td>
<td>4.35</td>
</tr>
<tr>
<td>25</td>
<td>1.46±0.07</td>
<td>0.467</td>
<td>4.28</td>
</tr>
<tr>
<td>30</td>
<td>1.14±0.04</td>
<td>0.438</td>
<td>4.05</td>
</tr>
<tr>
<td>35</td>
<td>0.87±0.04</td>
<td>0.392</td>
<td>3.59</td>
</tr>
<tr>
<td>37</td>
<td>0.82±0.03</td>
<td>0.401</td>
<td>3.68</td>
</tr>
<tr>
<td>40</td>
<td>0.71±0.04</td>
<td>0.384</td>
<td>3.52</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

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

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ± 1 K (compiler).

### Component 2

(2) Water; H\textsubscript{2}O [7732-18-5]

Original Measurements:

**Variables:**

- T/K = 298–313

**Prepared By:**

A. L. Horvath

#### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Oswald coefficient, L/dimensionless</th>
<th>100 w\textsubscript{1} (compiler)</th>
<th>10\textsuperscript{6} (X) \textsubscript{1} (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1.277±0.2</td>
<td>0.491</td>
<td>4.05</td>
</tr>
<tr>
<td>20</td>
<td>1.83±0.3</td>
<td>0.484</td>
<td>4.35</td>
</tr>
<tr>
<td>25</td>
<td>1.46±0.07</td>
<td>0.467</td>
<td>4.28</td>
</tr>
<tr>
<td>30</td>
<td>1.14±0.04</td>
<td>0.438</td>
<td>4.05</td>
</tr>
<tr>
<td>35</td>
<td>0.87±0.04</td>
<td>0.392</td>
<td>3.59</td>
</tr>
<tr>
<td>37</td>
<td>0.82±0.03</td>
<td>0.401</td>
<td>3.68</td>
</tr>
<tr>
<td>40</td>
<td>0.71±0.04</td>
<td>0.384</td>
<td>3.52</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

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

- **Estimated Errors:**
  - Solubility: see above.
  - Temperature: ± 0.5 K (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Oswald coefficient, ( L/\text{dimensionless} )</th>
<th>( 10^5 w_1 ) (compiler)</th>
<th>( 10^6 x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>0.86</td>
<td>0.421</td>
<td>3.86</td>
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### Auxiliary Information

**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; $\text{H}_2\text{O}$; [7732-18-5]
(2) 2-bromo-2-chloro-1,1,1-trifluoroethane; $\text{C}_2\text{HBrClF}_3$; [151-67-7]

Variables:
$T/K$ = 298

Experimental Data

<table>
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<tr>
<th>$T^\circ$ C</th>
<th>$100 \times x_1$ (compiler)</th>
<th>$100 \times \text{mol g}^{-1}$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>$3.0 \times 10^{-2}$</td>
<td>$3.28$</td>
</tr>
</tbody>
</table>

Auxiliary Information

- Source and Purity of Materials:
  1. Distilled.
  2. Not specified.

- Estimated Errors:
  Solubility: $\pm 7\%$
  Temperature: $\pm 0.1$ K

Components:
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; $\text{C}_2\text{HBrClF}_3$; [151-67-7]

Experimental Data

<table>
<thead>
<tr>
<th>$T^\circ$ C</th>
<th>Oswald coefficient, L/dm$^3$/mol/gaseous (compiler)</th>
<th>$100 \times x_1$ (compiler)</th>
<th>$10^3 \times x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.12 $\pm$ 0.02</td>
<td>0.359</td>
<td>3.28</td>
</tr>
<tr>
<td>29</td>
<td>1.06 $\pm$ 0.04</td>
<td>0.393</td>
<td>3.60</td>
</tr>
<tr>
<td>33</td>
<td>0.88 $\pm$ 0.05</td>
<td>0.376</td>
<td>3.44</td>
</tr>
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<td>37</td>
<td>0.76 $\pm$ 0.03</td>
<td>0.372</td>
<td>3.41</td>
</tr>
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</table>

Auxiliary Information

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

- Estimated Errors:
  Solubility: see above.
  Temperature: $\pm 0.5$ K (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>Oswald coefficient, ( L/\text{dimensionless} )</th>
<th>100 ( v_i ) (compiler)</th>
<th>10(^6) ( x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>0.82</td>
<td>0.40</td>
<td>3.67</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Mixture of 5 mL of bromo-2-chloro-1,1,1-trifluoroethane and 5 cm\(^3\), distilled water were added to 300 cm\(^3\) Erlenmeyer flask which were then placed in a water bath thermostat and agitated for 120 min. After equilibration, samples were taken and analysed for 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 results are the average of six determinations.

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

**Estimated Errors:**
Solubility: ± 0.03 mol.
Temperature: ± 0.5°C (compiler).
### Components:
(1) 2-bromo-2-chloro-1,1,1-trifluoroethane; C₂HBrClF₃
(2) 2-bromo-2-chloro-1,1,1-trifluoroethane; C₂HBrClF₃

### Original Measurements:

### Variables:
T/K = 297–100

### Prepared By:
A. L. Horvath

---

### Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
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<td></td>
</tr>
<tr>
<td>37</td>
<td></td>
<td></td>
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</tbody>
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### Experimental Data

<table>
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<tr>
<th>t/°C</th>
<th>100 w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
<th>10⁶ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### 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 recorder. Five parallel determinations were carried out.

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

**Estimated Errors:**
Solubility: ± 5%
Temperature: ± 0.5 °C (compiler).

**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-trifluorohene; C₂H₂Cl₂F₂ [306-83-2];
(2) Water; H₂O; [7732-18-5]

Evaluator:

21. 2,2-Dichloro-1,1,1-Trifluorohene wth Water

Critical Evaluation

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

Part 1. The solubility of 2,2-dichloro-1,1,1-trifluorohene (1) in water (2) has been reported in a du Pont bulletin, and by Zuckerman 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-trifluorohene (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>
<thead>
<tr>
<th>Temperature</th>
<th>Solubility</th>
<th>Source and Purity of Materials</th>
</tr>
</thead>
<tbody>
<tr>
<td>°C</td>
<td>K</td>
<td>10^4 w₁</td>
</tr>
<tr>
<td>21</td>
<td>294.15</td>
<td>—</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.46</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.21</td>
</tr>
</tbody>
</table>

References:
**Components:**

2. 2,2-Dichloro-1,1,1-trifluoroethane: C₂HCl₂F₃ [108-83-2]

**Original Measurement:**


**Variables:**

T/K = 298

**Prepared by:**

A. L. Horvath

---

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10⁵ x₁ (compleat)</th>
<th>10⁵ w₂ M⁻¹ mol g⁻¹ (compleat)</th>
</tr>
</thead>
<tbody>
<tr>
<td>21</td>
<td>4.7 × 10⁻³</td>
<td>3.58</td>
</tr>
</tbody>
</table>

---

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Details are not available.

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

**Estimated Errors:**
Solubility: not specified.
Temperature: ± 1 K (compleat).

---

**Components:**

1. 2,2-Dichloro-1,1,1-trifluoroethane: C₂HCl₂F₃ [108-83-2]

**Original Measurements:**


**Variables:**

T/K = 298

**Prepared by:**

A. L. Horvath

---

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10⁵ x₁ (compleat)</th>
<th>10⁵ w₂ (compleat)</th>
<th>10⁵ c₂ (compleat)</th>
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</thead>
<tbody>
<tr>
<td>21</td>
<td>2.10 × 10⁻³</td>
<td>2.48</td>
<td>6.62 × 10⁻³</td>
</tr>
</tbody>
</table>

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**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 (compleat).

**Estimated Errors:**
Solubility: not specified.
Temperature: ± 1 K (compleat).
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 253–333 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 sources was not used for the smoothing equation for a variety of reasons. The solubility data of Saltzmann et al.,1 Wright and Schofield,2 Newman et al.,3 Szyszka,4 and Orlandini et al.5 are markedly higher than other results and, therefore, have been rejected. The data of Riley et al.6 Sedmerova and Novak,7 Preuzmesic et al.,8 Cox and Diaz,9 McNally and Grah,10 and Yotishka et al.11 appear to be several percent lower than the smoothed solubility values and also have been rejected.

It may be noted that only two investigators2,12 showed the appearance of a solubility minimum over the reported temperature interval. In several studies, the solubility steadily increases13,14 or decreases15–19 with increasing temperature. The solubility data of Wright et al.20 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 et al.,21 Powell et al.,22 Tettamanti et al.,23 O’Connell,24 Lowe and Hageman,25 Astropv et al.,26 McConnell et al.,27 Pearson and McConnell,28 Chinn and Feed,29 Archer and Stevens,30 Hilday et al.,31 Ito and Nakajima,32 Goosen,33 Juncos and Calo,34 Bottomore et al.,35 Linscott and Goosen,36 Moore et al.,37 Miller et al.,38 Cossen,39 Wanner et al.,40 Howe et al.,41 and Wright et al.42 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 obtained to use the following mass percent (1) equation:

\[ \text{Solubility (wt.%) = 1.4049 - 82223 \times 10^{-3} (1/T) + 1.3218 \times 10^{-5} (1/T)^2} \]

This equation represents the combined data values from 23 studies which yielded a standard deviation of 1.59 × 10^{-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 31.0 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 1933. 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 Ellerbe,7 Sedmerova and Novak,7 and Pouyavan et al.2 are substantially lower than all other studies and are rejected. The data of Tettamanti et al.23 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,28 Martin,29 Riley et al.6 Hutchison and Lyon,30 McGovern,31 O’Connell,32 Lees and Sarram,33 Astropv et al.26 Coca and Diaz,9 and Ohtsuka and Kanemoto43 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:

\[ \log_{10} x_2 = 1.610 - 1291.0 / (T/F) \]

This equation yielded a standard deviation of 5.23 × 10^{-2}. The recommended solubility values at 5 K intervals for water (2) in trichloroethene (1) are presented in Table 2.
### Table 1: Tentative solubility of trichlorethene (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>K</th>
<th>10⁶ w₁</th>
<th>Solubility</th>
<th>10⁶ w₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.5</td>
<td>0.145</td>
<td>1.99</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>278.5</td>
<td>0.141</td>
<td>1.94</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>283.5</td>
<td>0.137</td>
<td>1.88</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>288.5</td>
<td>0.133</td>
<td>1.83</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>293.5</td>
<td>0.131</td>
<td>1.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>298.5</td>
<td>0.128</td>
<td>1.76</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>303.5</td>
<td>0.127</td>
<td>1.74</td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>308.5</td>
<td>0.126</td>
<td>1.73</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>313.5</td>
<td>0.126</td>
<td>1.73</td>
<td></td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>318.5</td>
<td>0.127</td>
<td>1.74</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>323.5</td>
<td>0.127</td>
<td>1.76</td>
<td></td>
<td></td>
</tr>
<tr>
<td>55</td>
<td>328.5</td>
<td>0.130</td>
<td>1.78</td>
<td></td>
<td></td>
</tr>
<tr>
<td>60</td>
<td>333.5</td>
<td>0.133</td>
<td>1.82</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Table 2: Recommended solubility of water (3) in trichlorethene (1)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>K</th>
<th>10⁶ w₁</th>
<th>Solubility</th>
<th>10⁶ w₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20</td>
<td>253.5</td>
<td>0.00477</td>
<td>3.477</td>
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<td></td>
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<tr>
<td>-15</td>
<td>258.5</td>
<td>0.00599</td>
<td>4.366</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-10</td>
<td>263.5</td>
<td>0.00745</td>
<td>5.433</td>
<td></td>
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<tr>
<td>-5</td>
<td>268.5</td>
<td>0.00920</td>
<td>6.507</td>
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</tr>
<tr>
<td>0</td>
<td>273.5</td>
<td>0.01213</td>
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</tr>
<tr>
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<td>303.5</td>
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<td>35</td>
<td>308.5</td>
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</tr>
<tr>
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<td>333.5</td>
<td>0.08041</td>
<td>58.377</td>
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<tr>
<td>65</td>
<td>338.5</td>
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<td>66.203</td>
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<tr>
<td>70</td>
<td>343.5</td>
<td>0.1041</td>
<td>73.688</td>
<td></td>
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</tr>
<tr>
<td>75</td>
<td>348.5</td>
<td>0.1180</td>
<td>81.670</td>
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<tr>
<td>80</td>
<td>353.5</td>
<td>0.1340</td>
<td>96.678</td>
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<td></td>
</tr>
</tbody>
</table>

References:

### Components:
- (1) Trichloroethene (trichloroethylene); C₂HCl₃ [79-01-6]
- (2) Water; H₂O [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 293
- 273

### Experimental Data

<table>
<thead>
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<th>10² V₁ / V₂ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
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</thead>
<tbody>
<tr>
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<td>1.8</td>
<td>0.263</td>
</tr>
<tr>
<td>25</td>
<td>5.50 × 10⁵</td>
<td>0.182</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:
- A volumetric method similar to that introduced by Alexejev
- Estimated Errors:
  - Solubility: not specified.
  - Temperature: ± 0.5 K (compiler).

#### Source and Purity of Materials:
- Commercial grade, further purified by washing with Na₂HPO₄ solution and then distilled.
- Estimated Errors:
  - Solubility: not specified.
  - Temperature: ± 0.5 K (compiler).
Components:
1. Water; H₂O; [7732-18-5]
2. Trichloroethene (trichloroethylene); C₂H₃Cl₂; [79-01-6]

Original Measurements:

Prepared by:
A. J. Horvath

Variables:
Temperature

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

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 g₁/g₂</th>
<th>100 w₁ (compiler)</th>
<th>F³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
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<td>1.7x10⁻²</td>
<td>1.24</td>
</tr>
<tr>
<td>18</td>
<td>2.6x10⁻¹</td>
<td>2.6x10⁻²</td>
<td>1.89</td>
</tr>
<tr>
<td>28</td>
<td>3.6x10⁻¹</td>
<td>3.6x10⁻²</td>
<td>2.62</td>
</tr>
</tbody>
</table>

Auxiliary Information

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

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K.
### Component:
- (1) Trichloroethane (trichloroethylene); C₂H₃Cl₃; [79-01-6]
- (2) Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 298

### Experimental Data

<table>
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<tr>
<th>t/°C</th>
<th>10ª w₁</th>
<th>10ª x₂</th>
<th>10ª w₂</th>
<th>10ª x₂</th>
</tr>
</thead>
<tbody>
<tr>
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<td>1.1 × 10⁻²</td>
<td>1.11</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>18</td>
<td>—</td>
<td>2.5 × 10⁻²</td>
<td>—</td>
<td>1.820</td>
</tr>
</tbody>
</table>

### 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 trichloroethane in water was accompanied by a quantitative hydrolysis reaction with aqueous KOH solution for 3 h at 120 °C in a sealed Carus tube. The chlorine content was determined by the Volhard method.

**Source and Purity of Materials:**
- (1) Imperial Chemical Industries Limited, further purified and freed from basic substances.
- (2) Distilled.

**Estimated Errors:**
Solvability: ±0.2 × 10⁻² mol L⁻¹.
Temperature: ±0.6 °C.

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

### Original Measurements:


### Variables:
Prepared By:
A. L. Horvath

**Experimental Data**

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 w_t</th>
<th>2 * 10^6 * x_t (compiler)</th>
<th>100 w_t</th>
<th>5 * 10^5 * x_t (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20</td>
<td></td>
<td>3.1105</td>
<td></td>
<td>1.44</td>
</tr>
<tr>
<td>0</td>
<td>3.1105</td>
<td>1.44</td>
<td>3.1105</td>
<td>7.14</td>
</tr>
<tr>
<td>10</td>
<td>3.107</td>
<td>1.47</td>
<td>3.1105</td>
<td>11.3</td>
</tr>
<tr>
<td>20</td>
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<td>1.48</td>
<td>3.1105</td>
<td>16.4</td>
</tr>
<tr>
<td>25</td>
<td>3.110</td>
<td>1.51</td>
<td>3.1105</td>
<td>23.3</td>
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<tr>
<td>30</td>
<td>3.113</td>
<td>1.55</td>
<td>3.1105</td>
<td>24.0</td>
</tr>
<tr>
<td>40</td>
<td>3.115</td>
<td>1.58</td>
<td>3.1105</td>
<td>33.7</td>
</tr>
<tr>
<td>60</td>
<td>3.125</td>
<td>1.72</td>
<td>3.1105</td>
<td>58.1</td>
</tr>
<tr>
<td>80</td>
<td></td>
<td>1.86 × 10^-1</td>
<td></td>
<td>91.2</td>
</tr>
</tbody>
</table>

Solubility data as a function of temperature were presented in graphical form only except for data values at 55 °C.

### 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 stirred with pyridine 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 not given, commercial grade.
(2) Distilled.

**Estimated Errors:**
Solubility: ±3.0%. Temperature: ±0.5 K (compiler).
Components:  
(1) Trichloroethene (trichloroethylene); [79-01-6]  
(2) Water; H₂O; [7732-18-5]

Original Measurements:  

Variables:  
T/K = 298

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>ϑ₀ x₁ (compiler)</th>
<th>100 w₁ M⁺/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.40</td>
<td>5.5</td>
<td>3.0×10⁻³</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:  
The equilibrium between trichloroethylene and water was established in a constant temperature water bath with sufficient agitation. The usual procedures were followed; the specific gravity was used as a mean of analysis.

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

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

References:  

Components:  
(1) Water; H₂O; [7732-18-5]  
(2) Trichloroethene (trichloroethylene); [79-01-6]

Original Measurements:  
E. Riehs, Wasser-Bestimmung mit Karl-Fischer-Lösung,  

Variables:  
T/K = 293

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>ϑ₀ x₁ (compiler)</th>
<th>100 w₁ M⁺/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.011±0.000</td>
<td>8.02</td>
<td>6.10×10⁻⁴</td>
</tr>
</tbody>
</table>

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) Trichloroethylene (trichloroethylens); C₂HCl₃; [79-01-6]
- (2) Water; H₂O; [7732-11-5]

### Original Measurements

### Variables
- T[K] = 313
- T[K] = 293

### Prepared By
- A. L. Horvath
- Z. Maczyna

### Experimental Data

<table>
<thead>
<tr>
<th>T[°C]</th>
<th>n=1000 ( w_1 )</th>
<th>( 10^5 ) ( x_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>2.3</td>
<td>0.873</td>
</tr>
<tr>
<td>20</td>
<td>0.10</td>
<td>1.37</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:
- Turbidimetric titrations were used for both the aqueous and the organic phases. First, the trichloroethylene was titrated with water from a microburet up to the appearance of turbidity.
- Then, afterwards, the water was titrated with trichloroethylene.
- The amounts of water or trichloroethylene in the flasks were weighted to an accuracy of 101 g. The temperature was maintained constant using a thermostat.

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

#### Estimated Errors:
- Solubility: ± 1.0%.
- Temperature: ± 0.1 K.
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w&lt;sub&gt;1&lt;/sub&gt;</th>
<th>10&lt;sup&gt;5&lt;/sup&gt; x&lt;sub&gt;1&lt;/sub&gt; (compiler)</th>
<th>100 w&lt;sub&gt;2&lt;/sub&gt;</th>
<th>10&lt;sup&gt;5&lt;/sup&gt; x&lt;sub&gt;2&lt;/sub&gt; (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.11</td>
<td>1.51</td>
<td>2.0 x 10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>1.46</td>
</tr>
<tr>
<td>19.85</td>
<td></td>
<td>1.0 x 10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>1.4</td>
<td>7.0 x 10&lt;sup&gt;-4&lt;/sup&gt;</td>
</tr>
<tr>
<td>20.85</td>
<td></td>
<td>1.5 x 10&lt;sup&gt;-3&lt;/sup&gt;</td>
<td>2.1</td>
<td>1.0 x 10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
<tr>
<td>39.85</td>
<td></td>
<td>2.0 x 10&lt;sup&gt;-2&lt;/sup&gt;</td>
<td>2.7</td>
<td>1.2 x 10&lt;sup&gt;-3&lt;/sup&gt;</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:

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

#### Source and Purify of Materials:

(1) Source not given, technical grade, distilled and dried over CaCl<sub>2</sub> before use, b.p. = 87.20 °C; d<sub>4</sub> = 1.4662.

(2) Twice distilled.

#### Estimated Errors:

Solubility: not specified.
Temperature: ± 0.5 K (compiler).
Components:  
(1) Trichloromethane (trichloroethylene); C₂HCl₃; [79-01-6]  
(2) Water; H₂O; [7732-18-5]

Original Measurements:  

Variables:  
T/K = 310

Prepared By:  
J. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Outward coefficient, L/dimensionless</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>1.51</td>
<td>0.30</td>
<td>1.784</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:  
The direct sample injection method was used. The sample containing the equilibrium mixture was injected into a Chromosorb column equipped with a detection 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:  
Stability: not specified.  
Temperature: ±0.05 K (compiler).

Components:  
(1) Water; H₂O; [7732-18-5]  
(2) Trichloromethane (trichloroethylene); C₂HCl₃; [79-01-6]

Original Measurements:  

Variables:  
T/K = 298

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
<th>100 w₁ M⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.0x10⁻³</td>
<td>1.46</td>
<td>1.1x10⁻³</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:  
The apparatus containing its 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); C₂HCl₃; [79-01-6]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
T/K = 283–373

### Prepared By:
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>10⁻² w₁</th>
<th>10⁻² x₁ (compiler)</th>
<th>10⁻² w₂</th>
<th>10⁻² x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1.01×10⁻¹</td>
<td>1.39</td>
<td>—</td>
<td>—</td>
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<tr>
<td>18</td>
<td>—</td>
<td>2.1×10⁻²</td>
<td>—</td>
<td>1.53</td>
</tr>
<tr>
<td>20</td>
<td>1.00×10⁻¹</td>
<td>1.50</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>22</td>
<td>—</td>
<td>2.4×10⁻²</td>
<td>—</td>
<td>1.75</td>
</tr>
<tr>
<td>26</td>
<td>1.22×10⁻¹</td>
<td>1.67</td>
<td>3.2×10⁻²</td>
<td>2.33</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:
Alexeev's synthetic solubility method of solubility determination was used. 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: ±4.5 K (compiler).

### References:

---

### Components:
1. Trichloroethene (trichloroethylene); C₂HCl₃; [79-01-6]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
T/K = 283–373

### Prepared By:
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>Distribution coefficient, a</th>
<th>10⁴ w₁</th>
<th>10⁵ x₁ (compiler)</th>
<th>10⁴ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>1.16×10⁴</td>
<td>3.469×10⁻³</td>
<td>4.757×10⁻²</td>
<td></td>
</tr>
<tr>
<td>21</td>
<td>9.2×10⁵</td>
<td>6.217×10⁻³</td>
<td>8.525×10⁻²</td>
<td></td>
</tr>
<tr>
<td>32</td>
<td>6.5×10⁵</td>
<td>1.440×10⁻¹</td>
<td>1.974×10⁻¹</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>4.5×10⁵</td>
<td>4.696×10⁻²</td>
<td>6.442×10⁻²</td>
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</tr>
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<td>9.74×10⁻²</td>
<td>1.33×10⁵</td>
<td></td>
</tr>
<tr>
<td>70.3</td>
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<td>2.06×10⁻¹</td>
<td>2.83×10⁵</td>
<td></td>
</tr>
<tr>
<td>80</td>
<td>1.6×10⁵</td>
<td>4.05×10⁻¹</td>
<td>5.71×10⁵</td>
<td></td>
</tr>
<tr>
<td>90.3</td>
<td>1.13×10⁵</td>
<td>7.12×10⁻¹</td>
<td>9.82×10⁵</td>
<td></td>
</tr>
<tr>
<td>96.6</td>
<td>1.0×10⁵</td>
<td>8.95×10⁻¹</td>
<td>1.23×10³</td>
<td></td>
</tr>
<tr>
<td>100</td>
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<td>1.08×10⁰</td>
<td>1.50×10⁵</td>
<td></td>
</tr>
</tbody>
</table>

*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 trichloroethene in both liquid and vapor phases was determined by using ³⁵Cl labeled compound.

#### 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) Water: H$_2$O; [7732-18-5]
(2) Trichloroethene (trichloroethylene): C$_2$HCl$_3$; [79-01-6]

Experimental Data

\[
\log a = \frac{917.18}{T/K} - 0.998, \\
\text{where } a = \text{distribution coefficient. At the normal boiling point of C$_2$HCl$_3$, } a = 39 \text{ and the activity coefficient, } \gamma = 63.
\]

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:

<table>
<thead>
<tr>
<th>$^\circ$C</th>
<th>$10^2 E_{1}/E_2$</th>
<th>100 $w_1$ (compiler)</th>
<th>$10^5 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.1$\times$10$^3$</td>
<td>0.1099</td>
<td>0.308</td>
</tr>
</tbody>
</table>

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); C₂HCl₃; [79-01-6]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 293

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10⁶ gR₁</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.1 × 10³</td>
<td>0.1099</td>
<td>1.508</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solutions were prepared in a constant temperature thermostated 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 ⁶³Ni electron capture detector.

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

Estimated Errors:
Solubility: not specified.
Temperature: ± 0.5 T (compiler).

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>1/V₂ g⁻¹ cm⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.78</td>
<td>0.178</td>
<td>2.44</td>
</tr>
<tr>
<td>20</td>
<td>1.50</td>
<td>0.150</td>
<td>2.06</td>
</tr>
<tr>
<td>34</td>
<td>1.46</td>
<td>0.147</td>
<td>2.02</td>
</tr>
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</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of 1-10 g trichloroethene was equilibrated with 100 cm³ of distilled water for 6 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a ⁶³Ni 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.

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

Estimated Errors:
Solubility: not specified.
Temperature: ± 0.5 K.

References:
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$10^3 \chi_1$</th>
<th>$10^3 \chi_2$</th>
<th>$D_2 \chi_3 / \chi_2$</th>
<th>$D_2 \chi_3 / \chi_1$</th>
<th>$10^3 \chi_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.10</td>
<td>1.37</td>
<td>&lt;0.1 x 10^-3</td>
<td></td>
<td>2.91</td>
</tr>
<tr>
<td>36.85</td>
<td>1.64</td>
<td>0.141</td>
<td>194</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
A constant flow of trichloroethylene 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) trichloroethylene. A Hilson 18A extractometer provided accurate estimations of phase concentrations of trichloroethylene. Five samples of aqueous solutions were analysed 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% (compiler).
Temperature: ±0.5 K (compiler).

---

**Notes:**
1. Dow Release from Dow Chemical USA (October 3, 1975).
<table>
<thead>
<tr>
<th>Component(s):</th>
<th>Original Measurements: C₃H₇Cl₂</th>
<th>Variables: T/K = 310</th>
</tr>
</thead>
</table>

| Preparied By: A. L. Horvath |

<table>
<thead>
<tr>
<th>Experimental Data:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Partition coefficient, K₂</td>
</tr>
<tr>
<td>T/K°C</td>
</tr>
<tr>
<td>37</td>
</tr>
</tbody>
</table>

*Gas–liquid chromatographic parameter, from instrument calibration.

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Trichloroethane vapor was equilibrated in an air-tight vial with warm and the overlaying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an air tight syringe and this sample was injected into a gas chromatograph for analysis. The chromatogram peak height was used to calculate the partition coefficient.

**Estimated Errors:**

Solubility: ± 0.1 std dev.
Temperature: ± 0.5 K (compiler).

**Source and Purity of Materials:**

(1) Pfa magnet, laboratory grade, further purified by distillation; middle fraction was used.
(2) Distilled.

**Estimated Errors:**

Solubility: not specified.
Temperature: ± 0.05 K.
### Components:
1. Trichloroethylene (trichloroethylene); CCl$_2$CHCl$_2$; [79-01-6]
2. Water; H$_2$O; [7732-18-5]

### Original Measurements:

### Variables:
- $\text{T/K} = 233 - 303$

### Prepared by:
- A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>$\nu/{}^\circ \text{C}$</th>
<th>Henry's law constant, $H/\text{m}^3 \text{atm} \text{mol}^{-1}$</th>
<th>$10^6 x_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>$0.01 \times 10^{-3}$</td>
<td>0.01526</td>
<td>2.095</td>
</tr>
<tr>
<td>15</td>
<td>$0.22 \times 10^{-3}$</td>
<td>0.01516</td>
<td>2.081</td>
</tr>
<tr>
<td>20</td>
<td>$0.74 \times 10^{-3}$</td>
<td>0.01504</td>
<td>2.065</td>
</tr>
<tr>
<td>25</td>
<td>$1.62 \times 10^{-3}$</td>
<td>0.01491</td>
<td>2.047</td>
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<tr>
<td>30</td>
<td>$1.09 \times 10^{-2}$</td>
<td>0.01481</td>
<td>2.033</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Henry's law constants were determined by a method similar to that described by Mackay et al. A water sample containing trichloroethylene 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-mined and carbon-treated.

**Estimated Errors:**
- Solubility: ±0.99% of determ.
- Temperature: ±0.5 K (compiler)

**References:**

**Auxiliary Data**

<table>
<thead>
<tr>
<th>$\nu/{}^\circ \text{C}$</th>
<th>$10^{-3} x_1/\text{mol dm}^{-3}$</th>
<th>$10^3 x_1$ (compiler)</th>
<th>$10^6 x_1$ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>25</td>
<td>$1.12 \times 10^{-3}$</td>
<td>0.144</td>
<td>2.02</td>
</tr>
</tbody>
</table>

**Source and Purity of Materials:**
- New England Naphtha, used as received.
- Distilled.

**Estimated Errors:**
- Solubility: ±3.5% std. dev.
- Temperature: ±0.3 K.
Components:  
(1) Trichloroethene (trichloroethylene); C₂HCl₃ [79-0-6]  
(2) Water; H₂O; [7732-18-5]

Original Measurements:  

Variables:  
T/E = 74–209

Prepared By:  
A. L. Horvath

Experiments Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>Distribution coefficient, D</th>
<th>100 w₁</th>
<th>10⁶ s₁</th>
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</thead>
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<td>compiler</td>
<td>compiler</td>
</tr>
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<td>2.5</td>
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<td>1.991</td>
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<td>12.0</td>
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<td>0.1468</td>
<td>2.016</td>
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<td>12.0</td>
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<td>12.9</td>
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<td>14.0</td>
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<td>18.0</td>
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<td>3.790 x 10⁵</td>
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<td>19.0</td>
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<td>19.2</td>
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<td>19.5</td>
<td>3.965 x 10⁵</td>
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<td>1.884</td>
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<tr>
<td>24.3</td>
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<td>26.0</td>
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<td>26.1</td>
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<td>1.820</td>
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</table>

Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>10⁻³ q₁ /mol dm⁻³</th>
<th>10⁶ s₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>1.66 x 10⁻²</td>
<td>0.126</td>
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</tbody>
</table>

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 high performance liquid chromatographic procedures, which has been described elsewhere.

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: ± 0.5 K.

References:  
**Components:**
(1) Water; H2O [7732-18-5]
(2) Trichloroethene (trichloroethylene); C2HCl3; [79-01-6]

**Original Measurements:**

**Variables:**
T/K = 298

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
<td>( t/\degree C )</td>
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<tr>
<td>25</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Water was added gradually to 50 cm\(^3\) trichloroethene in a tank which was then lowered into a thermostat bath. The flask was shaken vigorously until the first cloud (fugacity) appeared. The sample water content was determined by the Karl Fischer titration method.

**Source and Purity of Materials:**
(1) Distilled (compiler).
(2) Commercial J&J extra pure reagent, further purified by conventional methods.

**Estimated Errors:**
Solvency: not specified.
Temperature: ±0.5 K (compiler).

**Components:**
(1) Trichloroethene (trichloroethylene); C2HCl3; [79-01-6]
(2) Water; H2O [7732-18-5]

**Original Measurements:**

**Variables:**
T/K = 293

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/\degree C )</td>
</tr>
<tr>
<td>20</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Source and Purity of Materials:**
(1) Fluka reagent, purified by distillation before use.
(2) Distilled (compiler).

**Estimated Errors:**
Solvency: not specified.
Temperature: ±0.1 K.
Components: (1) Trichloroethene (trichlorethylene); C₂Cl₃H₂; [79-01-5] (2) Water; H₂O; [7732-18-5]


Variables: T/K = 293

Prepared By: A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Method</th>
<th>Henry's law constant, ( H ) m³ atm mol⁻¹</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10⁷ ( x_1 ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>EPICS method</td>
<td>20</td>
<td>7.68 x 10⁻³</td>
<td>0.119</td>
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<tr>
<td></td>
<td></td>
<td></td>
<td>1.810</td>
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<tr>
<td>log ( H ) = 11.94-4920(T/K)</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Batch air stripping method</td>
<td>20</td>
<td>6.54 x 10⁻³</td>
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<td></td>
<td></td>
<td></td>
<td>2.052</td>
</tr>
<tr>
<td>log ( H ) = 9.703-4300(T/K)</td>
<td></td>
<td></td>
<td></td>
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</tbody>
</table>

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 vials and the equilibrated headspace 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 Error:
Solubility: ± 5%. Temperature: ± 0.1 K.

Source and Purity of Materials:
(1) Chemical Service, West Chester, PA.; present grade available.
(2) Distilled and run through two Barnstead purification cartridges.

Estimated Errors:
Solubility: ± 3.2% at. dev. Temperature: ± 0.5 K (compiler).

References:

Prepared By:
A. L. Horvath

Experimental Data:

| Method Apparatus/Procedure | Standard trichloroethene solutions of increasing concentrations were prepared in volumetric flasks as described elsewhere. The aqueous organic liquid phase was 25 cm³ and the vapor phase above the mixture was 35 cm³. 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 a least five measurements. |
Components:
(1) Trichloroethylene (trichlorethylene); C₇H₅Cl₂ [79-01-6]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 283–303

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, ( \rho_1 ) kg m⁻³</th>
<th>( 100 \ t_1 ) (complete)</th>
<th>( 10^9 \ t_1 ) (complete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.192</td>
<td>1.21</td>
<td>0.1210</td>
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<td>20</td>
<td>0.326</td>
<td>1.18</td>
<td>0.1180</td>
</tr>
<tr>
<td>30</td>
<td>0.535</td>
<td>1.15</td>
<td>0.1150</td>
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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 reprecipitated by liquid–liquid extraction before analysis. The experiments were carried out in duplicate.

Source and Purity of Materials:
(1) J.T. Baker Chemicals Co., N.J., greater than 99.9% pure.
(2) Distilled and deionized.

Estimated Errors:
Solubility: ±0.0077 at. %
Temperature: ±0.5 K

Method/Apparatus/Procedure:
A saturated solution was prepared by passing of water through a column which was packed with glass beads coated with trichloroethylene. The saturated solution was then pumped through an extractor column and trichloroethylene was extracted directly into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both an UV absorbance and a fluoresence detector with excitation filters. The peak area was evaluated using a Hewlett-Packard recorder.

Source and Purity of Materials:
(1) Eastman Kodak Co., commercial quality, used as received.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±1 K (compiler).
Components:
1. Trichloroethene (trichloroethylene); C₂HCl₃; [79-01-6]
2. Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 293

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>ln°C</th>
<th>10⁸ p₁ g m⁻³</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁸ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.5²</td>
<td>2.5 × 10⁻¹¹</td>
<td>3.43</td>
</tr>
</tbody>
</table>

*Cited value in the original paper is in error (compiler).

Auxiliary Information

Method/Apparatus/Procedure:
A supersaturated solution of trichloroethylene 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 trichloroethylene 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.

Component:
1. Trichloroethene (trichloroethylene); C₂HCl₃; [79-01-6]
2. Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 283–308

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>ln°C</th>
<th>Henry’s law constant, H m³ atm mol⁻¹</th>
<th>CV² %</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁸ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.6</td>
<td>1.78 × 10⁻⁵</td>
<td>3.52</td>
<td>0.1611</td>
<td>2.212</td>
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<tr>
<td>17.5</td>
<td>6.32 × 10⁻⁵</td>
<td>1.32</td>
<td>0.1410</td>
<td>1.934</td>
</tr>
<tr>
<td>24.8</td>
<td>9.58 × 10⁻⁵</td>
<td>3.81</td>
<td>0.1334</td>
<td>1.832</td>
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<td>24.6</td>
<td>1.49 × 10⁻⁵</td>
<td>2.89</td>
<td>0.1347</td>
<td>1.849</td>
</tr>
</tbody>
</table>

*CV² = 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 trichloroethylene was injected into an erlenmeyer flask 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 ERCS 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%.

Source and Purity of Materials:
1. Fluka AG Chemicals F., greater than 99.5%, stabilized with 0.01% triethylamine.
2. Distilled.

Estimated Errors:
Solubility: see above.
Temperature: ± 0.1 K.
### Components:
- (1) Trichloroethene (trichloroethylene), C₂HCl₃; [79-01-6]
- (2) Water, H₂O; [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 298

### Prepared By:
- A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>t[°C]</th>
<th>Henry's law constant, 8H/m³ atm mol⁻¹</th>
<th>10⁹ x₁ (complex)</th>
<th>10⁵ x₁ (complex)</th>
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</thead>
<tbody>
<tr>
<td>24.85</td>
<td>1.17 x 10⁻²</td>
<td>0.110</td>
<td>1.511</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
The original method and apparatus for the determination of Henry's law constants are described elsewhere. The general procedure was to add an excess quantity of trichloroethylene to distilled de-ionized water, place the sample in a thermostated bath, and provide overnight mixing. A portion of this solution was returned to the stripping vessel. Trichloroethylene 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) Reagent grade available and was used without further purification, stated greater than 99% purity.
- (2) Distilled and de-ionized.

**Estimated Errors:**
- Solubility: ± 6% and dev.
- Temperature: ± 0.05°C.

**References:**

<table>
<thead>
<tr>
<th>t[°C]</th>
<th>10⁶ g₂ / l₂</th>
<th>10⁹ w₁ (compiler)</th>
<th>10⁶ w₂ (compiler)</th>
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<tbody>
<tr>
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<td>1.0574</td>
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<td>1.194 x 10³</td>
<td>0.1194</td>
<td>1.4388</td>
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<tr>
<td>30</td>
<td>1.401 x 10³</td>
<td>0.1401</td>
<td>1.9233</td>
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</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
250 cm³ bottles were fitted with distilled and de-ionized water and sealed. A measured volume of trichloroethylene was injected into the bottle through each septum using a microsyringe. Trichloroethylene was extracted from the water in the anticipated solubility limit. The bottles were shaken for 1 hr with a wrist-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbosieve column and a FID detector. The GC response was compared with calibration peaks.

**Source and Purity of Materials:**
- (1) Probably a commercial grade at least 99% pure, as received.
- (2) Distilled and de-ionized.

**Estimated Errors:**
- Solubility: not specified.
- Temperature: ± 0.5 K (compiler).
**Components:**
(1) Trichloroethylene (trichloromethylene), C₂HCl₃; [79-01-6]
(2) Water, H₂O; [7732-18-5]

**Variables:**
T/K = 293-313

<table>
<thead>
<tr>
<th>t/°C</th>
<th>γ_f</th>
<th>10^4 x₁</th>
<th>100 w₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>5418±160</td>
<td>1.83</td>
<td>0.135</td>
</tr>
<tr>
<td>30</td>
<td>5188±195</td>
<td>1.93</td>
<td>0.141</td>
</tr>
<tr>
<td>40</td>
<td>5509±290</td>
<td>1.79</td>
<td>0.130</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficients of trichloroethylene (γ_f) in water. Cells containing degassed water were submerged in a thermostated water bath. Trichloroethylene 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: ±0.05 mol/L.
Temperature: ±0.5 K.

**Component:**
(1) Trichloroethylene (trichloromethylene), C₂HCl₃; [79-01-6]
(2) MQ-Water

**Variables:**
T/K = 293

| 23. Trichloroethylene with MQ-Water
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental Data</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>Henry’s Law constant, H/dimensionless</td>
</tr>
<tr>
<td>20</td>
<td>0.44</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**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/dl, 0.75 mg COD/l.

**Estimated Errors:**
Solubility: ±0.015 mol/L.
Temperature: ±0.5 K.
Components:
(1) Trichloroethene (trichloroethylene); C₂HCl₃; [79-01-6]
(2) Municipal tap water (PASE)

Original Measurement:

Variables:
TK = 288

Prepared By:
A. L. Hervah

24. Trichloroethene with Municipal Tap Water (PASE)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Henry's law constant, H (dimensionless)</th>
<th>100 w₁ (complex)</th>
<th>10³ s₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.500</td>
<td>8.21×10⁻²</td>
<td>1.127</td>
</tr>
</tbody>
</table>

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 injected 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 reconstituted by liquid-liquid extraction before analysis. The experiments were carried out in duplicates.

Source and Purity of Materials:
(1) J. T. Baker Chemical Co., N.J., greater than 99.5% pure.
(2) 10 mg total organic carbon/10⁶; 40 mg COD/10⁶.

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

Components:
(1) Water-d₂; D₂O; [7789-20-0]
(2) Trichloroethene (trichloroethylene); C₂HCl₃; [99-01-6]

Original Measurements:

Variables:
TK = 298

Prepared By:
A. L. Hervah

25. Trichloroethene with Water-d₂

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w₁ (M⁻¹/mo l)</th>
<th>100 w₁ (complex)</th>
<th>10³ s₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.12×10⁻³</td>
<td>2.24×10⁻³</td>
<td>1.42</td>
</tr>
</tbody>
</table>

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 water bath thermostat. The assembly was shaken mechanically for about 90 min at constant temperature. The amount of heavy water in the equilibrated 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. 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: ±1.0×10⁻³ std. dev.
Temperature: ±0.05 K.

References:
### Table 1: Tensile stability of pentachloroethane (1) in Water (2)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>25</th>
<th>30</th>
<th>35</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stability (K)</td>
<td>205.5</td>
<td>208.1</td>
<td>210.6</td>
</tr>
</tbody>
</table>

Note: Stability values are in Kelvin (K).

*Estimated Values:
Temperature: 235.5 K (complex)*
### Components

- (1) Pentachloroethane; C₂HCl₅; [76-01-7]
- (2) Water; H₂O; [7732-18-5]

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w₁₂ (compiler)</th>
<th>10⁵ x₁₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>4.7×10⁻²</td>
<td>4.7×10⁻²</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **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; H₂O; [7732-18-5]
- (2) Pentachloroethane; C₂HCl₅; [76-01-7]

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
<th>100 w₁ M⁻¹mol⁻¹g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.62×10⁻²</td>
<td>1.82</td>
<td>8.99×10⁻⁴</td>
</tr>
<tr>
<td>25</td>
<td>3.47×10⁻²</td>
<td>3.91</td>
<td>1.93×10⁻⁴</td>
</tr>
<tr>
<td>30</td>
<td>4.14×10⁻²</td>
<td>4.65</td>
<td>2.30×10⁻⁴</td>
</tr>
</tbody>
</table>

### Auxiliary Information

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

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ±0.5 K (compiler).

---

**References**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$10^5 x_1$ (complete)</th>
<th>$10^5 x_2$ (complete)</th>
<th>$10^5 x_3$ (complete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>5.0 × 10^{-2}</td>
<td>445</td>
<td>3.0 × 10^{-2}</td>
</tr>
</tbody>
</table>

**Experimental Data**

**Auxiliary Information**

**Method/Apparatus/Procedure**

A mixture of 1 to 15 volume ratio of water and peracetic acid was introduced into an equilibration flask and then lowered into a water bath thermoregulated. 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. 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: ± 2.0 × 10^{-3} av. dev.

Temperature: ± 0.05 K.

**References**

Components:
(1) Pentachloroethylene; C₃Cl₅H ; [76-01-7]
(2) Water; H₂O; [7732-18-5]

Variables:
T/K = 293

Experimental Data

\[ t/°C \quad 10^2 w_1 \quad 10^2 c_1 \quad 10^2 w_2 \quad 10^2 c_2 \]
\[ 20 \quad 4.7×10^{-2} \quad 4.18 \quad 0.24 \quad 2.63 \]

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of pentachloroethylene and water was preheated to the desired temperature before rapid mixing. The resulting mixture was taredomated and the equilibrium was maintained by vigorous stirring. The concentration of pentachloroethylene is water was determined by gas chromatography.

Source and Purity of Materials:
(1) Soxy reagent, distilled before use, purity was 99.9% by GLC.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K.
Components:  
(1) Pentachloroethane; C₂H₂Cl₅; [76-01-7]  
(2) Water; H₂O; [7732-18-5]

Variables:  
T/K = 293

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>n₁ V₁ m⁻¹ s⁻¹</th>
<th>100 w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3.80 × 10⁻³</td>
<td>7.69 × 10⁻²</td>
<td>6.85</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess quantity of pentachloroethane was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactivity techniques. The activity of the water samples was measured in a liquid scintillation spectrometer by counting 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.

Original Measurements:

Components:
(1) Pentachloroethane; C₂H₂Cl₅; [76-01-7]  
(2) Water; H₂O; [7732-18-5]

Variables:  
T/K = 298

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>ρ₁ g/kg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.486</td>
<td>4.81 × 10⁻²</td>
<td>4.28</td>
</tr>
</tbody>
</table>

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 washed with cyclohexane. The samples were analyzed by an Aminco-Bowman spectrophotometer. A detailed description of the method has been reported elsewhere.1

Source and Purity of Materials:
(1) Aldrich Chemical, highest grade, used as received.  
(2) Double distilled.

Estimated Errors:
Solubility: not specified.  
Temperature: ± 0.2 K (compiler).

References:
### Components:
1. Water; H₂O; [7732-18-5]
2. Pentachloroethane; C₂HCl₅; [76-01-7]

### Original Measurements:

### Variables:
77K = 298

### Prepared By:
A. L. Harvath

### Experimental Data

<table>
<thead>
<tr>
<th>h°C</th>
<th>$g_1 V_2^1/2$ g dm⁻³</th>
<th>100 $w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.02</td>
<td>3.7 × 10⁻¹</td>
<td>4.14</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Water was added gradually to 50 cm³ 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 method.

**Estimated Errors:**
Solubility: not specified.
Temperature: ±0.5 °C (compiler).

---

### Components:
1. Water-$d_2$; D₂O; [7782-20-0]
2. Pentachloroethane; C₂HCl₅; [76-01-7]

### Original Measurements:

### Variables:
77K = 298

### Prepared By:
A. L. Forvath

### Experimental Data

<table>
<thead>
<tr>
<th>h°C</th>
<th>100 $w_M$¹/₂ mol g⁻¹</th>
<th>100 $w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.03 × 10⁻¹</td>
<td>3.26 × 10⁻²</td>
<td>3.28</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
A mixture of 1 to 15 volume ratio of heavy water and pentachloroethane was introduced into an equilibrium flask and then lowered into a water with thermostatic temperature of about 90 min at constant temperature. The mixture heavy water in the equilibrium phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate. This procedure was taken from a secondary source. 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: ±1.0 × 10⁻² at 25°C.
Temperature: ±0.05 K.

**References:**
28. 1,2-Dibromo-1,2-Dichloroethane with Water
Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 x.r./x</th>
<th>100 w1 (complete)</th>
<th>x03 x1</th>
<th>(complete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>7.0 x 10^-3</td>
<td>7.0 x 10^-3</td>
<td>9.68</td>
<td></td>
</tr>
</tbody>
</table>

Auxiliary Information

Source and Purity of Materials:
(1) Distilled (complect).
(2) Jow Chemicals Co., used as received.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (complete).

29. 1,1,2,2-Tetramethoxyethane with Water

Critical Evaluation

The 1,1,2,2-tetramethoxyethane (1) and water (2) binary system is treated in two parts: part 1 is 1,1,2,2-tetramethoxyethane (1) in water (2) and part 2 is water (2) in 1,1,2,2-tetramethoxyethane (1).

Part 1. The solubility of 1,1,2,2-tetramethoxyethane (1) in water (2) has been studied by five groups of workers. The compilation sheets immediately follow the Critical Evaluation. The approximate datum of Booth and Everson is rejected because the reported solubility is somewhat low as well as only approximate. The datum of Blumberg and Metzler 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 Groes et al. are believed to be more reliable than the other data by Groes et al. and O'Connell. All the data are classified as tentative and listed in Table 1 at 5 K intervals. The solubility values of Groes et al. were smoothed by least squares regression to give the following equation:

\[ \text{Solubility} = 920.55 \exp(0.93396 - 1.07375 \times \frac{1}{T} + 1.407921 \times \left(\frac{1}{T}\right)^2) \]

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Reported Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0521</td>
</tr>
<tr>
<td>5</td>
<td>0.0539</td>
</tr>
<tr>
<td>10</td>
<td>0.0556</td>
</tr>
<tr>
<td>15</td>
<td>0.0594</td>
</tr>
<tr>
<td>20</td>
<td>0.0630</td>
</tr>
<tr>
<td>25</td>
<td>0.0678</td>
</tr>
<tr>
<td>30</td>
<td>0.0724</td>
</tr>
<tr>
<td>35</td>
<td>0.0794</td>
</tr>
<tr>
<td>40</td>
<td>0.0876</td>
</tr>
<tr>
<td>45</td>
<td>0.0948</td>
</tr>
<tr>
<td>50</td>
<td>0.106</td>
</tr>
<tr>
<td>55</td>
<td>0.115</td>
</tr>
<tr>
<td>60</td>
<td>0.120</td>
</tr>
<tr>
<td>65</td>
<td>0.141</td>
</tr>
<tr>
<td>70</td>
<td>0.156</td>
</tr>
<tr>
<td>75</td>
<td>0.175</td>
</tr>
<tr>
<td>80</td>
<td>0.194</td>
</tr>
<tr>
<td>85</td>
<td>0.219</td>
</tr>
<tr>
<td>90</td>
<td>0.246</td>
</tr>
<tr>
<td>95</td>
<td>0.274</td>
</tr>
<tr>
<td>100</td>
<td>0.307</td>
</tr>
</tbody>
</table>

Part 2. A small difference exists between the data of Huncison and Lyon at 298.15 K and that of Blumberg and Metzler at 302.15 K and O'Connell at 295.15 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 probably the most accurate, that is, 0.039 (100 w.) at 298.15 K.

References:
**Components:**

(1) 1,1,2,3-tetramethoxypropane; \( \text{C}_9\text{H}_{14}\text{O}_4 \); [79-7-6]
(2) Water; \( \text{H}_2\text{O} \); [7732-18-5]

**Variables:**

\( T/\text{K} = 298 \)

**Prepared By:**

A. L. Horvath

---

### Experimental Data

<table>
<thead>
<tr>
<th>( \Delta \text{C} )</th>
<th>( 10^3 \text{ g} \times \text{ g}^{-1} )</th>
<th>( 100 \omega_1 ) (compiler)</th>
<th>( 10^6 \chi_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.65</td>
<td>6.51×10^{-2}</td>
<td>3.39</td>
</tr>
<tr>
<td>25</td>
<td>2.113×10^{-1}</td>
<td>3.807×10^{-2}</td>
<td>*0.254</td>
</tr>
</tbody>
</table>

---

**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 Zeta combination liquid and gas interferometer described elsewhere. A detailed description of the complete procedure is given in a K. A. thesis.

**Source and Purity of Materials:**

(1) Eastman Kodak Co., purified by fractional distillation before use, b. p. range 124.4 to 125.0 °C.
(2) Distilled.

**Estimated Errors:**

Solubility: ±2.0%. Temperature: ±0.02 K.

**References:**

### Components
(1) 1,1,2,2-tetrachloroethane; C₂H₂Br₄; [79-27-6]
(2) Water; H₂O; [7732-11-5]

### Original Measurements

### Variables
T/K = 298

### Prepared By
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 V₁/V₂ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>&lt;2.6×10⁻²</td>
<td>&lt;5.9×10⁻²</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **Method/Apparatus/Procedure:**
  The sample equilibrium was established and ensured through repeated shaking and centrifuging of the sample mixture into a stopped Goetz tube and returned to the tube to a constant temperature water bath. The difference between the total amount of 1,1,2,2-tetrachloroethane which was added and the amount remaining in excess at equilibrium was taken as the amount of water added, dissolved in the known volume of water. The determination of the excess amount of water added has been described elsewhere.²

- **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:**

### Components
(1) 1,1,2,2-tetrachloroethane; C₂H₂Br₄; [79-27-6]
(2) Water; H₂O; [7732-11-5]

### Original Measurements

### Variables
T/K = 302–324

### Prepared By
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>10⁵ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10⁵ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>29</td>
<td>—</td>
<td>—</td>
<td>0.04±0.01</td>
<td>7.62</td>
</tr>
<tr>
<td>51</td>
<td>1.30±0.07</td>
<td>1.57</td>
<td>0.15±0.04</td>
<td>28.0</td>
</tr>
</tbody>
</table>

### 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. Commercial reagent.
  2. (2) Distilled (compiler).

- **Estimated Errors:**
  Solubility: see above.
  Temperature: ±1 K.
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 $x_1$</th>
<th>$10^2 x_1$ (compiler)</th>
<th>100 $x_2$</th>
<th>$10^2 x_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3.19</td>
<td>3.39</td>
<td>4.3 x 10^{-2}</td>
<td>7.62</td>
</tr>
<tr>
<td>30</td>
<td>6.5 x 10^{-2}</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **Source and Purity of Materials:**
  - Dow Chemical Co., used as received.
  - Distilled (compiler).

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ±0.5 K (compiler).

### Method/Apparatus/Procedure:

The equilibrium between 1,1,2,2-tetrafluoroethane 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 by 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.\(^3\)

### References:

31. 1,1-Dichloroethylene with Water

Critical Evaluation

The 1,1-dichloroethylene (1) and water (2) binary system is treated in two parts: part 1 is 1,1-dichloroethylene (1) in water (2) and part 2 is water (2) in 1,1-dichloroethylene (1).

Part 1. The solubility of 1,1-dichloroethylene (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, which to not include details on the origin of data, method of experimental determinations, and the purity of the component. Nevertheless, these two sources of information cannot be disregarded. The likely origin of the solubility data is from industrial reports, bulletins, or brochures.

The data reported in the early publications, particularly of McComett et al., Pearson and McComett, and Horne et al., are substantially lower than all other studies and are rejected. The datum of Warner et al. at 298.15 K is substantially higher than the selected value and is therefore rejected. The data of Winer at 298.15 K and at two different 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 Stirling, DeLeau and Schmidt, Leighton and Calo, and Kirk-Othmer, are given in Table I. The data of Gomperz et al. in the temperature range between 273.15 and 363.65 K are generally in reasonable agreement. The available solubility data of 1,1-dichloroethylene in water were first observed by DeLeau and Schmidt in 1918. They found that the solubility had 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.

![Graph showing solubility of 1,1-dichloroethylene (1) in water (2)](image-url)
The experimental data discussed above 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:

\[ \text{Solubility} = 100 \times e^{-1.5 \times 10^{-12} \times T + 1.25 \times 10^{-5} \times T^2} \]

The above equation, representing the combined data, yielded a standard deviation of 3.1 \times 10^{-3}. 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 2 K intervals for 1,1-dichloroethane in water are presented in Table 1.

**TABLE 1. Recommended solubility of 1,1-dichloroethane (1) in water (2)**

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>100 ( w_f )</th>
<th>Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.310</td>
<td>5.77</td>
</tr>
<tr>
<td>10</td>
<td>282.15</td>
<td>0.289</td>
<td>5.08</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.270</td>
<td>5.03</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.255</td>
<td>4.72</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.242</td>
<td>4.51</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.233</td>
<td>4.35</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.226</td>
<td>4.21</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.223</td>
<td>4.15</td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.222</td>
<td>4.12</td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.225</td>
<td>4.19</td>
</tr>
<tr>
<td>55</td>
<td>328.15</td>
<td>0.230</td>
<td>4.28</td>
</tr>
<tr>
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<td>90</td>
<td>363.15</td>
<td>0.355</td>
<td>6.62</td>
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</table>

Part 2. The solubility of water (2) in 1,1-dichloroethane (1) has been reported in three secondary sources only. They neither disclosed the original sources nor described the experimental methods and purity of components. Two sources reported identical solubilities of 0.035 [100 \( w_f \)] at 298.15 K, while the third reference (Ref. 1) gives the solubility of 0.4 [100 \( w_f \)] at 293.15 K. This latter value is too high and consequently it is rejected. The solubility values of 0.035 [100 \( w_f \)] 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:**
Components:  
(1) 1,1-dichloroethylene (1,1-dichloroethylen); $\text{C}_2\text{H}_4\text{Cl}_2$;  
[75-35-4]  
(2) Water; $\text{H}_2\text{O}$; [7732-18-5]  

<table>
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<th>Auxiliary Information</th>
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<th>Auxiliary Information</th>
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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).  

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).
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<th>100 w₂M₁⁻¹ mol g⁻¹ (compiler)</th>
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</thead>
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<td>16</td>
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<td>25</td>
<td>0.25</td>
<td>465</td>
<td>2.58×10⁻³</td>
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**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: ±10% (compiler).

---

**Components:**
(1) 1,1-dichloroethene (1,1-dichloroethylene): C₂H₄Cl₂;
(2) Water: H₂O; [7732-18-5]

**Original Measurements:**
Components:
(1) 1,1-dichloroethene (1,1-dichloroethylene); C₂H₂Cl₂;
[75-35-4]
(2) Water; H₂O; [7732-18-5]

Variables:
T/K = 293

Prepared By:
A. L. Horvath

Experimental Data:

<table>
<thead>
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<th>t/°C</th>
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<th>10⁵ x₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
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<tbody>
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<td>7.44</td>
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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 7% electron capture detector.

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

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

Original Measurements:

Components:
(1) 1,1-dichloroethene (1,1-dichloroethylene); C₂H₂Cl₂;
[75-35-4]
(2) Water; H₂O; [7732-18-5]

Variables:
T/K = 288–364

Prepared By:
A. L. Horvath

Experimental Data:

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<th>10⁵ x₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
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<td>0.225</td>
<td>4.19</td>
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<td>28.5</td>
<td>0.24</td>
<td>4.47</td>
<td>2.47×10⁻³</td>
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<td>29.5</td>
<td>0.255</td>
<td>4.35</td>
<td>2.63×10⁻³</td>
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<td>38.5</td>
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<td>4.09</td>
<td>2.27×10⁻³</td>
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<td>2.17×10⁻³</td>
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<td>55</td>
<td>0.21</td>
<td>3.51</td>
<td>2.17×10⁻³</td>
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<td>4.47</td>
<td>2.47×10⁻³</td>
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<tr>
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<td>71</td>
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<td>74.5</td>
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<td>81</td>
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<td>85.5</td>
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<td>90.5</td>
<td>0.35</td>
<td>6.52</td>
<td>3.61×10⁻³</td>
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</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Approximately 60 cm³ 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 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).
### Component: 1,1-dichloroethane (1,1-dichloroethylene; C₂H₂Cl₂)


#### Variables:

\( T/K = 276-299 \)

#### Experimental Data

<table>
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<tr>
<th>( \mu^\circ C )</th>
<th>( D_{\text{dimentionless}} )</th>
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<th>( 10^6 x_1 ) (compiler)</th>
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<td>25</td>
<td>5.33 \times 10^2</td>
<td>0.314</td>
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<td>70</td>
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<td>4.9299</td>
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<td>72.9</td>
<td>1.16 \times 10^3</td>
<td>0.228</td>
<td>4.2599</td>
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<td>18.0</td>
<td>1.334 \times 10^3</td>
<td>0.249</td>
<td>4.3227</td>
</tr>
<tr>
<td>19.5</td>
<td>1.732 \times 10^3</td>
<td>0.195</td>
<td>3.6572</td>
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<td>24.3</td>
<td>1.714 \times 10^3</td>
<td>0.243</td>
<td>4.5158</td>
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<td>26.1</td>
<td>2.148 \times 10^3</td>
<td>0.297</td>
<td>3.8115</td>
</tr>
</tbody>
</table>

*Gas-liquid system analysis parameter, from calibration measurement.

### Auxiliary Information

**Method/Apparatus/Procedure:**

A 5 mL 1,1-dichloroethane sample was injected into a 2.3 L equilibrium cell containing distilled water. 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-dichloroethane content was extracted and measured using a gas chromatograph equipped with a dual flame ionization detector.

**Source and Purity of Materials:**

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

**Estimated Errors:**

Solubility: ± 14.0%. Temperature: ± 0.5 K (compiler).

---

### Component: Water (H₂O)


#### Variables:

\( T/K = 298 \)

#### Experimental Data

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<th>( 10^5 x_1 ) (compiler)</th>
<th>( 10^6 w_2 ) (compiler)</th>
<th>( 10^6 x_2 ) (compiler)</th>
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</thead>
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<td>4.65</td>
<td>3.5 \times 10^{-2}</td>
<td>1.88</td>
</tr>
</tbody>
</table>

---

**Source and Purity of Materials:**

1. Source and purity not given.
2. Distilled (compiler).
Components: (1) 1,1-dichloroethene (1,1-dichloroethylene); C₂H₄Cl₂; [75-35-4]
(2) Water; H₂O; [7732-18-5]

Variables: T/K = 303

Prepared By: A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>H₂O</th>
<th>100 w₁ (compiler)</th>
<th>10¹⁰ x₁ (compiler)</th>
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<td>30</td>
<td>2222</td>
<td>0.2237</td>
<td>4.165</td>
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Estimated Errors:
Source and Purity of Materials:
(1) Chemical Service, West Chester, PA., USA, purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

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 at 18–24 h at four desired temperatures in a reciprocating shaking 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 4.76.

Source and Purity of Materials:
(1) Riedel-De-Haen A.R., greater than 99.9% by OIC analysis.
(2) Distilled.

Estimated Errors:
Solubility: see above.
Temperature: ±0.1 K.
### Experimental Data

<table>
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<tr>
<th>$T/°C$</th>
<th>$H/m^3$ am mol$^{-1}$</th>
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<th>$10^6 x_i$ (compiler)</th>
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<td>24.85</td>
<td>1.50×10$^{-2}$</td>
<td>0.506</td>
<td>9.410</td>
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</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
The original method and apparatus for the determination of Henry’s law constants are described elsewhere. The general procedure was as follows: 1. A sample of distilled water, heated to a known temperature, was placed in a stirred vessel. The 1,1-dichloroethylene was added to the solution and the mixture was stirred. The gas concentration in the headspace above the solution was monitored over time. 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) Liquid, not further specified. (2) Distilled and de-ionized.

**Estimated Errors:**
- Solubility: ± 0.6% std. dev.
- Temperature: ± 0.05°C

**References:**

### Experimental Data

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<th>$10^6 x_i$ (compiler)</th>
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<td>6.30×10$^{-2}$</td>
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<td>7.50×10$^2$</td>
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<td>6.56×10$^2$</td>
<td>6.56×10$^{-2}$</td>
<td>1220</td>
</tr>
</tbody>
</table>

### 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-dichloroethylene was injected into the bottles through each septum using a microsyringe. The 1,1-dichloroethylene was in excess of the solubility limit. The bottles were sealed for 1 hour with a wire-action shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a Carbopack C 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: ± 0.05 K (compiler).
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 in 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 CCl₄, CCl₃, CH₂Cl₂, CH₃Cl, and CH₄Cl in water. Both the measured values of McGovern2 and those of Sat0 and Nakajima3 are noticeably low and were not used for the smoothing equation.

The combined data of Gossen1 and Wright et al.4 were correlated to obtain the following mass percent (1) equation:

\[
\text{Solubility } [\%] = 27.735 - 0.178316(7K) + 2.92328 \times 10^{-5}(7K)^2,
\]

which yielded a standard deviation of 5.32×10⁻³ in the temperature range from 283.15 to 33.15 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 solute values for this system are given in Table 1, with 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 literature.

### TABLE 1. Tentative solubility of cis-1,2-dichloroethene (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature (K)</th>
<th>Solubility (10⁻³ w₁)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.755</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.705</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.667</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.641</td>
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<td>30</td>
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<td>0.631</td>
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<td>35</td>
<td>308.15</td>
<td>0.636</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.656</td>
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</table>

Part 2. The solubility of water (2) in cis-1,2-dichloroethene (1) has been studied by McGovern2 and Ohtsubo and Kuzum5 between 273.15 and 298.15 K. The solubility data of McGovern2 are believed to be more reliable than those of Ohtsubo and Kuzum5 because McGovern made measurements at more than one temperature. However, the data at 298.15 K is a misprint, and it should be read as 0.055 [100 w₂]. 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)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature (K)</th>
<th>Solubility (10⁻³ w₂)</th>
</tr>
</thead>
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<tr>
<td>0</td>
<td>273.15</td>
<td>0.019</td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.024</td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.028</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.034</td>
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<tr>
<td>20</td>
<td>293.15</td>
<td>0.039</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.055</td>
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</table>

References:


---

<table>
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<tr>
<th>T/K</th>
<th>0.25</th>
<th>0.30</th>
<th>0.35</th>
<th>0.40</th>
<th>0.45</th>
<th>0.50</th>
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<td>0.85</td>
<td>0.90</td>
<td>0.95</td>
<td>1.00</td>
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</table>

![Fig. 8. Solubility of cis-1,2-dichloroethene (1) in water (2).](image-url)
### Components:
1. cis-1,2-dichloroethylene (cis-1,2-dichloroethene); C₅H₄Cl₂; [196-59-3]
2. Water; H₂O: [7732-18-5]

### Original Measurements:

### Variables:

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<th>Temperature (°C)</th>
<th>100 w₁</th>
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<th>10³ x₂ (complex)</th>
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<td>—</td>
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</tr>
<tr>
<td>20</td>
<td>—</td>
<td>—</td>
<td>3.5 × 10⁻²</td>
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<tr>
<td>25</td>
<td>3.5 × 10⁻¹</td>
<td>4.52</td>
<td>5.5 × 10⁻¹</td>
</tr>
</tbody>
</table>

### Experimental Data

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 data at 25°C for (2) under 100 w₁ column is a misprint and should be 5.5 × 10⁻².

### Auxiliary Information

#### Method/Apparatus/Procedure:
 cis-1,2-dichloroethylene vapor sample was equilibrated in an air-tight vial between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vial 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 not given of the commercial grade.
(2) Distilled (complex)

#### Estimated Errors:
Solubility: not specified
Temperature: ± 0.5 K (compiler)

#### Source and Purity of Materials:
(1) Source not given of the commercial grade.
(2) Distilled
### Original Measurements:
2. cis-1,2-dichloroethene (cis-1,2-dichloroethylene): C₅H₄Cl₂ [156-59-2]

### Components:
2. cis-1,2-dichloroethene (cis-1,2-dichloroethylene): C₅H₄Cl₂ [156-59-2]

### Variables:
T/K = 298

### Experimental Data

<table>
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<th>Temperature (°C)</th>
<th>100 w₁ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.17</td>
<td>9.1×10⁻²</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Components:**
2. cis-1,2-dichloroethene (cis-1,2-dichloroethylene): C₅H₄Cl₂ [156-59-2]

**Variables:**
T/K = 298

**Original Measurements:**

**Prepared By:**
A. L. Lervagh

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Henry's law constant, ( H ip ) ( \text{mm} \text{ mol}^{-1} )</th>
<th>CV(^a)</th>
<th>100 w₁ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.3</td>
<td>172×10⁻²</td>
<td>3.99</td>
<td>€7632</td>
<td>1.427</td>
</tr>
<tr>
<td>17.5</td>
<td>265×10⁻²</td>
<td>2.44</td>
<td>€7037</td>
<td>1.315</td>
</tr>
<tr>
<td>24.8</td>
<td>408×10⁻²</td>
<td>6.32</td>
<td>€6359</td>
<td>1.188</td>
</tr>
<tr>
<td>34.6</td>
<td>545×10⁻²</td>
<td>5.04</td>
<td>€7186</td>
<td>1.343</td>
</tr>
</tbody>
</table>

\(^{a}\)CV = coefficient of variation (+100 S.D./mean).

**Source and Purity of Materials:**
(1) Aldrich Chemical Co., 97% pure.
(2) Distilled.

**Estimated Errors:**
Solubility; not specified.
Temperature: ± 0.5 K (compiler).
### Components:
1. cis-1,2-dichloroethylene (cis-1,2-dichloroethylene); C_{2}H_{4}Cl_{2}; [55-59-2]
2. Water; H_{2}O; [7732-18-5]

### Original Measurements:

### Variables:
77K = 283–333

### Prepared By:
A. L. Horvath

### Experimenal Data

<table>
<thead>
<tr>
<th>°C</th>
<th>10^6 ( x_{1}/t_2 )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10^5 ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.52×10^2</td>
<td>1.52×10^{-2}</td>
<td>2.825</td>
</tr>
<tr>
<td>30</td>
<td>2.73×10^2</td>
<td>2.73×10^{-2}</td>
<td>5.075</td>
</tr>
<tr>
<td>40</td>
<td>1.76×10^2</td>
<td>1.76×10^{-2}</td>
<td>3.271</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
250 cm³ bottles were filled with distilled and de-ionized water and sealed. A measured volume of cis-1,2-dichloroethylene was injected into the bottles through each system using a microsyringe. The cis-1,2-dichloroethylene 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, as received.
(2) Distilled and de-ionized.

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

### Components:
1. cis-1,2-dichloroethylene (cis-1,2-dichloroethylene); C_{2}H_{4}Cl_{2}; [55-59-2]
2. Water; H_{2}O; [7732-18-5]

### Original Measurements:

### Variables:
77K = 293–313

### Prepared By:
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>°C</th>
<th>( \gamma_i )</th>
<th>10^5 ( x_1 )</th>
<th>100 ( w_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>856±44</td>
<td>1.17</td>
<td>0626</td>
</tr>
<tr>
<td>30</td>
<td>884±43</td>
<td>1.13</td>
<td>0605</td>
</tr>
<tr>
<td>40</td>
<td>866±65</td>
<td>1.20</td>
<td>0616</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of cis-1,2-dichloroethylene (\( \gamma_i \)) in water. Cells containing degassed water were submerged in a thermostated water bath. The cis-1,2-dichloroethylene 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.
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 and those of Sato and Nakajima are believed to be higher than the expected solubility and are rejected. The solubility determination of Horw et al. tend to appear low in general as discussed in the critical evaluation of solubilities of CCl₄, chloroform, CCl₃CH₂Cl, CH₂Cl₂, and cis-1,2-CH₂=CHCl in water, and they are also rejected.

The remaining solubility data of Gosset, Warner et al., and Weight et al. were used to obtain by regression the following mass percent (1) equation:

\[ \text{Solubility} = 7.803 \times 10^{-4} + 5.453 \times 10^{-7} (\text{T/K}) - 6.967 \times 10^{-11} (\text{T/K})^2. \]

This equation represents the combined data points and it yields a standard deviation of 2.722 × 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) as 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).](image)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperatures K</th>
<th>100 w_i</th>
<th>Solubility 10^5 g/L</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.525</td>
<td>9.83</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.497</td>
<td>9.27</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.472</td>
<td>8.85</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.452</td>
<td>8.46</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.433</td>
<td>8.08</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.419</td>
<td>7.82</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.408</td>
<td>7.60</td>
</tr>
</tbody>
</table>

Part 2. The solubility of water (2) in trans-1,2-dichloroethene (1) has been studied only by McGovern 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:
**Component:**
- C₆H₅Cl₂; [30-60-5]
- Water; H₂O; [7732-18-5]

**Prepared By:**
A. L. Horwitz

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w₁ (compiler)</th>
<th>100 w₂ (compiler)</th>
<th>10² Kₑ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>6.3 × 10⁻³</td>
<td>1.18</td>
<td>1.14</td>
</tr>
</tbody>
</table>

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 data at 25°C for (2) under the 100 w₁ column is a misprint and should be 5.5 × 10⁻².

**Auxiliary Information:**

**Method/Apparatus/Procedure:**
A sample of trans-1,2-dichloroethene vapor was equilibrated in an air-tight vial between water and the overlying air. When equilibrium was established, a portion of the equilibrated air in the vessel was withdrawn using an air tight 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:**
- Source and purity not given.
- Distilled.

**Estimated Errors:**
Solubility: ±0.4 std. dev.
Temperature: ±0.5 K (compiler).
Original Measurements:

Variables:
77K = 283-308

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>Henry's Law Constant, ( H/m^2 \text{ atm} \text{ mol}^{-1} )</th>
<th>CV(^*)</th>
<th>( 10^6 w_1 ) (compiler)</th>
<th>( 10^6 x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>4.20x10(^{-8})</td>
<td>1.76</td>
<td>0.5354</td>
<td>9.993</td>
</tr>
<tr>
<td>17.5</td>
<td>6.60x10(^{-8})</td>
<td>2.27</td>
<td>0.4738</td>
<td>8.819</td>
</tr>
<tr>
<td>24.8</td>
<td>9.38x10(^{-8})</td>
<td>2.07</td>
<td>0.4344</td>
<td>8.873</td>
</tr>
<tr>
<td>34.6</td>
<td>3.80x10(^{-8})</td>
<td>1.75</td>
<td>0.4339</td>
<td>8.566</td>
</tr>
</tbody>
</table>

\(^*\)CV=coefficient of variation (= 100 S.D./mean).

Auxiliary Information

Method/Apparatus/Procedure:
The original method and apparatus for the determination of Henry's law constants, as described by Mackay et al., 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 thermostatic bath, and mix overnight. A portion of this solution was filtered and the filtrate was analyzed for trans-1,2-dichloroethene. 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) Redel-De Haen adL, greater than 99.9% pure.
(2) Distilled and de-ionized.

Estimated Errors:
Solubility: ±0.5% rel. dev.
Temperature: ±0.05 K.

Reference:
**Components:**
1. trans-1,2-dichloroethylene (trans-1,2-dichloroethylene); \( \text{C}_2\text{H}_4\text{Cl}_2 \); [15-69-5]
2. Water; \( \text{H}_2\text{O} \); [7732-18-5]

**Variables:**
\( T/K = 283-303 \)

**Prepared By:**
A. L. Forath

**Experimental Data**

<table>
<thead>
<tr>
<th>( T/^\circ C )</th>
<th>( 10^5 \gamma_1 )</th>
<th>( 10^5 x_1 )</th>
<th>( 100 w_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>4.188 \times 0^3</td>
<td>0.4188</td>
<td>7.810</td>
</tr>
<tr>
<td>20</td>
<td>3.599 \times 0^3</td>
<td>0.3599</td>
<td>6.691</td>
</tr>
<tr>
<td>30</td>
<td>3.863 \times 0^3</td>
<td>0.3863</td>
<td>7.198</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
250 cm³ bottles were filled with distilled and de-ionized water and sealed. A measured volume of trans-1,2-dichloroethylene was injected into the bottles through a septum using a microsyringe. The trans-1,2-dichloroethylene was in excess of the anticipated solubility limit. The bottles were shaken for 1 h with a wrist-action shake 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 cuts.

**Source and Purity of Materials:**
(1) Probably a commercial reagent, at least 99% pure as received.
(2) Distilled and de-ionized.

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

---

**Components:**
1. trans-1,2-dichloroethylene (trans-1,2-dichloroethylene); \( \text{C}_2\text{H}_4\text{Cl}_2 \); [15-69-5]
2. Water; \( \text{H}_2\text{O} \); [7732-18-5]

**Variables:**
\( T/K = 293-313 \)

**Prepared By:**
A. L. Forath

**Experimental Data**

<table>
<thead>
<tr>
<th>( T/^\circ C )</th>
<th>( y_1 )</th>
<th>( 10^5 x_1 )</th>
<th>( 100 w_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>200±60</td>
<td>8.33</td>
<td>0.407</td>
</tr>
<tr>
<td>30</td>
<td>1310±65</td>
<td>7.63</td>
<td>0.409</td>
</tr>
<tr>
<td>40</td>
<td>1370±75</td>
<td>7.30</td>
<td>0.392</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of trans-1,2-dichloroethylene (\( y_1 \)) in water. Cells containing degassed water were submerged in a thermostated water bath. The trans-1,2-dichloroethylene 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.
### 34. 1,2-Dichloro-1,1-Difluoroethane with Water

**Experimental Data:**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 x₁</th>
<th>100 x₂</th>
<th>100 x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>0.49</td>
<td>5.57</td>
<td>8.1×10⁻²</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Source and Purity of Materials:**
  - (1) Source and purity not given.
  - (2) Extracted (compiler).

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ±1 K (compiler).

**Components:**
- (1) 1,1,1,2-tetrafluoroethane; C₂F₄Cl₂ [600-29-6]
- (2) Water; H₂O [7732-18-5]

**Original Measurements:**

**Prepared By:**
- A. L. Horváth

**Method/Apparatus/Procedure:**
Details are not available. The original report is not obtainable; therefore, the solubility data were taken from a secondary source.

---

**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 237.15 to 323.15 K. There is a reasonable agreement among the reported results except for those of Chou and Freed whose measurements are markedly lower than other data and are therefore rejected.

The combined data of van der Waals, Schreinemakers et al., Sato and Nishi, and Weight et al. were correlated to obtain the following mass percent (1) equation:

\[
\text{Solubility (100 g sol.)} = 2.17896 - 1.966 \times 10^{-3} (1/k) + 2.83507 \times 10^{-5} (1/k)^2
\]

which shows a standard deviation of 4.97×10⁻³ in the temperature range from 237.15 to 323.15 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 0. The curve shows a distinct minimum at 296.76 K. The appearance of the solubility minimum for aprotic 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.

**Components:**
- (1) 1,1,1,2-tetrachloroethane; C₂Cl₄ [600-29-6]
- (2) Water; H₂O [7732-18-5]

**Evaluator:**

![Graph](image-url)

**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)

<table>
<thead>
<tr>
<th>Temperature</th>
<th>X</th>
<th>100 w₁</th>
<th>10⁶ x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.120</td>
<td>1.289</td>
</tr>
<tr>
<td>5</td>
<td>273.15</td>
<td>0.115</td>
<td>1.236</td>
</tr>
<tr>
<td>10</td>
<td>288.15</td>
<td>0.111</td>
<td>1.192</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.108</td>
<td>1.160</td>
</tr>
<tr>
<td>20</td>
<td>299.15</td>
<td>0.107</td>
<td>1.150</td>
</tr>
<tr>
<td>25</td>
<td>299.15</td>
<td>0.107</td>
<td>1.150</td>
</tr>
<tr>
<td>30</td>
<td>308.15</td>
<td>0.108</td>
<td>1.160</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.110</td>
<td>1.182</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.113</td>
<td>1.214</td>
</tr>
<tr>
<td>45</td>
<td>313.15</td>
<td>0.117</td>
<td>1.257</td>
</tr>
<tr>
<td>50</td>
<td>322.15</td>
<td>0.123</td>
<td>1.322</td>
</tr>
</tbody>
</table>

Part 2: The solubility of water (2) in 1,1,1,2-tetrachloroethane has been reported in a paper. Only the data of Sturman⁶ are available for the solubility of water in 1,1,1,2-tetrachloroethane and no critical evaluation is possible. These data are classified as tentative. For further details the reader is referred to the relevant compilation.

References:
Components:
(1) Water; H₂O [7732-18-5]
(2) 1,1,2-trichloroethane; C₃H₅Cl₂ [620-20-6]

Variables:
77K = 273.15K

Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>100 w₃</th>
<th>100 w₃ M⁺⁻¹ mol⁻¹ g⁻¹ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.30×10⁻²</td>
<td>2.3×10⁻²</td>
</tr>
<tr>
<td>25</td>
<td>5.55×10⁻²</td>
<td>5.8×10⁻²</td>
</tr>
<tr>
<td>30</td>
<td>6.08×10⁻²</td>
<td>6.0×10⁻²</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
A mixture of 1,1,2-trichloroethane and water was shaken for about 12 hours in a paraffin bath held at a constant temperature. 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:
Components:
(1) 1,1,1,2-tetrachloroethane; C₂H₂Cl₄; [630-2-6]
(2) Water; H₂O; [7732-18-5]

Original Measurements:
C. T. Chieh and V. F. Freid, "Chromodynamic Studies on Beach

Variables:
T/K = 296.07

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>S (V₂/g)</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>0.23</td>
<td>2.15 × 10⁻⁴</td>
<td>2.31</td>
</tr>
<tr>
<td>20</td>
<td>0.20</td>
<td>2.00 × 10⁻⁴</td>
<td>2.15</td>
</tr>
<tr>
<td>34</td>
<td>0.20</td>
<td>2.02 × 10⁻⁴</td>
<td>2.17</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of 5–10 g 1,1,1,2-tetrachloroethane was equilibrated
with 100 cm³ 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 3% SE-30 column and a
deuterated polystyrene 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: ±0.5 L.

References:
¹C. T. Chieh and D. V. Schmeling, Text. Protec. Environ. Fate

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

Estimated Errors:
Solubility: ±0.5 ± 0.1 K (compiler).
Components:
(1) 1,1,2,2-tetrachloroethane: C₆H₄Cl₄ [630-20-6]
(2) Water: H₂O [7732-18-5]

Original Measurements:

Variables:
\( T(K) = 293-313 \)

Prepared By:
A. L. Horvath

Experimental Data

$$t(C) \quad \gamma \quad 10^6 x_1 \quad 100 \% w_1$$

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>82862.730</td>
<td>1.08</td>
<td>0.101</td>
</tr>
<tr>
<td>30</td>
<td>85505.635</td>
<td>1.17</td>
<td>0.109</td>
</tr>
<tr>
<td>40</td>
<td>88385.645</td>
<td>1.13</td>
<td>0.105</td>
</tr>
</tbody>
</table>

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 (\( \gamma \)) in water. Cells containing degassed water were immersed in a thermostat at a desired temperature. 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.

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 Hojo and Leavell \(^1\) and Persnyosov 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 Veen \(^4\), Othmer et al. \(^5\), McElroy et al. \(^6\), Gierowski et al. \(^7\), Chiba and Frenz \(^8\), Sato and Nishijima \(^9\), Stack \(^10\), and Stack et al. \(^11\), Bunsell et al. \(^12\), Sauer and Miller \(^13\), Lighton and Cabo \(^14\), McNally and Grob \(^15\), and Riedel and Wille \(^16\), Howe et al. \(^17\), Vogel \(^18\), and Wright and Schaffer \(^19\) were used to obtain the following mass percent (\(\gamma\)) equation:

$$\text{Solubility} \gamma = 4.87993 - 1.40377 \times 10^{-3} (T/K) + 5.20513 \times 10^{-5} (T/K)^2,$$

which shows a standard deviation of 4.344 x 10\(^{-3}\) 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).](image-url)
Table 1. Recommended solubility of 1,1,2,2-tetrachloroethene (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>ζ</th>
<th>100 w₁</th>
<th>Solubility</th>
<th>10⁵ xₐ</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>271.15</td>
<td>0.302</td>
<td>3.35</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>271.1</td>
<td>0.293</td>
<td>3.3</td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>271.1</td>
<td>0.287</td>
<td>3.4</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>271.1</td>
<td>0.284</td>
<td>3.36</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>271.1</td>
<td>0.283</td>
<td>3.25</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>271.1</td>
<td>0.285</td>
<td>3.27</td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>271.1</td>
<td>0.290</td>
<td>3.16</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>271.1</td>
<td>0.296</td>
<td>3.18</td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>271.1</td>
<td>0.306</td>
<td>3.29</td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>271.1</td>
<td>0.318</td>
<td>3.32</td>
<td></td>
</tr>
</tbody>
</table>

Table 2. Recommended solubility of water (2) in 1,1,2,2-tetrachloroethene (1)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>K</th>
<th>100 w₂</th>
<th>Solubility</th>
<th>10⁵ xₐ</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.0605</td>
<td>0.56</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.0803</td>
<td>0.65</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.0861</td>
<td>0.75</td>
<td></td>
<td></td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.0931</td>
<td>0.86</td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.107</td>
<td>0.94</td>
<td></td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.121</td>
<td>1.12</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.138</td>
<td>1.27</td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.155</td>
<td>1.43</td>
<td></td>
<td></td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.174</td>
<td>1.60</td>
<td></td>
<td></td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.195</td>
<td>1.79</td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.219</td>
<td>2.00</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Part 2. The solubility of water (2) in 1,1,2,2-tetrachloroethene (1) has been studied by 11 groups of workers, mostly at 298.5 K. The data of Lee and Sarrat3 is markedly lower than other results and is therefore rejected. The measurements of Offen et al.,4 McGovern,5 and Ziemlinski6 are several percent higher than the smoothed solubility value and are also rejected. The solubilities calculated from the distribution coefficients of Prystytny et al.7 are in very good agreement, giving no confidence in the values which are regarded as doubtful. The remaining data of Swanson,33 Hilitz and Lyon,4 Johnson et al.,34 Johnson,35 Cristian et al.,36 and Barr and Newham37 were compiled or used for its smoothing equation. The fitting equation used was:

\[ \log_{10} x_a = 3.1715 - 974.64(1/T) \]

This equation represents the combined data with a standard deviation of 3.36 x 10⁻² in the 23–323 K temperature range.

The recommended solubilities at 5 K intervals for water in 1,1,2,2-tetrachloroethene are given in Table 2.

Measured values and the curve obtained from the smoothing equation for solubility expressed as \( \log_{10} x_a \) 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, \( \log_{10} x_a \) versus \( 1/(T/K) \), in which case a straight line usually represents the curve, at least over some limited temperature range.
References:


Components: 1
Original Measurements:
1. 1,2,2-trichloroethane: C₃H₆Cl₃ [79-345]

Variables:
77K = 298
Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>V₃₅g⁻¹/dm³kg⁻¹</th>
<th>100 w₁ (compiler)</th>
<th>92 x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.50 x 10⁻⁵</td>
<td>0.286</td>
<td>3.08</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The solubility was determined by mixing definite quantities of 1,2,2-trichloroethane with large volumes of water and measuring the volume of the unsaturated 1,2,2-trichloroethane.

Source and Purity of Materials:
(1) Commercial grade, further purified by washing with a NaClO₃ solution and redistilled.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.5 K (compiler).
### Components

1. 1,1,2,2-tetrachloroethane; C₃H₇Cl₄ [79-34-3]
2. Water; H₂O [7732-18-5]

### Original Measurements


### Variables

T/K = 293–303

### Prepared By

A. L. Horvah

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 x₁</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.288</td>
<td>0.287</td>
<td>3.09</td>
</tr>
<tr>
<td>55.5</td>
<td>0.33x²</td>
<td>0.335</td>
<td>3.61</td>
</tr>
</tbody>
</table>

### 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).

### Original Measurements


### Variables

T/K = 273–303

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>10³ x₁</th>
<th>100 w₁Mᵢkg⁻¹mol⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>5.84x¹⁰⁻²</td>
<td>5.73x₁₀⁰</td>
<td>3.24x¹⁰⁻³</td>
</tr>
<tr>
<td>25</td>
<td>1.095x¹⁰⁻⁷</td>
<td>1.09x₁₀⁰</td>
<td>6.09x¹⁰⁻³</td>
</tr>
<tr>
<td>30</td>
<td>1.32x¹⁰⁻⁷</td>
<td>1.23x₁₀⁰</td>
<td>7.33x¹⁰⁻³</td>
</tr>
</tbody>
</table>

### 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:

<table>
<thead>
<tr>
<th>Component:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1,1,2,2-tetrachloroethane: $\text{C}_4\text{H}_2\text{Cl}_4$ [79-3-5]</td>
<td>D. P. Ohmer, R. E. White, and E. Trüger, Ind. Eng. Chem. 33, 1513 (1941).</td>
</tr>
<tr>
<td>(2) Water: $\text{H}_2\text{O}$ [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$77K=299$</td>
<td>A. L. Sorvath</td>
</tr>
</tbody>
</table>

**Experimental Data**

<table>
<thead>
<tr>
<th>$\mu^\circ$C</th>
<th>0.9 $w_1$</th>
<th>0.9 $w_2$</th>
<th>10$^3$ $x_1$ (compiler)</th>
<th>10$^5$ $x_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.5</td>
<td>0.28</td>
<td>0.13</td>
<td>1.2</td>
<td>1.06</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>0.115</td>
<td></td>
</tr>
</tbody>
</table>

**Auxiliary Information**

Method/Apparatus/Procedure:
The determination of the solubility was carried out in a 125 cm$^3$ Erlenmeyer flask, containing about 8 cm$^3$ of water. 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 acceptable 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:

<table>
<thead>
<tr>
<th>Component:</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) 1,1,2,2-tetrachloroethane: $\text{C}_4\text{H}_2\text{Cl}_4$ [79-3-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$77K=299$</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

**Experimental Data**

<table>
<thead>
<tr>
<th>$\mu^\circ$C</th>
<th>100 $w_1 M_1^{-1}$/mol $g^{-1}$</th>
<th>10$^5$ $x_1$ (compiler)</th>
<th>10$^8$ $w_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>6.41 × 10$^{-3}$</td>
<td>1.06</td>
<td>0.115</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

Method/Apparatus/Procedure:
A 1 to 15 volume ratio mixture of 1,1,2,2-tetrachloroethane and water was introduced into an equilibration flask and then lowered into the water-bath thermometer. The assembly was shaken mechanically for about 30 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. 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: ± 3.0 × 10$^{-3}$ wt. dev.
Temperature: ± 0.05 K.

References:
## Experimental Data

<table>
<thead>
<tr>
<th>n°C</th>
<th>$10^4 w_1$</th>
<th>$10^5 x_1$</th>
<th>100 $w_2$</th>
<th>$10^5 x_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.8×10^{-1}</td>
<td>3.01</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>25</td>
<td>2.9×10^{-1}</td>
<td>3.12</td>
<td>1.13</td>
<td>9.62</td>
</tr>
<tr>
<td>30</td>
<td>3.0×10^{-1}</td>
<td>3.23</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>40</td>
<td>3.0×10^{-1}</td>
<td>3.28</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>50</td>
<td>3.1×10^{-1}</td>
<td>3.54</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

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).

### Source and Purity of Materials:
1. Water, H$_2$O [7732-18-5]
2. 1,1,2,2-tetrafluoroethane, C$_2$H$_2$Cl$_2$ [79-34-5]

### 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.

Source and Purity of Materials:
1. Distilled (compiler).
2. Glaxo Chemical, washed and redissolved before use.

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

References:
### Experimental Data

<table>
<thead>
<tr>
<th>( T/K )</th>
<th>( \Delta H/\text{cmol} )</th>
<th>( % \text{w}_1 )</th>
<th>( 10^5 x_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>97.9</td>
<td>10</td>
<td>8.60</td>
<td>1.60</td>
</tr>
<tr>
<td>94.5</td>
<td>5.1</td>
<td>32.37</td>
<td>5.1</td>
</tr>
<tr>
<td>94.0</td>
<td>17.79</td>
<td>65.85</td>
<td>17.79</td>
</tr>
<tr>
<td>93.4</td>
<td>33.0</td>
<td>84.55</td>
<td>37.0</td>
</tr>
<tr>
<td>94.1</td>
<td>53.1</td>
<td>91.34</td>
<td>33.1</td>
</tr>
<tr>
<td>94.1</td>
<td>85.87</td>
<td>98.26</td>
<td>85.87</td>
</tr>
<tr>
<td>94.0</td>
<td>91.8</td>
<td>99.05</td>
<td>91.8</td>
</tr>
<tr>
<td>95.3</td>
<td>96.85</td>
<td>99.65</td>
<td>96.85</td>
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<tr>
<td>116.0</td>
<td>96.9</td>
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<td>96.9</td>
</tr>
<tr>
<td>131.5</td>
<td>99.01</td>
<td>99.89</td>
<td>99.01</td>
</tr>
<tr>
<td>146.3</td>
<td>100.0</td>
<td>100.0</td>
<td>100.0</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

Samples of the organic-water solutions were equilibrated in isothermal waterbaths. A solvent isoporous apparatus was used which has been described elsewhere. The water solubilities were determined using a Beckman Model KFP-1 Analyzer.

**Source and Purity of Materials:**

(1) Distilled (compiler)

(2) Source not given. Reagent grade, distilled in an Okenhaw oven before use.

**Estimated Errors:**

Solubility: ± 0.0012.

Temperature: ± 0.1 K.

**References:**

**Components:**
(1) Water, H₂O [7732-18-5]
(2) 1,1,2,2-tetrachloroethane, C₂H₂Cl₄ [79-35-2]

**Original Measurements:**

**Variables:**
T/K = 298

**Prepared By:**
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10⁻² C₁ /mol dm⁻³</th>
<th>10⁵ w₁ (complete)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.141</td>
<td>0.115</td>
<td>1.06</td>
</tr>
</tbody>
</table>

### 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 refractometer 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, H₂O [7732-18-5]
(2) 1,1,2,2-tetrachloroethane, C₂H₂Cl₄ [79-34-0]

**Original Measurements:**

**Variables:**
T/K = 298

**Prepared By:**
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>n₁V₂⁻¹/mol dm⁻³</th>
<th>10⁵ w₁ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.1030±0.0012</td>
<td>0.1143</td>
<td>13.55</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
The solube imporatent method was used without modifiasion. 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-1-A analyzer. The Karl Fischer reagent was standardized against crystalline sodium acetate-hydrate.

**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:
(1) Water, H₂O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane, C₂H₄Cl₄; [79-34-5]

Variables:
T/K = 298

Prepared By:
A. L. Horvath

Experimental Data:

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>100 w₁, mol g⁻¹</th>
<th>100 w₁, mol g⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>4.0×10⁻³</td>
<td>3.71</td>
<td>2.2×10⁻²</td>
</tr>
</tbody>
</table>

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 torsion magnet for about 48 h. The concentration of water in the organic liquid phase was determined by the Karl Fisher titration method.

Estimated Errors:
Solubility: ±7%.
Temperature: ±0.1 °.

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

Original Measurements:

Components:
(1) 1,1,2,2-tetrachloroethane, C₂H₄Cl₄; [79-34-5]
(2) Water, H₂O; [7732-18-5]

Variables:
T/K = 287–373

Prepared By:
A. L. Horvath

Experimental Data:

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Distribution coefficient,² n₁/n₂</th>
<th>100 w₁, mol g⁻¹ (compiler)</th>
<th>100 w₁, mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>1.36×10¹</td>
<td>1.05×10⁻²</td>
<td>2.09×10⁻¹</td>
</tr>
<tr>
<td>32</td>
<td>8.80×10¹</td>
<td>1.00×10⁻²</td>
<td>1.07×10⁻¹</td>
</tr>
<tr>
<td>50</td>
<td>5.90×10¹</td>
<td>4.20×10⁻¹</td>
<td>4.50×10⁻¹</td>
</tr>
<tr>
<td>60</td>
<td>5.50×10¹</td>
<td>7.30×10⁻¹</td>
<td>8.06×10⁻¹</td>
</tr>
<tr>
<td>70</td>
<td>4.50×10¹</td>
<td>1.47×10⁻¹</td>
<td>1.37×10⁻¹</td>
</tr>
<tr>
<td>80</td>
<td>4.40×10¹</td>
<td>2.32×10⁻¹</td>
<td>2.59×10⁻¹</td>
</tr>
<tr>
<td>90</td>
<td>3.55×10¹</td>
<td>4.37×10⁻¹</td>
<td>4.92×10⁻¹</td>
</tr>
<tr>
<td>90.4</td>
<td>2.95×10¹</td>
<td>6.61×10⁻¹</td>
<td>7.14×10⁻¹</td>
</tr>
<tr>
<td>100</td>
<td>2.80×10¹</td>
<td>7.95×10⁻¹</td>
<td>8.59×10⁻¹</td>
</tr>
</tbody>
</table>

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 H₂ in 1,1,2,2-tetrachloroethane in both liquid and vapor phases was determined by using a ³⁵Cl labeled compound.

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

Source and Purity of Materials:
(1) Source and purity not given.
(2) Distilled (compiler).
Components:
(1) Water: H₂O; [7732-18-5]
(2) 1,1,2,2-tetrachloroethane; CH₂Cl₂; [79-09-5]

Variables:
T/K = 298–363

Original Measurements:

Prepared By:
A. L. Horvath

Experimental Data

\[ \log D_{298} = 1317.16 \]

where \( D \) = distribution coefficient.

At the normal boiling point of CHCl₂–C₂Cl₄, \( D = 25 \) and the activity coefficient, \( \gamma = 1.5 \).

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:

Components:
(1) 1,1,2,2-tetrachloroethane; CH₂Cl₂; [79-09-5]
(2) Water; H₂O; [7732-18-5]

Variables:
T/K = 283–353

Original Measurements:

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:

\[ \log_{10} (S_{mol} \text{ dm}^{-3}) = \frac{270}{(T/K)} - 15.316 + 3.0222(T/K) \]

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 x 10⁻³ mol dm⁻³ at 298.5 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) Solyt chemical, rectified before use; purity was 99.9% by GLC analysis.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ± 0.5 K.
### Components

1. 1,1,2,2-tetrachloroethane; C₂H₄Cl₄; [79-5-5]
2. Water; H₂O; [7732-18-5]

### Original Measurements


### Variables

\( T/K = 298-373 \)

### Experimental Data

<table>
<thead>
<tr>
<th>( T/°C )</th>
<th>100 ( \nu_1 ) ( \nu_2 )</th>
<th>10⁸ ( \chi_1 ) ( \chi_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>3.8</td>
<td>0.379</td>
</tr>
<tr>
<td>37</td>
<td>3.57*10²</td>
<td>0.3041</td>
</tr>
<tr>
<td>37</td>
<td>3.57*10²</td>
<td>0.3041</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:
An excess of 8.10 g 1,1,2,2-tetrachloroethane was equilibrated with 100 cm³ of distilled water for 24 h in airtight vessel. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a 0.016 in. internal diameter detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on determination and evaluation of the procedure were 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:
### Components:
- C₆H₅Cl₂ [79-34-5]
- H₂O, [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 297

### Prepared By:
- A. L. Hoehn

### Experimental Data

<table>
<thead>
<tr>
<th>℃</th>
<th>10⁻² x₁ (compiler)</th>
<th>10⁻⁴ M⁻₁ mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23.5</td>
<td>0.296</td>
<td>1.76 x 10⁻³</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
- The aqueous solubility was determined by elution chromatography. The solution (3 mm i.d., 2 mm i.d., and 40 cm long) was 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:
- C₆H₅Cl₂ [79-34-5]
- H₂O, [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 203

### Prepared By:
- A. L. Hoehn

### Experimental Data

<table>
<thead>
<tr>
<th>℃</th>
<th>n₁ V⁠⁻¹/mmol cm⁻² (compiler)</th>
<th>10⁻⁴ M⁻¹ mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.78 x 10⁻³</td>
<td>0.298</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure**
- An excess of C₆H₅Cl₂ was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radiometric techniques. The ¹⁴C activity of the water sample 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.
<table>
<thead>
<tr>
<th>Component</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1,1,2,2-tetrachloroethane: C₃H₇Cl₄</td>
<td>[79-36-5]</td>
</tr>
<tr>
<td>(2) Water: H₂O</td>
<td>[7732-18-5]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>Prepared By</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K=298</td>
<td>A. L. Horváth</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>µg</td>
</tr>
<tr>
<td>25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Auxiliary Information</th>
</tr>
</thead>
</table>

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) Prew England Nuclear, used as received.
(2) Distilled.

Estimated Errors:
Solubility: ±0.6% std. dev.
Temperature: ±0.3 L

<table>
<thead>
<tr>
<th>Component</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) 1,1,2,2-tetrachloroethane: C₃H₇Cl₄</td>
<td>[79-36-5]</td>
</tr>
<tr>
<td>(2) Water: H₂O</td>
<td>[7732-18-5]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variable</th>
<th>Prepared By</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K=293-303</td>
<td>A. L. Horváth</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>µg</td>
</tr>
<tr>
<td>10.0</td>
</tr>
<tr>
<td>20.0</td>
</tr>
<tr>
<td>30.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Auxiliary Information</th>
</tr>
</thead>
</table>

Method/Apparatus/Procedure:
The aqueous solubility was determined by elution chromatography. The solute columns (3 mm id., 1.8 mm id.) 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).
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Distribution Coefficient, $D_p/\text{density}$</th>
<th>$10^3 \gamma_1$ (compt.)</th>
<th>$10^5 \beta_1$ (compt.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.0</td>
<td>1.94</td>
<td>0.194</td>
<td>2.0892</td>
</tr>
<tr>
<td>13.0</td>
<td>1.52</td>
<td>0.197</td>
<td>2.1150</td>
</tr>
<tr>
<td>21.0</td>
<td>1.03</td>
<td>0.253</td>
<td>2.7305</td>
</tr>
<tr>
<td>23.0</td>
<td>1.40</td>
<td>0.236</td>
<td>2.5647</td>
</tr>
<tr>
<td>27.2</td>
<td>2.04</td>
<td>0.309</td>
<td>3.3030</td>
</tr>
</tbody>
</table>

*Gas-liquid system analysis parameter, from calibration measurements.*

### Auxiliary Information

#### Method/Apparatus/Procedure:
- A 3 μL 1,1,2,2-tetrachloroethane sample was injected into a 2.3 dm$^3$ equilibrium 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 monitored 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) Certified.

#### Estimated Errors:
- Solubility: ±5.6%.
- Temperature: ±0.5 K.

#### Auxiliary Information

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$\gamma_1 V_2^{1/2} \alpha$ (compt.)</th>
<th>$100 w_i$ (compt.)</th>
<th>$K^2 x_i$ (compt.)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>2.915 x 10$^3$</td>
<td>0.2919</td>
<td>1.141</td>
</tr>
</tbody>
</table>

### Source and Purity of Materials:
- (1) Chemical Service, West Chester, Pa., USA, pure grade available.
- (2) Distilled and run through two Bunnstead purification cartridges.

### Estimated Errors:
- Solubility: ±5.43% and dev.
- Temperature: ±0.5 K (compt.).

### References:
### Components:
- (1) 1,1,2,2-tetrachloroethane: C₂H₄Cl₄ [79-34-5]
- (2) Water: H₂O [7732-18-5]

### Original Measurements:

### Variables:
- T/K = 293–323
- T/K = 283–393

## Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10⁴ x₁</th>
<th>10⁵ x₂</th>
<th>10⁴ x₃</th>
<th>10⁵ x₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.52</td>
<td>0.234</td>
<td>11.3</td>
<td>0.123</td>
</tr>
<tr>
<td>35</td>
<td>2.89</td>
<td>0.269</td>
<td>15.4</td>
<td>0.168</td>
</tr>
<tr>
<td>50</td>
<td>3.32</td>
<td>0.308</td>
<td>20.6</td>
<td>0.255</td>
</tr>
</tbody>
</table>

Mole fraction of 1,1,2,2-tetrachloroethane (x₁) was calculated from the activity coefficients at infinite dilution (γ_i*) using the relation

\[ x_1 = \frac{1}{1 + \gamma_1} \]

### Auxiliary Information

**Method/Apparatus/Procedure:**
The water-rich mixture was studied using gas-liquid chromatography in which a mixture of methanol 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 isopropyl method in which CeCl₃ 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) 1,1,2,2-tetrachloroethane: 99.9% pure, as received.
- (2) Distilled and de-ionized.

**Estimated Errors:**
- Solubility: not specified.
- Temperature: ±0.02 K (compiler).
**Components:**
(1) 1,1,2,2-tetrachloroethane: C₂H₄Cl₄; [79-34-5]
(2) Water: H₂O; [7732-18-5]

**Variables:**
77K = 293

**Original Measurements:**

**Prepared By:**
A. L. Horvath

---

**Experimental Data**

<table>
<thead>
<tr>
<th>t°C</th>
<th>10⁻² x₁ (compile)</th>
<th>10⁻⁴ M⁻¹ cm² mol⁻¹ g⁻¹ (compile)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.0</td>
<td>0.29</td>
<td>3.2</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.73 x 10⁻⁷</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

Method/Equipment/Procedure:
The solubility determination was carried out in small test tube (e.g., 100x12 mm) to permit rigorous shaking of the solvent and solute mixture. During the experiment, 0.20 cm³ 1,1,2,2-tetrachloroethane was added to 3.0 cm³ of water and agitated. The concentration of 1,1,2,2-tetrachloroethane in water was analyzed by passing the sample through a chromatographic column.

**Sources 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: C₂H₄Cl₄; [79-34-5]
(2) Water: H₂O; [7732-18-5]

**Variables:**
77K = 293 - 313

**Prepared By:**
A. L. Horvath

---

**Experimental Data**

<table>
<thead>
<tr>
<th>t°C</th>
<th>γ₂</th>
<th>10⁻⁴ x₁ (compiler)</th>
<th>10⁻² w₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3850±666</td>
<td>2.60</td>
<td>0.242</td>
</tr>
<tr>
<td>30</td>
<td>2970±627</td>
<td>3.37</td>
<td>0.173</td>
</tr>
<tr>
<td>40</td>
<td>3570±247</td>
<td>2.80</td>
<td>0.260</td>
</tr>
</tbody>
</table>

**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 (γ₂⁻) in water. Cells containing degassed water were submerged in a thermostatic 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. Thus, the stirrer was turned off and the differential pressure was recorded. The experiment was repeated at least three times at each temperature.

**Sources and Purity of Materials:**
(1) Source and purity not given.
(2) Distilled, filtered and deionized.

**Estimated Errors:**
Solubility: see above.
Temperature: ± 0.05 K.
37. 1,1,2,2-Tetrachloroethane with Water-d$_2$

**Experimental Data**

<table>
<thead>
<tr>
<th>$t{^\circ}$C</th>
<th>$10^3 x_1$ (compiler)</th>
<th>$0.0 w_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>5.56 x 10^{-3}</td>
<td>9.23</td>
</tr>
</tbody>
</table>

**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 Fisher titration method. The determination was done in triplicate. This procedure description was taken from a secondary source. 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 freed before use.

**Estimated Errors:**

Solubility: ±1.0 x 10^{-3} mol g^{-1}.

Temperature: ± 0.05 °C.

**References:**


---

38. Cis-1,2-Dilodoethene with Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$t{^\circ}$C</th>
<th>$c_1$ (mol m^{-2})</th>
<th>$10^2 w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>1.65</td>
<td>4.63 x 10^{-2}</td>
<td>2.98</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**

Water was mixed with cis-1,2-dilodoethene in a glass-stopped Erlenmeyer flask which was then placed in a constant temperature bath and stirred for 30 h. The organic halide content in 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.

**Source and Purity of Materials:**

(1) Prepared by isomerization of crude trans-1,2-dilodoethene 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:**

### 39. Trans-1,2-Diiodoethene with Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>$c_i$ / mol L⁻¹</th>
<th>100 $w_i$ (compiler)</th>
<th>$10^6 x_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>0.527</td>
<td>1.48 x 10⁻²</td>
<td>9.53</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Water was mixed with trans-1,2-diiodoethene in a glass stopped Erlenmeyer flask which was then placed in a constant temperature bath and rotated for 30 h. The organic halide constituent of the aqueous phase was extracted with n-hexane. Theoretical density of the extract was measured against a pure-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 iodine in 95% ethyl alcohol and purified by repeated crystallization.
2. Distilled (compiler).

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

**References:**

### 40. 1,2-Dibromo-1-Chloroethene with Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>$g_i$ / g₂</th>
<th>100 $w_i$ (compiler)</th>
<th>$10^3 x$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>6.0 x 10⁻²</td>
<td>6.0 x 10⁻²</td>
<td>7.35</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
Solubility: not specified.
Temperature: ±0.5 K (compiler).

**Source and Purity of Materials:**
1. Distilled (compiler).
2. Dow Chemical Co., used as received.

**Estimated Errors:**
### 41. 1,1,2-Trichloroethane with Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$t$ (°C)</th>
<th>$10^3 w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>5.0×10⁻²</td>
<td>7.35</td>
</tr>
</tbody>
</table>

**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).

### 42. 1,1-Dichloro-1-Fluoroethane with Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$t$ (°C)</th>
<th>$10^3 w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
<th>$10^3 x_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>6.6×10⁻³</td>
<td>1.02</td>
<td>2.72</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Method/Apparatus/Procedure:** Details are not available.
- **Source and Purity of Materials:**
  - (2) Distilled (compiler).
- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ±0.5 K (compiler).
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 McNeeley et al.1,2 Pearson and McConnell,3 Azac and Stevens4,5 Croce and Diaz6 Hinchliffe et al.7 and McNally and Gros8 are markedly lower than the solubility values calculated from the smoothing equation and are therefore rejected. The measurements of Lowant and Miller9 and Warner et al10 are several percent higher than the smoothed solubility values and are also rejected.

The remaining data of von Arx and Veis,11 O'Connell,12 Warner and Veis13 Chion and Proux14 Sano and Nakajima,15 Shifan,16 Vebit et al.17 Bauder et al.18 Leggot and Calo,19 Hunter-Smith et al.19 Extendi et al.1,9 Linoff and Gessert,20 Munt,21 Bar and Newham,22 Kroner,23 Howart et al.24 and Wight et al.25 were compiled or used for the smoothing equation. The combined set of 17 laboratories were used to obtain the following mass percent (v) equation:

\[
\text{Solubility} = 100 \times \left[ 1.0909 - 0.52776 \times 10^{-3} (\text{K}) + 1.09747 \times 10^{-7} (\text{K})^2 \right],
\]

where the standard deviation of 1.73 x 10^{-2} is in the temperature range from 273 to 323 K.

The measurements and the curve obtained from the smoothing equation as shown in Fig. 3. A solubility minimum calculated from the above 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.

---

Table 1. Recommended solubility of 1,1,1-trichloroethane (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature (K)</th>
<th>100 x_1</th>
<th>Solubility (mol/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.184</td>
<td>1.81</td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.200</td>
<td>1.78</td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.130</td>
<td>1.76</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.129</td>
<td>1.74</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.159</td>
<td>1.74</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.129</td>
<td>1.74</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.130</td>
<td>1.76</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.131</td>
<td>1.77</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.133</td>
<td>1.80</td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.135</td>
<td>1.82</td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.138</td>
<td>1.87</td>
</tr>
</tbody>
</table>

---

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 smoothing equation with the following exclusions. Both results of Leow and Storm26 and Archer and Stevens27 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,28 Crocc and Diaz,4 O'Connell,12 Olzewski and Kozuma,29 Cateniti et al.30 and Bar and Newham,22 were used for the smoothing equation:

\[
\text{log}_{10} x_2 = 0.43885 - 9.09.356 (\text{K})^{-1}
\]

This equation represents the combined data with a standard deviation of 9.63 x 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)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature (K)</th>
<th>100 x_2</th>
<th>Solubility (mol/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.0174</td>
<td>1.285</td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.0199</td>
<td>1.475</td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.0228</td>
<td>1.685</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.0259</td>
<td>1.916</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.0294</td>
<td>2.170</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.0331</td>
<td>2.445</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.0371</td>
<td>2.743</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.0416</td>
<td>3.072</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.0464</td>
<td>3.423</td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.0515</td>
<td>3.802</td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.0571</td>
<td>4.214</td>
</tr>
</tbody>
</table>

---

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 \(1/(\text{K})\) 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 $\gamma$ vs 1000/(T/K).

References

Components:
1. 1,1,1-trichloroethane; C₃H₇Cl₂ : [71-55-6]
2. Water; H₂O : [7732-18-5]

Original Measurements:

Variables:
$T$/K = 273–333

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>$10^6 \gamma$</th>
<th>$100 \gamma_1 \gamma_2$</th>
<th>$100 \gamma_1$</th>
<th>$10^6 \gamma_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.159</td>
<td>0.159</td>
<td>2.15</td>
</tr>
<tr>
<td>20</td>
<td>0.152</td>
<td>0.132</td>
<td>1.78</td>
</tr>
<tr>
<td>35</td>
<td>0.126</td>
<td>0.126</td>
<td>1.70</td>
</tr>
<tr>
<td>50</td>
<td>0.128</td>
<td>0.128</td>
<td>1.73</td>
</tr>
</tbody>
</table>

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).

HORVATH ET AL.
### Components:

1. Water: H₂O \[7732-18-5\]
2. 1,1,1-Trichloroethane: C₂H₅Cl \[71-55-6\]

### Original Measurements:


### Variables:

- T/K = 273–308

### Prepared By:

- A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁</th>
<th>10⁶ x₁ (compiler)</th>
<th>10² w₂M²⁻¹mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.62×10⁻²</td>
<td>1.35×10⁻²</td>
<td>8.99×10⁻⁴</td>
</tr>
<tr>
<td>25</td>
<td>3.39×10⁻²</td>
<td>2.57×10⁻²</td>
<td>1.88×10⁻³</td>
</tr>
<tr>
<td>30</td>
<td>4.22×10⁻²</td>
<td>3.72×10⁻²</td>
<td>2.34×10⁻³</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

A mixture of 1,1,1-Trichloroethane and water was shaken for about 12 h in a separatory funnel. It was then filtered. 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 not specified.

**Temperature:** ±0.5 K (compiler).

**Estimated Errors:**

- Error not specified.

**Solubility:** not specified.

**References:**

**Components:**
(1) Water, H$_2$O; [7732-18-5]
(2) 1,1,1-trichloroethane; C$_2$H$_3$Cl$_3$; [71-55-6]

**Original Measurements:**

**Variables:**
T/K = 298

**Prepared By:**
A. L. Horvath

---

**Components:**
(1) 1,1,1-trichloroethane; C$_2$H$_3$Cl$_3$; [71-55-6]
(2) Water, H$_2$O [7732-18-5]

**Original Measurements:**

**Variables:**
T/K = 283–353

**Prepared By:**
A. L. Horvath

---

**Experimental Data**

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w$_1$</th>
<th>10$^3$ x$_1$</th>
<th>100 w$_1$.M$^{-3}$mol g$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>5.0×10$^{-2}$</td>
<td>.69</td>
<td>2.8×10$^{-3}$</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The apparatus containing the organic-water system was held in a waterbath thermostated. The stirring of the mixture was affected 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.

---

**Experimental Data**
The temperature dependence of the solubility of 1,1,1-trichloroethane in water versus absolute temperature was expressed by the equation:

$$\log_{10}(S/mol dm^{-3}) = \frac{270}{(7K)} - 14.860 + 0.0200(T/K),$$

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 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 gaschromatography.

**Source and Purity of Materials:**
(1) Solvay, rectified before use, the purity was 99.9% by GLC analysis.
(2) Distilled.

**Estimated Errors:**
Solubility: not specified.
Temperature: ±0.5 K (compiler).
### Components:
1. 1,1,1-trichloroethane: C₂H₂Cl₃ [71-55-6]

### Original Measurements:

### Variables:
T/K = 293

### Prepared By:
A.L. Borvah

### Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>10⁶ x₁</th>
<th>10⁶ x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>4.80E+10</td>
<td>4.80E-10</td>
</tr>
</tbody>
</table>

### 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 mass spectrometry (MS) method.

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

**Estimated Errors:**
Solubility: ±0.2 K (compiler).

---

### Components:
1. 1,1,1-trichloroethane: C₂H₂Cl₃ [71-55-6]

### Original Measurements:

### Variables:
T/K = 293

### Prepared By:
A.L. Hevath

### Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>10⁷ g₁/µl</th>
<th>10⁷ g₂/µl</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>4.80E+3</td>
<td>4.80E-3</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Saturated solutions were prepared in a constant temperature thermostatic bath. Water samples were extracted with n-pentane and an aliquot of the extract was gas-liquid chromatographed. A gas chromatograph was fitted with a 63Ni electron capture detector.

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

**Estimated Errors:**
Solubility: ±0.2 K (compiler).
### Components:
1. 1,1,1-trichloroethane; C₃H₅Cl₃; [71-55-6]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
T/K = 276-307

### Prepared By:
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>e₆/V²/mg m⁻³</th>
<th>10⁶ w₁</th>
<th>10⁸ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>1.29</td>
<td>0.179</td>
<td>2.42</td>
</tr>
<tr>
<td>20</td>
<td>1.37</td>
<td>0.137</td>
<td>1.85</td>
</tr>
<tr>
<td>34</td>
<td>1.35</td>
<td>0.156</td>
<td>2.11</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
An excess of 5-10 g 1,1,1-trichloroethane was equilibrated with 100 cm³ 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 60 electron capture detector. The GLC column was packed with porous polypropylene 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:**
### Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
<th>100 w,M⁻²/mol g⁻¹ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>37</td>
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<td>1.798</td>
<td></td>
</tr>
<tr>
<td>23.5</td>
<td>0.120</td>
<td>1.62</td>
<td>8.99×10⁻⁴</td>
</tr>
<tr>
<td></td>
<td>0.115</td>
<td>1.55</td>
<td>8.62×10⁻⁴</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
- The aqueous solubility was determined by static chromatography. The solute columns (3 mm o.d., 2 mm i.d., and 40 cm long) were filled with Chromosorb 7. 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% (3σ).
- Temperature: ±1.5 K.
<table>
<thead>
<tr>
<th>Component(s):</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 298</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Auxiliary Information</th>
</tr>
</thead>
</table>

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: ± 0.0. K.

<table>
<thead>
<tr>
<th>Component(s):</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 293</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>20</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Auxiliary Information</th>
</tr>
</thead>
</table>

Method/Apparatus/Procedure:
An excess of 1,1,1-trichloroethane was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ³⁵Cl 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; C₃H₇Cl₃ [71-55-6]
(2) Water; H₂O [7732-18-5]

### Original Measurements:

<table>
<thead>
<tr>
<th>Variables</th>
<th>Prepared By</th>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 298</td>
<td>A. L. Hovath</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>t/°C</th>
<th>p₁/ kg m⁻³</th>
<th>10⁶ x₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.72X</td>
<td>7.22×10⁻⁵</td>
<td>9.76</td>
</tr>
</tbody>
</table>

### 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 41 h, the solution was extracted with cyclohexane. The samples were analyzed using an Ambico-Bowman spectrophotometer. A detailed description of the method has been reported elsewhere.¹

**Source and Purity of Materials:**
(1) Aldrich Chemical, highest grade used as received.
(2) Ethanol distilled.

**Estimated Errors:**
Solubility: not specified.
Temperature: ±0.2 °C (compiler).

### References:
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Distribution coefficient, (D_L)</th>
<th>(10^4 x_1) (compiler)</th>
<th>(100 , \text{w}_1, M^{-1} \text{mol}^{-1} ) (compiler)</th>
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</table>

\(^a\)Gas-liquid system analysis per parameter, from calibration measurements.

### Auxiliary Information

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

**Estimated Errors:**
- Solubility: ±2.5%.
- Temperature: ±0.5 K.

**Method/Apparatus/Procedure:**
- 2.3 dm³ 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 determined using a dual flame ionization detector gas chromatograph.

**Prepared By:**
- A. L. Horvath

---

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>(100 , \text{w}_1) (compiler)</th>
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</table>

\(^a\)Gas-liquid system analysis per parameter, from calibration measurements.

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

**Estimated Errors:**
- Solubility: ±2.5%.
- Temperature: ±0.5 K.

**Method/Apparatus/Procedure:**
- A 5 µL, 1,1,1-trichloroethane sample was injected into a 2.3 dm³ 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 determined using a dual flame ionization detector gas chromatograph.
Components:
(1) Water: H₂O [7732-18-5]
(2) 1,1,1-trichloroethane: C₃H₅Cl₃ [71-55-6]

Original Measurements:

Variables:
T/K = 298

Experimental Data

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<tr>
<th>°C</th>
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<tbody>
<tr>
<td>25</td>
<td>0.42</td>
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Auxiliary Information

Method/Apparatus/Procedure:
Water was added gradually to 50 cm³ 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 (mellibility) appeared. The water content in the sample was determined by the Karl Fischel 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: C₃H₅Cl₃ [71-55-6]
(2) Water: H₂O [7732-18-5]

Original Measurements:

Variables:
T/K = 278–306

Experimental Data

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</table>

*The Henry’s law constant (H, dimensionless) was derived from a van’t Hoff plot best-fit equation: log H=9.15-2915/(T/K).

Auxiliary Information

Method/Apparatus/Procedure:
The multiple equilibration technique was used to measure the Henry’s law constant as described elsewhere. 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:
### Components:  
(1) 1,1,1-trichloroethane; C₂H₃Cl₃; [71-55-6]  
(2) Water; H₂O; [7732-18-5]

### Original Measurements:  

### Variables:  
T/K = 293

### Prepared By:  
A. L. Horvath

### Experimental Data

<table>
<thead>
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<th>Temperature (°C)</th>
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<th>10° x₂ (compiler)</th>
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### Experimental Data

**EPICS method**

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log, $H=1.21-4260/(T/K)$

**Batch air stripping method**

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</table>

log, $H=9.375-4186/(T/K)$

### Auxiliary Information

**Source and Purity of Materials:**  
(1) Prolabo reagent, purified by distillation before use.  
(2) Distilled (compiler).

**Estimated Errors:**  
Solubility: not specified.  
Temperature: ±0.1 K.

### 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 AT20) was equipped with a Shimadzu Chromatopac C1A integrator. A stainless steel column packed with 100-120 mesh Chromosorb W DMCD coated with hexadecane nitrile was used for analysis.

**Henry's law constant, $H/m^3$ atm mol⁻¹**

### Original Measurements:  

### Variables:  
T/K = 293

### Prepared By:  
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10° x₁ (compiler)</th>
<th>10° x₂ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>1.32×10⁻²</td>
<td>0.1313</td>
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</tbody>
</table>

log, $H=1.21-4260/(T/K)$

**Estimated Errors:**  
Solubility: ±5%–10%.  
Temperature: ±0.1 K.
Components:
(1) 1,1,1-trichloroethane; C₃H₅Cl₃; [71-55-4]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>ρ₁ (kg m⁻³)</th>
<th>100 w₁ (composite)</th>
<th>10⁹ x₁ (composite)</th>
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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 23 cm³ and the vapor phase above the mixture was 35 cm³. 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 used through two Barnstead purification cartridges before use.

Estimated Errors:
Solubility: ± 5.17% ± 0.05, Temperature: ± 0.5 °C (compiler).

References:

Components:
(1) 1,1,1-trichloroethane; C₃H₅Cl₃; [71-55-4]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>Henry's law constant, H/dimensionless</th>
<th>ρ₂ (kg m⁻³)</th>
<th>100 w₂ (composite)</th>
<th>10⁹ x₂ (composite)</th>
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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. Both vapor samples were injected directly into the 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: ± 3.5%.
Temperature: ± 0.5 K.
Components:
(1) 1,1,1-trichloroethane; C₂H₇Cl₁ \( \text{[71-55-6]} \)
(2) Water; H₂O; \( \text{[7732-18-5]} \)

Original Measurements:

Variables
\( T/K = 293-323 \)

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
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<th>( 10^5 x_2 )</th>
<th>( 10^5 w_1 ) (compiler)</th>
<th>( 10^5 w_2 ) (compiler)</th>
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<td>5.90x10⁻²</td>
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Mole fraction of 1,1,1-trichloroethane \( x_1 \) was calculated from the activity coefficients to infinite dilution \( \gamma_1^\infty \) using the relation \( x_1 = \frac{u}{(\gamma_1^\infty)} \).

Auxiliary Information

Method/Apparatus/Procedure:
The water-rich mixture was studied using gas-liquid chromatography in which a mixture of methanol and 1,1,1-trichloroethane vapor passed through the sampling loop. The column was purged with Ar carrier gas. The effluent of 1,1,1-trichloroethane was monitored with a flame ionization detector. The organic-rich mixture was studied using an air-sparged method in which water was controlled using a partial pressure of water. The water concentration of the organic phase was determined by using a Karl Fisher titration apparatus.

Source and Purity of Materials:
(1) Koch Light Laboratory Limited, redistilled in glass furnace. Prepared by:
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.8 K.

CV = coefficient of variation (±100 S.D./mm).

Component:
(1) 1,1,1-trichloroethane; C₂H₇Cl₁ \( \text{[71-55-6]} \)
(2) Water; H₂O; \( \text{[7732-18-5]} \)

Original Measurements:

Variables
\( T/K = 283-308 \)

Prepared By:
A. L. Horvath

Experimental Data

<table>
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<tr>
<th>( T/°C )</th>
<th>Henry's law constant, ( \mu \text{m}^2 \text{atm} \text{mol}^{-1} )</th>
<th>CV ( % )</th>
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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: C₂₃H₃₅Cl [71-55-6]
(2) Water: H₂O [7732-18-5]

Original Measurements:
P. Warner, J. M. Creem, and J. C. Ireland, "Determination of
Henry's Law Constants of Selected Indoor Pollutants," U.S.
EPA Technical Report, PB87-21200, Cincinnati, OH (July
1987).

Prepared By:
A. L. Horvath

Variables:
T/K = 298

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Henry's law constant, ( \frac{H}{m^3 \text{atm} \text{mol}^{-1}} )</th>
<th>100 ( w_1 ) ( (\text{compile}) )</th>
<th>10^4 ( x_4 ) ( (\text{compile}) )</th>
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<tbody>
<tr>
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<td>6.193</td>
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Auxiliary Information

Method/Apparatus/Procedure:
The original method and apparatus for the determination of
Henry's law constants, as described by Mackey, et al., 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
thermostated 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) Haynes quality available, used without further purification,
standard purity greater than 99%.
(2) Distilled and de-ionized.

Estimated Errors:
Solubility: ± 0.5% and dev.
Temperature: ± 0.05 K

References:

Components:
1) 1,1,1-trichloroethane: C₂₃H₃₅Cl [71-55-6]
2) Water: H₂O [7732-18-5]

Original Measurements:
G. B. Howe, M. E. Mullins, and T. V. Rogers, AFESC Treadway
(September 1987), 106 pp. (AD-A185, 541.)

Prepared By:
A. L. Horvath

Variables:
T/K = 283-303

Experimental Data

<table>
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<tr>
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<th>100 ( w_1 ) ( \text{(compiler)} )</th>
<th>10^4 ( x_4 ) ( \text{(compiler)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.399 x 10^4</td>
<td>0.1369</td>
<td>1.3915</td>
</tr>
<tr>
<td>20</td>
<td>1.559 x 10^4</td>
<td>0.1559</td>
<td>2.1081</td>
</tr>
<tr>
<td>30</td>
<td>1.420 x 10^4</td>
<td>0.1420</td>
<td>1.5199</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
150 cm³ bottles were filled with distilled, de-ionized water and
sealed. Measured volumes of 1,1,1-trichloroethane were
injected into the system through each bottle septum using a
microliter syringe. The solution was in excess of the anticipated
solubility limit. The bottle was shaken for 1 h with a
vibratory shaker and allowed to equilibrate for about three
weeks. Samples were then injected into a gas chromatograph
equipped with a Carbowax 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).
### 44. 1,1-Trichloroethane with MQ-Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>Henry's Law Constant, $H$ (dimensionless)</th>
<th>$10^3 x_1$</th>
<th>$100 w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.617</td>
<td>1.70</td>
<td>0.126</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td></td>
<td>1.82</td>
<td>0.135</td>
<td></td>
</tr>
<tr>
<td>40</td>
<td></td>
<td>1.85</td>
<td>0.137</td>
<td></td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The multiple equilibrium technique with direct aqueous injection into 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 placed on an equilibrator. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into the 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) Mallon Coleman & Bell, OHI, greater than 99.9% pure.
(2) Mill-Q water; 0.25 mg total organic carbon per mL and 0.75 mg COD per mL.

**Estimated Errors:**
Solubility: ±0.017 std. dev.
Temperature: ±0.5 K.
45. 1,1,1-Trichloroethane with Municipal Tap Water (PASE)

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Henry’s law constant, H/dimensionless</th>
<th>100 w1 (compiler),%</th>
<th>10^6 x1 (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.066</td>
<td>0.1049</td>
<td>1.488</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The multiple-equilibrium technique with direct aqueous injection into gas chromatograph was used to determine the dimethylsulfoxide 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 the gas chromatograph, the liquid samples were concentrated with liquid–liquid extraction before analysis. The experiments were carried out in duplicate.

Source and Purity of Materials:
(1) Matheson Coleman & Bell, OH, purer than 99.5% pure.
(2) 10 µg total organic carbon/dm³ ad 40 mg COD/liter.

Estimated Errors:

- Solubility: ± 0.028 at. dev.
- Temperature: ± 0.5 K

46. 1,1,1-Trichloroethane with Seawater

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Henry’s law constant, H/dimensionless</th>
<th>100 w1 (compiler)</th>
<th>10^6 x1 (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.368</td>
<td>1.002×10⁻¹</td>
<td>1.554</td>
</tr>
<tr>
<td>10</td>
<td>0.4714</td>
<td>9.92×10⁻²</td>
<td>1.549</td>
</tr>
<tr>
<td>15</td>
<td>0.5993</td>
<td>9.79×10⁻²</td>
<td>1.524</td>
</tr>
<tr>
<td>20</td>
<td>0.7552</td>
<td>9.66×10⁻²</td>
<td>1.505</td>
</tr>
<tr>
<td>25</td>
<td>0.9442</td>
<td>9.50×10⁻²</td>
<td>1.284</td>
</tr>
</tbody>
</table>

The Henry’s law constant (H, dimensionless) was derived from a van’t Hoff plot best-fit equation: log [H] = 13.03 - 3905/(T/K).

Auxiliary Information

Method/Apparatus/Procedure:
The multiple equilibration technique was used to measure the Henry’s law constant as described by McAuliffe. 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 sparged 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, 45° N to 5° S latitudes, in late 1981.

Estimated Errors:

- Solubility: ± 5.5% at. dev.
- Temperature: ± 0.2 K.

References:
1 C. D. McAuliffe, Chem. Technol, 46 (971).
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 in 1,1,2-trichloroethane (1) in water (2) and part 2 is 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 used in the data smoothing procedure. The solubility data of Wright and Schaffers and Bows et al. are significantly lower than other results and are therefore rejected. Even though there appears to be some inaccuracy in the reported solubility data of Litgahe and Calo and Howe et al., it is not possible to give a minimum and the latter shows a maximum in solubility. The combined results of 16 laboratories have been used for the smoothing equations. The data of van Acker and Voss, McGovern, Trewky et al., Newman et al., Winters and Nakanishi, and Cava and Danis were included to obtain the following mass percent (1) equation:

\[ \text{Solubility (100 \, w_{12})} = 2.8976 - 1.8598 \times 10^{-2} \times (1/T) + 3.4692 \times 10^{-5} \times (1/T) \]

which shows a standard deviation of 341 \times 10^{-3} in the temperature range from 273.15 to 328.15 K. The above equation represents the combined data with a maximum deviation of 15%, usually less, and may be considered tentative for solubility if 1,1,2-trichloroethane is 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 hydrogen cyanide solutions are provided in the text.

The tentative values for this system are given in Table 1 as smoothed values at 5 K intervals.

![Graph of solubility vs. temperature](image)

**Fig. 15. Solubility of 1,1,2-trichloroethane (1) in water (2).**

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Solubility (100 , w_{12})</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.15</td>
<td>0.0478</td>
</tr>
<tr>
<td>278.15</td>
<td>0.0586</td>
</tr>
<tr>
<td>283.15</td>
<td>0.0694</td>
</tr>
<tr>
<td>288.15</td>
<td>0.0802</td>
</tr>
<tr>
<td>293.15</td>
<td>0.0909</td>
</tr>
<tr>
<td>298.15</td>
<td>0.1016</td>
</tr>
<tr>
<td>303.15</td>
<td>0.1123</td>
</tr>
<tr>
<td>308.15</td>
<td>0.1231</td>
</tr>
<tr>
<td>313.15</td>
<td>0.1336</td>
</tr>
<tr>
<td>318.15</td>
<td>0.1442</td>
</tr>
<tr>
<td>323.15</td>
<td>0.1548</td>
</tr>
<tr>
<td>328.15</td>
<td>0.1654</td>
</tr>
</tbody>
</table>

The remaining data of Litgahe, Trewky et al., and Bowers and Nakanishi were compiled or used for the smoothing equations. The fitting equation is

\[ \text{Solubility (100 \, w_{12})} = 2.8976 - 1.8598 \times 10^{-2} \times (1/T) + 3.4692 \times 10^{-5} \times (1/T) \]

This equation yields a standard deviation of 341 \times 10^{-3} in the temperature range from 268.15 to 328.15 K. The recommended solubility at 5 K intervals is in 1,1,2-trichloroethane as shown in Table 2.

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Solubility (100 , w_{12})</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.15</td>
<td>0.0478</td>
</tr>
<tr>
<td>278.15</td>
<td>0.0586</td>
</tr>
<tr>
<td>283.15</td>
<td>0.0694</td>
</tr>
<tr>
<td>288.15</td>
<td>0.0802</td>
</tr>
<tr>
<td>293.15</td>
<td>0.0909</td>
</tr>
<tr>
<td>298.15</td>
<td>0.1016</td>
</tr>
<tr>
<td>303.15</td>
<td>0.1123</td>
</tr>
<tr>
<td>308.15</td>
<td>0.1231</td>
</tr>
<tr>
<td>313.15</td>
<td>0.1336</td>
</tr>
<tr>
<td>318.15</td>
<td>0.1442</td>
</tr>
<tr>
<td>323.15</td>
<td>0.1548</td>
</tr>
<tr>
<td>328.15</td>
<td>0.1654</td>
</tr>
</tbody>
</table>

Measured values and the curve obtained from a smoothing equation for solubility expressed as \( \log_{10} x_2 \) versus the reciprocal of absolute temperature are shown in Fig. 6.
FIG. 16. Solubility of water (1) in 1,1,2-trichloroethane; log $x_1 = 1000/(T/K)$.
Components:  
(1) 1,1,2-trichloroethane; C₃H₇Cl₂  \[ 79-00-5 \]
(2) Water; H₂O  \[ 7732-18-5 \]

Variables:  
T/K = 273 - 320

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>℃</th>
<th>100 g₁/g₂</th>
<th>100 w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.460</td>
<td>0.464</td>
<td>6.29</td>
</tr>
<tr>
<td>20</td>
<td>0.436</td>
<td>0.434</td>
<td>5.88</td>
</tr>
<tr>
<td>35</td>
<td>0.438</td>
<td>0.456</td>
<td>6.18</td>
</tr>
<tr>
<td>55</td>
<td>0.532</td>
<td>0.529</td>
<td>7.18</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Water was obtained 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

Estimated Errors:
Solvency: not specified.
Temperature: ±0.5 K (compiler).

References:
### Components:
1. 1,1,2-trichloroethane; C₃H₆Cl₂; [79-00-5]
2. Water; H₂O; [7732-18-5]

### Original Measurements:
- (2) Water; H₂O; [7732-18-5]

### Variables:
- T/K = 264-298

### Prepared By:
- A. L. Horvath

#### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>10⁸ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10⁸ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-9</td>
<td>—</td>
<td>2.5 × 10⁻²</td>
<td>1.85</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>4.4 × 10⁻¹</td>
<td>5.96</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

#### 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; C₆H₅Cl₃; [79-00-5]
(2) Water; H₂O; [7732-18-5]

Variables:
T/R = 298

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10² x₀ (compiler)</th>
<th>100 w₀ x₀⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.44</td>
<td>5.96</td>
</tr>
</tbody>
</table>

Auxiliary Information

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:
Components:
(1) 1,1,2-trichloroethane; C₃H₅Cl₃; [79-00-5]
(2) Water; H₂O; [7732-18-5]

Variables:
T/K = 310

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Partition coefficient*; $K_d$ (dimensionless)</th>
<th>$10^3 x_1$ (compiler)</th>
<th>$10^5 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>0.77</td>
<td>0.50</td>
<td>6.836</td>
</tr>
</tbody>
</table>

*Gas-liquid chromatographic parameter; from instrument calibration.

Method/Apparatus/Procedure:
A 1,1,2-trichloroethane vapor sample was equilibrated in an air tight vial with water and the overlying air. When equilibrium was reached, a portion of the equilibrated air was 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:
Sensitivity: ±1.3 std dev.
Temperature: ±0.5 K (compiler).

Source and Purity of Materials:

Variables:
T/K = 298

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>$10^3 w_1$ (compiler)</th>
<th>$10^5 w_1$ (compiler)</th>
<th>$10^5 w_2$ (compiler)</th>
<th>$10^7 w_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.51</td>
<td>6.92</td>
<td>8.0×10⁻²</td>
<td>5.80</td>
</tr>
</tbody>
</table>

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-air thermostat while maintaining a constant agitation using an amagnetic stirrer.

Source and Purity of Materials:
(1) Laboratory grade Fluka reagent, further purified by distillation, only middle fraction was used.
(2) Distilled.

Estimated Errors:
Sensitivity: not specified.
Temperature: ±0.05 K.
Components:
(1) 1,1,2-trichloroethane; C₃H₆Cl₃ [79-06-5]
(2) Water; H₂O [7732-18-5]

Original Measurements:

Variables:
T/K = 298

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>θ°C</th>
<th>10⁴ x₁ (complex)</th>
<th>10⁴ x₂ (complex)</th>
<th>10⁴ x₃ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.50</td>
<td>6.78</td>
<td>8.5 × 10⁻³</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The mutual solubility data were determined by a method described by Othomer, et al. A 10 cm³ 1,1,2-trichloroethane sample was added to water from a buret and agitated until the solution became turbid. The appearance of 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 (complex).

References:
### Components:
1. 1,1,2-trichloroethane; C₂H₃Cl₃; [79-00-5]
2. Water; H₂O; [7732-18-5]

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10² x₁</th>
<th>10⁶ w₁ (complex)</th>
<th>10⁶ w₁ M₁⁻¹ mol g⁻¹ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.5</td>
<td>5.86</td>
<td>0.532</td>
<td>2.54 x 10⁻³</td>
</tr>
<tr>
<td>14.0</td>
<td>5.73</td>
<td>0.423</td>
<td>3.17 x 10⁻³</td>
</tr>
<tr>
<td>21.0</td>
<td>5.77</td>
<td>0.426</td>
<td>3.19 x 10⁻³</td>
</tr>
<tr>
<td>21.6</td>
<td>5.87</td>
<td>0.433</td>
<td>3.25 x 10⁻³</td>
</tr>
<tr>
<td>25.0</td>
<td>5.83</td>
<td>0.430</td>
<td>3.22 x 10⁻³</td>
</tr>
<tr>
<td>30.0</td>
<td>6.19</td>
<td>0.56</td>
<td>3.42 x 10⁻³</td>
</tr>
<tr>
<td>35.0</td>
<td>6.00</td>
<td>0.42</td>
<td>3.31 x 10⁻³</td>
</tr>
<tr>
<td>40.0</td>
<td>6.46</td>
<td>0.76</td>
<td>3.57 x 10⁻³</td>
</tr>
<tr>
<td>50.0</td>
<td>7.58</td>
<td>0.558</td>
<td>4.18 x 10⁻³</td>
</tr>
</tbody>
</table>

### 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 Porapack Q 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 (complex).
### Component: 1,1,2-trichloroethane; C₃H₇Cl₂; [79-09-3]

- Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
- 77K = 321; 76mm Hg = 648

### Prepared By:
- A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>p₁ [mm Hg]</th>
<th>10⁵ x₁</th>
<th>100 w₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>48.2</td>
<td>639</td>
<td>0.39</td>
<td>2.85 x 10⁻⁵</td>
</tr>
<tr>
<td>48.2</td>
<td>122</td>
<td>0.66</td>
<td>4.36 x 10⁻⁵</td>
</tr>
<tr>
<td>48.2</td>
<td>145</td>
<td>1.00</td>
<td>1.54 x 10⁻⁴</td>
</tr>
<tr>
<td>48.2</td>
<td>183</td>
<td>1.24</td>
<td>5.82 x 10⁻⁴</td>
</tr>
<tr>
<td>48.2</td>
<td>314</td>
<td>2.77</td>
<td>2.00 x 10⁻³</td>
</tr>
<tr>
<td>48.2</td>
<td>476</td>
<td>4.49</td>
<td>3.31 x 10⁻¹</td>
</tr>
</tbody>
</table>

### Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>Distribution coefficient, D₂/Dimensionless</th>
<th>100 w₁ (compiler)</th>
<th>10₀ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.5</td>
<td>0.17</td>
<td>0.3705</td>
<td>1.0191</td>
</tr>
<tr>
<td>7.0</td>
<td>0.35</td>
<td>0.3591</td>
<td>0.2719</td>
</tr>
<tr>
<td>12.9</td>
<td>0.33</td>
<td>0.3433</td>
<td>0.8505</td>
</tr>
<tr>
<td>18.0</td>
<td>0.34</td>
<td>0.4523</td>
<td>1.3327</td>
</tr>
<tr>
<td>19.5</td>
<td>0.34</td>
<td>0.4985</td>
<td>1.7619</td>
</tr>
<tr>
<td>24.3</td>
<td>0.44</td>
<td>0.4922</td>
<td>1.6761</td>
</tr>
<tr>
<td>26.1</td>
<td>0.48</td>
<td>0.4902</td>
<td>1.6486</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**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 °C

---

### Component: 1,1,2-trichloroethane; C₃H₇Cl₂; [79-09-3]

- Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
- 77K = 321; 76mm Hg = 648

### Prepared By:
- A. L. Horvath

### Auxiliary Information

- One-liquid system analysis parameter, from dilution measurements.
<table>
<thead>
<tr>
<th>Component</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) 1,1,2-trichloroethane; C₃H₇Cl₂; [79-00-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables</th>
<th>Prepared By</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 298</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

### Experimental Data

<table>
<thead>
<tr>
<th>T°C</th>
<th>g₁V₂⁻¹/kg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.30</td>
<td>9.0 x 10⁻¹</td>
<td>6.63</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Water was added gradually to 50 cm³ 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 Fisher titration method.

**Source and Purity of Materials:**
(1) Distilled (compiler).
(2) Commercial JIS extra pure reagent, further purified by conventional method.

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

---

<table>
<thead>
<tr>
<th>Component</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; HO; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables</th>
<th>Prepared By</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 303</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

### Experimental Data

<table>
<thead>
<tr>
<th>T°C</th>
<th>g₁V₂⁻¹/kg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>4.3653</td>
<td>0.4565</td>
<td>5.917</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Standard 1,1,2-trichloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere. The aqueous organic liquid phase was 25 cm³ and the vapor phase above the mixture was 25 cm³. 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., pure grade available.
(2) Distilled and run through two Barnstead purification cartridges.

**Estimated Errors:**
Solubility: ± 7.5% std. dev.
Temperature: ± 0.5 K (compiler).

**References:**
Components:  
(1) 1,1,2-trichloroethane; C₈H₅Cl_₂; [79-09-5]  
(2) Water; H₂O; [7732-18-5]

Original Measurements:  

Variables:  
T/K = 283-323

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>υ°C</th>
<th>10² s₁</th>
<th>10² w₁ (compiler)</th>
<th>10³ s₂</th>
<th>10² w₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>6.67</td>
<td>0.492</td>
<td>8.11</td>
<td>0.110</td>
</tr>
<tr>
<td>35</td>
<td>6.58</td>
<td>0.483</td>
<td>12.3</td>
<td>0.168</td>
</tr>
<tr>
<td>50</td>
<td>6.99</td>
<td>0.515</td>
<td>17.5</td>
<td>0.170</td>
</tr>
</tbody>
</table>

Mole fraction of 1,1,2-trichloroethane (x₁) was calculated from the activity coefficient at infinite dilution (γ₁*) using the relation

\[ x₁ = \frac{1}{1 + γ₁*} \]

Auxiliary Information

Method/Apparatus/Procedures:

The water-rich mixture was studied using gas-liquid chromatography in which a mixture of trimethyl and 1,1,2-trichloroethane vapor passed through a sampling loop. The eluted 1,1,2-trichloroethane was determined with a flame ionization detector. The organic-rich mixture was studied using an isoperibol method in which CaCl₂ solution controlled the partial pressure of water. The water concentration of the organic phase was determined by using a Karl Fisher titration apparatus.

Source and Purity of Materials:

(1) Aldrich Chemical Co. Ltd., re-distilled in a glass sieve tray column before use.  
(2) Double distilled tap water.

Estimated Errors:

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

Original Measurements:

Components:
(1) 1,1,2-trichloroethane; C₂H₃Cl₃; [79-00-5]
(2) Water; H₂O; [7732-18-5]

Variables:
T/K = 293–323

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Y / (mm Hg)</th>
<th>10⁹ x₁</th>
<th>100 w₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1320±20</td>
<td>6.58</td>
<td>0.485</td>
</tr>
<tr>
<td>35</td>
<td>1410±25</td>
<td>7.09</td>
<td>0.523</td>
</tr>
<tr>
<td>50</td>
<td>1220±30</td>
<td>8.20</td>
<td>0.604</td>
</tr>
</tbody>
</table>

Auxiliary Information:

Method/Apparatus/Procedure:
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficients of 1,1,2-trichloroethane (Y) in water. Cells containing degassed water were submerged in a thermostat 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.

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 range between the solubility data of Gros et al. and Chittwood, the agreement is very poor. 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.

References:
Components:  
(1) 1-bromo-2-chloroethane; C\textsubscript{2}H\textsubscript{4}BrCl; [107-04-0]  
(2) Water; H\textsubscript{2}O; [7732-18-5]

Original Measurements:  
85, 653 (1933).

Variables:  
77K = 303

Prepared By:  
A. L. Hervath

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$10^6 g_1$</th>
<th>$10^6 g_2$</th>
<th>100 w (compiler)</th>
<th>10$^6 x_2$</th>
<th>(compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>6.88</td>
<td>8.63</td>
<td>0.685</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Experimental Data**

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 spectrophotometer and gas chromatograph described elsewhere. A detailed description of the complete procedure is given in a M. A. Gorman thesis.  

Source and Purity of Materials:  
(1) Eschenbach 60, distilled fractionally before use, b.p. 106.62-106.71 °C.  
(2) Distilled.

Estimated Errors:  
Solubility: ±1%.  
Temperature: ±0.02 °C.

References:  

Components:  
(1) 1-bromo-2-chloroethane; C\textsubscript{2}H\textsubscript{4}BrCl; [107-04-0]  
(2) Water; H\textsubscript{2}O; [7732-18-5]

Original Measurements:  

Variables:  
77K = 298

Prepared By:  
A. L. Hervath

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w (compiler)</th>
<th>$10^5 x_2$ (compiler)</th>
<th>100 w Mo\textsuperscript{2+} (1mol g\textsuperscript{-1}) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.69</td>
<td>8.72</td>
<td>4.81 × 10\textsuperscript{-3}</td>
</tr>
</tbody>
</table>

**Experimental Data**

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).
46. 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 L2-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 to 348 K. The data of Booth and Iversen are notably higher than the likely solubility and are rejected. Similar conclusions were drawn for the poor solubility of other solubility data (e.g., CCl₄, CHB₄, CH₂Cl₂, C₂H₄Cl₂, and C₂H₆Cl₂), which justifies the rejection of these data. The measurements of Wade and Dredfick 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.² is used as a guide for the other measured data and therefore the data 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 Syder,³ van Arkel and Visscher,⁴ Shenakovsky and Zeulina,⁵ Drozhdin and Shoutovskaya,⁶ Chervod,⁷ Call,⁸ O’Connell,¹¹ China and Freest,¹² Mackay et al.,¹³ and Teves et al.¹⁴ were used to obtain the following mass percent (1) equation:

\[
\text{Solubility (100 w₁)} = 3.8651 - 1.7921 \times 10^{-3}(75K) + 5.4565 \times 10^{-5}(75K)^2,
\]

which shows a standard deviation of 3.72 x 0.01 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 significant overlap above the temperature interval used for the measurement. Additional details concerning the appearance of the solubility minimum in most aqueous biphased 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.

![Graph showing solubility vs. temperature](image)

Fig. 17. Solubility of 1,2-dibromoethane (1) in water (2).

### Table 1. Tentative solubility of 1,2-dibromoethane (1) in water (2)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>100 w₁</th>
<th>Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.11</td>
<td>0.309</td>
<td>2.971</td>
</tr>
<tr>
<td>5</td>
<td>278.11</td>
<td>0.320</td>
<td>3.077</td>
</tr>
<tr>
<td>10</td>
<td>283.11</td>
<td>0.334</td>
<td>3.172</td>
</tr>
<tr>
<td>15</td>
<td>288.11</td>
<td>0.350</td>
<td>3.287</td>
</tr>
<tr>
<td>20</td>
<td>293.11</td>
<td>0.369</td>
<td>3.359</td>
</tr>
<tr>
<td>25</td>
<td>298.11</td>
<td>0.391</td>
<td>3.576</td>
</tr>
<tr>
<td>30</td>
<td>303.11</td>
<td>0.415</td>
<td>3.792</td>
</tr>
<tr>
<td>35</td>
<td>308.11</td>
<td>0.442</td>
<td>4.045</td>
</tr>
<tr>
<td>40</td>
<td>313.11</td>
<td>0.472</td>
<td>4.346</td>
</tr>
<tr>
<td>45</td>
<td>318.11</td>
<td>0.505</td>
<td>4.625</td>
</tr>
<tr>
<td>50</td>
<td>323.11</td>
<td>0.540</td>
<td>5.018</td>
</tr>
<tr>
<td>55</td>
<td>328.11</td>
<td>0.578</td>
<td>5.478</td>
</tr>
<tr>
<td>60</td>
<td>333.11</td>
<td>0.619</td>
<td>5.960</td>
</tr>
<tr>
<td>65</td>
<td>338.11</td>
<td>0.663</td>
<td>6.326</td>
</tr>
<tr>
<td>70</td>
<td>343.11</td>
<td>0.709</td>
<td>6.684</td>
</tr>
<tr>
<td>75</td>
<td>348.11</td>
<td>0.758</td>
<td>7.024</td>
</tr>
</tbody>
</table>

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 Shenakovsky and Zeulina are significantly higher than the other measurements and are therefore rejected. These data are an order of magnitude too high. The data of Mackay et al.¹³ is several percent lower than other results and is also rejected.

The remaining data of Boët,¹⁵ Straverman,¹⁵ Hutchison and Lyon,¹⁷ and O’Connell¹¹ were used for data smoothing. The fitting equation used was:

\[
\log_{10} w_2 = 0.7213 - 886.78/(75K),
\]

which gave a standard deviation of 5.15 x 10⁻² in the narrow temperature range from 288 to 306 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)

<table>
<thead>
<tr>
<th>°C</th>
<th>Temperature</th>
<th>100 w₂</th>
<th>Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>288.11</td>
<td>0.0526</td>
<td>5.489</td>
</tr>
<tr>
<td>20</td>
<td>293.11</td>
<td>0.0593</td>
<td>6.146</td>
</tr>
<tr>
<td>25</td>
<td>298.11</td>
<td>0.0665</td>
<td>6.899</td>
</tr>
<tr>
<td>30</td>
<td>303.11</td>
<td>0.0743</td>
<td>7.697</td>
</tr>
</tbody>
</table>

Measured values and the linear relationship between the solubility expressed as log₁₀ w₂ versus 1/(75K) 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:


Components:
1. 1,2-dibromoethane: C₉H₈Br₂, [106-93-4]

Original Measurements:

Variables:
T/K = 288-363

Prepared By:
A. L. Forthath

Experimental Data

<table>
<thead>
<tr>
<th>T°C</th>
<th>10⁵ x₂ / L₂</th>
<th>10⁵ w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>3.92</td>
<td>0.390</td>
<td>3.75</td>
</tr>
<tr>
<td>30</td>
<td>4.31</td>
<td>0.429</td>
<td>4.13</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of 1,2-dibromoethane in 500 g water was shaken for 12 h in a water bath thermostated. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss. A detailed description of the complete procedure is given in a Ph.D. thesis.

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:
### Components
(1) Water; H₂O; [7732-18-5]
(2) 1,2-dichloroethane; C₂H₅Cl₂; [106-93-4]

### Experimental Data

<table>
<thead>
<tr>
<th>°C</th>
<th>10⁰ g₁ / g₂</th>
<th>10⁰ w₁ (compiler)</th>
<th>10⁰ c₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>1.04</td>
<td>4.75 × 10⁻³</td>
<td>4.93</td>
</tr>
<tr>
<td>20</td>
<td>1.30</td>
<td>5.97 × 10⁻²</td>
<td>6.19</td>
</tr>
<tr>
<td>25</td>
<td>1.61</td>
<td>7.42 × 10⁻²</td>
<td>7.68</td>
</tr>
</tbody>
</table>

### Auxiliary Information

Method/Apparatus/Procedure:
A mixture of water and 1,2-dichloroethane of about 1 to 5 volume ratio was placed in a sample vessel and rotated in a thermostated flask 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 naphthol yellow dihydrochlorphosphate. The evolved HCl gas was absorbed in water and titrated with NaOH solution. Two to three successive determinations were carried out with the samples.

Source and Purity of Materials:
(1) Distilled (compiler).
(2) Knoch reagent, analytical grade, redistilled before use.

Estimated Errors:
Solubility: ± 1.5% main dev.
Temperature: ± 0.02 °C

References:
### Components

1. Water; H₂O. [7732-18-5]
2. 1,2-dibromoethane; C₂H₂Br₂. [106-93-4]

### Original Measurements


### Variables

T/K = 298–303

### Experimental Data

<table>
<thead>
<tr>
<th>T°C</th>
<th>10⁶ w₁</th>
<th>10⁶ w₂ M⁻¹ mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>6.565×10⁻³</td>
<td>0.85×10⁻²</td>
</tr>
<tr>
<td>30</td>
<td>7.145×10⁻³</td>
<td>0.46×10⁻²</td>
</tr>
</tbody>
</table>

### Experimental Data (continued)

<table>
<thead>
<tr>
<th>T°C</th>
<th>10⁶ w₁</th>
<th>10⁶ w₂ M⁻¹ mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.25</td>
<td>2.40</td>
</tr>
<tr>
<td>25</td>
<td>0.36</td>
<td>3.46</td>
</tr>
<tr>
<td>35</td>
<td>0.42</td>
<td>4.04</td>
</tr>
<tr>
<td>50</td>
<td>0.54</td>
<td>5.20</td>
</tr>
<tr>
<td>75</td>
<td>0.77</td>
<td>7.43</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **Method/Apparatus/Procedure:**
  - Water was shaken with 1,2-dibromoethane for about 12 h in a paraffin liquid bath thermostated. 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.

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

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ± 0.5 K (compiler).

- **References:**

### Additional Information

- **Auxiliary Information:**
  - Source and Purity of Materials:
    - (1) Source and purity not given.
    - (2) Distilled.

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ± 0.5 K (compiler).

- **References:**
Components:  
(1) 1,2-dibromomethane; C₂H₂Br₂ [106-95-4]  
(2) Water; H₂O [7732-18-5]

Original Measurements:  

Variables:  
77K = 308

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>10² x₁ (compiler)</th>
<th>100 w₁ M⁻¹·l·mol⁻¹·g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>0.42</td>
<td>4.44</td>
</tr>
<tr>
<td></td>
<td>2.23 × 10⁻³</td>
<td></td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:  
A 20 cm³ 1,2-dibromomethane sample was mixed with 40 cm³ water in a flask fitted with a thermometer 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic-rich phase was calculated by the method of Kursan.¹

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

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

References:  

Components:  
(1) Water; H₂O [7732-18-5]  
(2) 1,2-dibromomethane; C₂H₂Br₂ [106-93-4]

Original Measurements:  

Variables:  
77K = 298

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temp (°C)</th>
<th>100 w₁ M⁻¹·l·mol⁻¹·g⁻¹ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>5.84 × 10⁻²</td>
<td>6.06</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:  
A 1 to 15 volume ratio mixture of water and 1,2-dibromomethane was introduced into an equilibrium flask and then lowered into the water bath 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: ±1.0 × 10⁻⁵ mol·l⁻¹·g⁻¹.  
Temperature: ±0.05 K.

References:  
### Components
1. 1,2-dibromomethane, $\text{CH}_2\text{Br}_2$; [106-93-4]
2. Water, $\text{H}_2\text{O}$; [7732-18-5]

### Original Measurements

### Variables
$T/K=298$

### Prepared By
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>$1/\text{C}$</th>
<th>$100 V_1, N_2$</th>
<th>$100 w_1$ (complex)</th>
<th>$10^6 x_1$ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.40</td>
<td>0.85</td>
<td>8.3</td>
</tr>
</tbody>
</table>

### Experimental Data

<table>
<thead>
<tr>
<th>$1/\text{C}$</th>
<th>$100 w_1$ (complex)</th>
<th>$10^6 x_1$ (complex)</th>
<th>$100 w_{M_1}^{1/1//mol g^{-1}}$ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.43</td>
<td>4.14</td>
<td>2.29 x 10^{-3}</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

The equilibrium was established through repeated shaking and centrifuging of a 1,2-dibromomethane and water mixture in a stopped glass tube and returned the tube to a constant temperature water bath. The difference between the total amount of 1,2-dibromomethane 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 Hanlick.\(^1\)

**Source and Purity of Materials:**

(1) Commercial reagent, G. F. grade, used as received.
(2) Distilled.

**Estimated Errors:**

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

**References:**

Components:
(1) 1,2-dibromoethane, C₂H₅Br₂; [106-93-4]
(2) Water, H₂O; [7732-18-5]

Original Measurements:

Prepared By:
A. L. Horvath

Variables:
T/K = 293

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>0.01V/I·Ag m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁹ x₁ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>0.411</td>
<td>4.31×10⁻⁴</td>
<td>4.15</td>
</tr>
</tbody>
</table>

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 exit and 1,2-dibromoethane was determined by the catalytic thermal decomposition procedure. The decomposition products were absorbed in a solution of NaOH containing H₂O₂. The generated bromide was titrated with AgNO₃ solution.¹

Source and Purity of Materials:
(1) Laboratory sample, washed with NaHCO₃ solution, dried over Na₂SO₄ and recrystallised twice.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ±0.05 K (compiler).

References:

Original Measurements:

Prepared By:
A. L. Forman

Variables:
T/K = 293

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>ρ₁ /kg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁹ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3.37×10⁻²</td>
<td>0.338</td>
<td>3.25</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
100 cm³ distilled water and a known amount of 1,2-dibromoethane were placed in a scintillation flask. The equilibrium was attained by placing the flask in a mechanical shaker for one hour. The experiment was performed in a constant temperature room. The results were obtained from two separate experiments.³

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

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

References:
### Components
(1) Water, Li2O; [7732-18-5]
(2) 1,2-dibromoethane; C2H4Br2; [106-93-4]

### Original Measurements

### Variables
\( T/K = 298 \)

### Prepared By
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>( T^\circ C )</th>
<th>( \gamma_{1} )</th>
<th>( 10^{6} x_{1} ) (compiler)</th>
<th>( 100 , \text{mol} , \text{g}^{-1} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>7.1 \times 10^{-1}</td>
<td>7.35</td>
<td>3.94 \times 10^{-3}</td>
</tr>
</tbody>
</table>

### Auxiliary Information

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<thead>
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</thead>
<tbody>
<tr>
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</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Source and Purity of Materials:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Distilled.</td>
</tr>
<tr>
<td>(2) Dow Chemical Co., 99.91% pre, purified by distillation before use.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Estimated Errors:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility: not specified.</td>
</tr>
<tr>
<td>Temperature: ± 1 K (compiler).</td>
</tr>
</tbody>
</table>

### Components
(1) 1,2-dibromoethane; C2H4Br2; [106-93-4]
(2) Water; H2O; [7732-18-5]

### Original Measurements

### Variables
\( T/K = 293-298 \)

### Prepared By
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>( T^\circ C )</th>
<th>( 100 , \text{g} / \text{g} )</th>
<th>( 10^{6} x_{2} ) (compiler)</th>
<th>( 100 , \text{mol} , \text{g}^{-1} ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td></td>
<td>7.4 \times 10^{-2}</td>
<td></td>
</tr>
<tr>
<td>25</td>
<td>4.17 \times 10^{-2}</td>
<td>4.00</td>
<td></td>
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### Auxiliary Information

<table>
<thead>
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<th>Method/Apparatus/Procedure:</th>
</tr>
</thead>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Source and Purity of Materials:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dow Chemical Co., used as received.</td>
</tr>
<tr>
<td>(2) Distilled (compiler).</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Estimated Errors:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility: not specified.</td>
</tr>
<tr>
<td>Temperature: ± 0.5 K (compiler).</td>
</tr>
</tbody>
</table>
### Components:
1. 1,2-dibromoethane; C₂H₄Br₂; [106-93-4]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
1. T/K = 276–367

### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>( \rho V_2^{-1}/kg )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10⁵ ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>2.97</td>
<td>0.296</td>
<td>2.85</td>
</tr>
<tr>
<td>20</td>
<td>3.52</td>
<td>0.351</td>
<td>3.38</td>
</tr>
<tr>
<td>34</td>
<td>4.14</td>
<td>0.415</td>
<td>3.99</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
An excess of 5–10 g 1,2-dibromoethane was equilibrated with 100 cm³ 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 30-m electron capture detector. The GLC column was packed with porous pumice Chromosorb 101. Further details on determination and evaluation of the procedure have been reported by Chien and Schmieding.¹

**Estimated Errors:**
Solubility: not specified.
Temperature: ± 0.5 K.

**References:**
### Components:
1. 1,2-dibromoethane; C₂H₂Br₂; [106-93-4]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
T/K = 298

<table>
<thead>
<tr>
<th>Experimetal Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>10°C</td>
</tr>
<tr>
<td>25</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
A saturated aqueous solution of 1,2-dibromoethane was filtered and samples of 30, 100, and 200 μL were diluted in a 0.1 N methylethylammonium perchlorate aqueous solution. A cathodoluminescence on the RMD3 was recorded. Quantification was done by standard addition using 0.01 M solute in ethanol as the standard.

**Source and Purity of Materials:**
(1) Fisher Scientific Co., EL73 certified, 99.9% pure. Used as received.

**Estimated Errors:**
Solubility: ±4.0×10⁻⁵ g₁/ε₂.
Temperature: ±0.2 K.

### Components:
1. 1,2-dibromoethane; C₂H₂Br₂; [106-93-4]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
T/K = 283–309

<table>
<thead>
<tr>
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</tr>
</thead>
<tbody>
<tr>
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</tr>
<tr>
<td>10</td>
</tr>
<tr>
<td>20</td>
</tr>
<tr>
<td>30</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
250 cm² 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 microsyringe. 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.

**Estimated Errors:**
Solubility: not specified.
Temperature: ±0.3 K (compiler).
### 50. 1,2-Dibromomethane with Magnesium Chloride and Water

#### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$w_2$</th>
<th>$w_1$</th>
<th>$10^3 x_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>12.28</td>
<td>1.9x10^{-1}</td>
<td>2.36</td>
</tr>
<tr>
<td></td>
<td>21.27</td>
<td>4.3x10^{-1}</td>
<td>0.507</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

**Method/Apparatus/Procedure:**
A 20 cm³ 1,2-dibromomethane sample was mixed with 40 cm³ aqueous electrolyte solution in a flask fitted with a thermostatic 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Kuznetsov.

**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:**

### 51. 1,2-Dibromomethane with Magnesium Chloride, Magnesium Sulfate, and Water

#### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$w_2$</th>
<th>$w_1$</th>
<th>$w_3$</th>
<th>$100 w_3$</th>
<th>$100 w_1$</th>
<th>$100 w_2$</th>
<th>$100 w_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>8.4</td>
<td>6.5</td>
<td>0.6</td>
<td>6.51 x10^{-2}</td>
<td>8.46 x10^{-2}</td>
<td>6.51 x10^{-2}</td>
<td></td>
</tr>
<tr>
<td>12.10</td>
<td>4.65</td>
<td>6.51</td>
<td>0.61</td>
<td>6.51 x10^{-2}</td>
<td>6.51 x10^{-2}</td>
<td>6.51 x10^{-2}</td>
<td></td>
</tr>
<tr>
<td>19.3</td>
<td>2.17</td>
<td>6.51</td>
<td>0.61</td>
<td>6.51 x10^{-2}</td>
<td>6.51 x10^{-2}</td>
<td>6.51 x10^{-2}</td>
<td></td>
</tr>
</tbody>
</table>

#### Auxiliary Information

**Method/Apparatus/Procedure:**
A 20 cm³ 1,2-dibromomethane sample was mixed with 40 cm³ aqueous electrolyte solution in a flask fitted with a thermostatic 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Kuznetsov.

**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:**
52. 1,2-Dibromoethane with Magnesium Sulfate and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>°C</th>
<th>100 w₂</th>
<th>100 w₁</th>
<th>10⁴ x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>23.3</td>
<td>2.6×10⁻¹</td>
<td>2.15</td>
</tr>
<tr>
<td>9.36</td>
<td>1.9×10⁻¹</td>
<td>2.27</td>
<td></td>
</tr>
<tr>
<td>15.74</td>
<td>9.0×10⁻²</td>
<td>1.14</td>
<td></td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Method/Apparatus/Procedure:**
  A 20 cm³ 1,2-dibromoethane sample was mixed with 40 cm³ 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 in the organic phase was determined by adding AgNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Carini.¹

- **Source and Purity of Materials:**
  1. Source and purity not given.
  2. Source and purity not given.
  3. Entitled.

- **Estimated Errors:**
  Solubility: not specified.
  Temperature: ±0.5 K (compiler).

- **References:**

---

53. 1,2-Dibromoethane with Sodium Chloride and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>°C</th>
<th>100 w₂</th>
<th>100 w₁</th>
<th>10⁴ x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>3.68</td>
<td>30×10⁻¹</td>
<td>4.36</td>
</tr>
<tr>
<td>11.24</td>
<td>27×10⁻¹</td>
<td>3.19</td>
<td></td>
</tr>
<tr>
<td>26.42</td>
<td>9.0×10⁻²</td>
<td>1.20</td>
<td></td>
</tr>
</tbody>
</table>

**Auxiliary Information**

- **Method/Apparatus/Procedure:**
  A 20 cm³ 1,2-dibromoethane sample was mixed with 40 cm³ 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 in the organic phase was determined by adding AgNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Kriuse.¹

- **Source and Purity of Materials:**
  1. Source and purity not given.
  2. Source and purity not given.
  3. Entitled.

- **Estimated Errors:**
  Solubility: not specified.
  Temperature: ±0.5 K (compiler).

- **References:**
### Components
1. 1,2-dibromoethane; C₆H₅Br₂; [106-93-4]
2. Sodium chloride; NaCl; [7647-14-5]
3. Magnesium chloride; MgCl₂; [7786-30-3]
4. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
77K = 308 K and Concentration

| 54. 1,2-Dibromoethane with Sodium Chloride, Magnesium Chloride, and Water |
|---|---|---|---|
| n°C | 0°C w₀ | 100 w₀ | 100 w₁ |
| 350 | 11.20 | 13.07 | 1.6×10⁻³ |
| 17.93 | 6.36 | 1.2×10⁻³ |

### Auxiliary Information
- **Method/Apparatus/Procedure:** A 20 cm³ 1,2-dibromoethane sample was mixed with 40 cm³ 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic riche phase was calculated by the method of Kama.

### 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:

### Components:
1. 1,2-dibromoethane; C₆H₅Br₂; [106-93-4]
2. Sodium chloride; NaCl; [7647-14-5]
3. Sodium sulfate; Na₂SO₄; [7778-04-6]
4. Water; H₂O; [7732-18-5]

### Original Measurements:

### Variables:
77K = 308 K and Concentration

| 55. 1,2-Dibromoethane with Sodium Chloride, Sodium Sulfate, and Water |
|---|---|---|---|
| n°C | 0°C w₀ | 100 w₀ | 100 w₁ |
| 35.6 | 19.6 | 12.24 | 1.5×10⁻³ |
| 16.46 | 15.82 | 1.0×10⁻² |
| 10.08 | 21.16 | 1.1×10⁻² |

### Auxiliary Information
- **Method/Apparatus/Procedure:** A 20 cm³ 1,2-dibromoethane sample was mixed with 40 cm³ 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Kama.

### 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:
56. 1,2-Dibromoethane with Sodium Sulfate and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>τ°C</th>
<th>100 w₂</th>
<th>100 w₁</th>
<th>10² z₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>5.47</td>
<td>7.8 x 10⁻¹</td>
<td>8.94</td>
</tr>
<tr>
<td>17.89</td>
<td>1.1 x 10⁻¹</td>
<td>1.42</td>
<td></td>
</tr>
<tr>
<td>24.13</td>
<td>6.0 x 10⁻²</td>
<td>0.868</td>
<td></td>
</tr>
<tr>
<td>32.56</td>
<td>1.2 x 10⁻³</td>
<td>0.185</td>
<td></td>
</tr>
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</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A 20 cm³ 1,2-dibromoethane sample was mixed with 40 cm³ 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Karius.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).

---

57. 1,2-Dibromoethane with Sodium Sulfate, Magnesium Sulfate, and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>τ°C</th>
<th>100 w₂</th>
<th>100 w₁</th>
<th>100 w₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>35.0</td>
<td>10.2</td>
<td>12.76</td>
<td>6.0 x 10⁻²</td>
</tr>
<tr>
<td>18.87</td>
<td>9.81</td>
<td>8.2 x 10⁻²</td>
<td></td>
</tr>
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<td>23.9</td>
<td>4.35</td>
<td>1.6 x 10⁻²</td>
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</tr>
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<td>28.0</td>
<td>1.54</td>
<td>5.2 x 10⁻²</td>
<td></td>
</tr>
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**Auxiliary Information**

**Method/Apparatus/Procedure:**
A 20 cm³ 1,2-dibromoethane sample was mixed with 40 cm³ 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 HNO₃ to the solution and the free bromine was titrated with AgNO₃ solution. The water content of the organic rich phase was calculated by the method of Karius.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).

---

Components:
(1) Water-$\text{d}_2$: D$_2$O; [7782-26-0]
(2) 1,2-Dibromoethane: C$_2$HBr$_2$: [106-93-4]

Original Measurements:
C. A. Hutchison and M. Lyon, Columbus University Report A-745 (July 1, 1943).

Variables:
$T/K = 298$

Prepared By:
A. L. Sorvath

58. 1,2-Dibromoethane with Water-$\text{d}_2$

Experimental Data

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>100 $w_1$ [mol g$^{-1}$]</th>
<th>100 $w_x$ (compiler)</th>
<th>$10^5 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.79 x 10$^{-3}$</td>
<td>5.59 x 10$^{-4}$</td>
<td>5.22</td>
</tr>
</tbody>
</table>

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. The original university report is no longer available.

Source and Purity of Materials:
(1) Source and purity as given.
(2) Probably a commercial reagent, further purified and dried beforehand.

Estimated Errors:
Solubility: ±1.0 x 10$^{-4}$ avg. dev.
Temperature: ±0.05 K

References:

59. 1-Chloro-2-Fluoroethane with Water

Experimental Data

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$g_1 V_x^{1/2}$ [kg m$^{-3}$]</th>
<th>100 $w_x$ (compiler)</th>
<th>$10^5 x_x$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>25</td>
<td>2.44</td>
<td>5.41</td>
</tr>
</tbody>
</table>

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).
60. 1,1-Dichlorehane with Water

Critical Evaluation

The 1,1-dichlorehane (1) and water (2) binary system is rated in two parts; part 1 is 1,1-dichlorehane (1) in water (2) and part 2 is water (2) in 1,1-dichlorehane (1).

Part 1. The solubility of 1,1-dichlorehane (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 data of Ley et al. is significantly lower than all other measurements and is therefore rejected. The solubility values of Heine et al. are several percent higher than those calculated from the smoothing equation and are also rejected.

The remaining data of Rees, Wright and Scheller, van Artikel and Vins, Waldherr et al., Satow and Nakajima, Newham, McCall and Gore, Buxton and Newham, Wexler et al., and Wright et al. are used to obtain the following mass percent (1) equation:

\[ \text{Solubility (100 w/w)} = 9.4136 - 5.249 \times 10^{-5} (\text{m} - 273) + 9.1789 \times 10^{-3} (\text{m} - 273)^2 \]

which shows a standard deviation of 3.70x10^-2 in the temperature range from 273 to 323 K.

The measurements and the curve obtained from the smoothing equation are shown in Fig. 15. A solubility minimum calculated from the above regression equation is 0.487 [100 w/w] 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-dichlorehane (1) in water (2) are presented in Table 1.

![Graph showing solubility of 1,1-dichlorehane (1) in water (2).](image)

**Table 1. Recommended solubility of 1,1-dichlorehane (1) in water (2)**

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>Solubility (100 w/w)</th>
</tr>
</thead>
<tbody>
<tr>
<td>273.15</td>
<td>0.624</td>
</tr>
<tr>
<td>278.15</td>
<td>0.591</td>
</tr>
<tr>
<td>283.15</td>
<td>0.562</td>
</tr>
<tr>
<td>288.15</td>
<td>0.538</td>
</tr>
<tr>
<td>293.15</td>
<td>0.519</td>
</tr>
<tr>
<td>298.15</td>
<td>0.504</td>
</tr>
<tr>
<td>303.15</td>
<td>0.493</td>
</tr>
<tr>
<td>308.15</td>
<td>0.488</td>
</tr>
<tr>
<td>313.15</td>
<td>0.478</td>
</tr>
<tr>
<td>318.15</td>
<td>0.469</td>
</tr>
<tr>
<td>323.15</td>
<td>0.458</td>
</tr>
</tbody>
</table>

Part 2. The solubility of water (2) in 1,1-dichlorehane (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. The combined data of Newham et al. and Buxton and Newham were used for the smoothing equation:

[^1]: 9.4136 - 5.249 \times 10^{-5} (\text{m} - 273) + 9.1789 \times 10^{-3} (\text{m} - 273)^2

[^2]: This equation expresses the combined data with a standard deviation of 4.13x10^-3 in the temperature range from 273 to 323 K. The recommended solubility values at 5 K intervals for water (2) in 1,1-dichlorehane (1) are presented in Table 2.

[^3]: Measured values and the curve obtained from the smoothing equation for solubility expressed as log_{10} s_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} s_2 versus 1/T(K). Such straight line plots are characteristic for water solubility in halogenated hydrocarbons. The reader should consult the Preface for further details.
Components:
(1) 1,1-dichloroethane; C₂H₄Cl₂; [75-34-3]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
77K = 298

Prepared By:
A. L. Hervath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g; 8₁ (compiler)</th>
<th>10₀ w₁ (compiler)</th>
<th>10^6 x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.50 a</td>
<td>0.503</td>
<td>9.19</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
A weighted amount of 1,1-dichloroethane was mixed with 1000 g water in a bottle and heated on a water-bath thermostat. The bottle was placed in 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 spectrophotometer. One or more samples were prepared as 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 °C.

References:
¹P. N. Gross, Z. Phys. Chem. 68, 21 (1929).

Components:
(1) 1,1-dichloroethane; C₂H₄Cl₂; [75-34-3]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
77K = 298

Prepared By:
A. L. Hervath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>V₂₉⁷/°C cm³ g⁻¹</th>
<th>10₀ w₁ (compiler)</th>
<th>10^6 x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.80 x 10⁴</td>
<td>0.554</td>
<td>1.01</td>
</tr>
</tbody>
</table>

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 NaHCO₃ solution and redistilled.
(2) Distilled.

Estimated Errors:
Solubility: not specified.
Temperature: ± 0.5 °C (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 g (\times 1)</th>
<th>100 (w_1) (\times 10^3)</th>
<th>20° (x_1) (\times 10^{-3})</th>
<th>100 (w_1) (\times 10^{-3}) (\text{mol}^{-1}) (\text{g}^{-1}) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.590</td>
<td>10.79</td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.503</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>35</td>
<td>0.480</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>0.516</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
Water was shaken with 1,1-dichloroethane for about 12 h in a paraffin liquid water thermostat. The water content of the organic phase was determined by the Karl Fiechter titration method. All measurements were carried out in duplicate. The result is an average of two measurements. A full description of the method and 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: \(\pm 0.5\) K (compiler).

**References:**
<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

**Variables:**

| T/K = 298 |

| Prepared By: | A. L. Horvath |

**Experimental Data**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁</th>
<th>0° x₁ (compiler)</th>
<th>100 w₂ M⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.0×10⁻³</td>
<td>1.36</td>
<td>1.03×10⁻⁴</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**

(1) Sample used,

(2) High grade, purified by distillation and recrystallisation.

**Estimated Errors:**

Solubility: ±0.05%.

Temperature: ±0.5 K.

---

**Components:**

(1) 1,1-dichloroethane; C₂H₃Cl₂; [75-34-3]

(2) Water; H₂O; [7732-18-5]

**Original Measurements:**


**Variables:**

| T/K = 283-350 |

| 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:

\[
\log_{10}(\text{solubility} \text{ (mol dm}^{-3}\text{)}) = \frac{2070}{T(K)} - 15.116 + 0.0230(T/K),
\]

where S = solubility, and T = absolute temperature.

For example, the calculated solubility derived from the above equation is 1.77×10⁻¹ [100 w₁] at 298.15 K (compiler).

**Auxiliary Information**

**Method/Apparatus/Procedure:**

A mixture of 1,1-dichloroethane and water was prepared 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.

**Estimated Errors:**

Solubility: ±0.05%.

Temperature: ±0.5 K.
Components:
(1) 1,1-dichloroethane; C₃H₅Cl₂ [75-34-3]
(2) Water; H₂O [7732-18-5]

Variables:
\( T/K = 310 \)

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>( T/°C )</th>
<th>Partition coefficient, ( k ) (dimensionless)</th>
<th>100 ( w_1 ) (complete)</th>
<th>10² ( x_1 ) (complete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>2.7</td>
<td>0.512</td>
<td>9.36</td>
</tr>
</tbody>
</table>

*Gas–liquid chromatographic parameter, from instrument calibration.

Auxiliary Information

Method/Apparatus/Procedure:
A 1,1-dichloroethane vapor sample was equilibrated in an airight vessel between water and the overlying air. When equilibrium was reached, a portion of the equilibrated air in the vessel was withdrawn using an airight syringe and then injected into a gas chromatograph and analyzed. The signal peak height in the chromatogram was used to calculate the partition coefficient.

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

Estimated Errors:
Solubility: \( ±0.6 \) mol dl⁻¹.
Temperature: \( ±0.5 \) K (complete).

Source and Purity of Materials:

Variables:
\( T/K = 273–323 \)

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>( T/°C )</th>
<th>10³ ( v_1 )</th>
<th>100 ( w_2 ) (complete)</th>
<th>10² ( x_2 )</th>
<th>100 ( w_2 ) (complete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>--</td>
<td>2.71</td>
<td>4.94x10⁻²</td>
<td></td>
</tr>
<tr>
<td>11.4</td>
<td>8.9</td>
<td>0.462</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>20.0</td>
<td>8.5</td>
<td>0.465</td>
<td>4.53</td>
<td>8.28x10⁻²</td>
</tr>
<tr>
<td>25.0</td>
<td>8.1</td>
<td>0.49</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>30.0</td>
<td>8.0</td>
<td>0.6</td>
<td>6.45</td>
<td>1.28x10⁻¹</td>
</tr>
<tr>
<td>35.0</td>
<td>8.0</td>
<td>0.444</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>40.0</td>
<td>--</td>
<td>8.99</td>
<td>1.54x10⁻¹</td>
<td></td>
</tr>
<tr>
<td>50.0</td>
<td>8.2</td>
<td>0.49</td>
<td>1.96x10⁻¹</td>
<td></td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Samples were equilibrated for at least 10 days in water bath thermostat. Water analysis was performed with an automatic Karl Fischer titration apparatus. The concentration of 1,1-dichloroethane in water was determined with a Perkin-Elmer model 900 gas chromatograph equipped with a flame ionization detector and an automatic digitizer. A helium carrier gas and a Porapak 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 (complete).

Estimated Errors:
Solubility: \( ±1 \) %.
Temperature: \( ±0.1 \) K.
### Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>pH</th>
<th>10¹ x₁</th>
<th>100 w₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.9</td>
<td>8.30±0.14</td>
<td>0.454</td>
</tr>
<tr>
<td></td>
<td>5.6</td>
<td>8.63±0.23</td>
<td>0.472</td>
</tr>
<tr>
<td></td>
<td>10.6</td>
<td>8.66±0.16</td>
<td>0.474</td>
</tr>
<tr>
<td>50</td>
<td>2.2</td>
<td>8.00±0.27</td>
<td>0.438</td>
</tr>
<tr>
<td></td>
<td>7.7</td>
<td>8.20±0.23</td>
<td>0.449</td>
</tr>
<tr>
<td></td>
<td>10.0</td>
<td>8.30±0.20</td>
<td>0.454</td>
</tr>
</tbody>
</table>

### 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-dichloroethene 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; C₂H₂Cl₂ [75-34-3]
(2) Water; H₂O [7732-18-5]

Variables:
T/K = 303

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^6 g₁ / c₁</th>
<th>100 w₁ (compiler)</th>
<th>10^6 a₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>4.8344×10⁻³</td>
<td>0.4811</td>
<td>8.795</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Standard solutions were prepared in 100 cm³ flasks. 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 into headspace vials, sealed, thermostatted and then
examined by gas chromatographic headspace analysis
technique. AnF&K 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. Purity grade
available.
(2) Distilled and run through two Isotrac purification
cartridges.

Estimated Errors:
Solubility: ±0.1% R. E.
Temperature: ±0.5 K (compiler).

References:
Components:  
(1) 1,1-dichloroethane; C₂H₄Cl₂; [75-34-3]  
(2) Water; H₂O; [7732-18-5]

Variables:  
T/K = 293–323

Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>10⁻³ x₁ (compiler)</th>
<th>10⁻² w₁ (compiler)</th>
<th>10⁻⁳ x₂ (compiler)</th>
<th>10⁻² w₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>9.26</td>
<td>0.007</td>
<td>5.82</td>
<td>0.106</td>
</tr>
<tr>
<td>35</td>
<td>8.91</td>
<td>0.018</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>50</td>
<td>9.26</td>
<td>0.007</td>
<td>D.5</td>
<td>0.193</td>
</tr>
</tbody>
</table>

Mole fraction of 1,1-dichloroethane (x₁) was calculated from the activity coefficient at infinite dilution (γᵢ) using the relation 
\[ x₁ = \frac{1}{γᵢ} \gamma_i \]

Auxiliary Information

Method/Apparatus/Procedure:
The water-rich mixture was studied using gas-liquid chromatography in which a mixture of methanol 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 CH₂Cl₂ 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) Fluka Limited. Redistilled in a glass still by the column.  
(2) Distilled water.

Estimated Errors:
Solubility: not specified  
Temperature: ±0.05 K.

Components:  
(1) 1,1-dichloroethane; C₂H₄Cl₂; [75-34-3]  
(2) Water; H₂O; [7732-18-5]

Variables:  
T/K = 283–308

Experimental Data

<table>
<thead>
<tr>
<th>T/K</th>
<th>Henry’s law constant, ( H/\text{m}^3\text{atm mol}^{-1} )</th>
<th>CV%</th>
<th>10⁻² w₁ (compiler)</th>
<th>10⁻² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.6</td>
<td>2.4 × 10⁻³</td>
<td>3.60</td>
<td>0.850</td>
<td>1.116</td>
</tr>
<tr>
<td>17.5</td>
<td>3.8 × 10⁻³</td>
<td>1.15</td>
<td>0.550</td>
<td>1.036</td>
</tr>
<tr>
<td>24.8</td>
<td>5.0 × 10⁻³</td>
<td>4.13</td>
<td>0.520</td>
<td>0.9554</td>
</tr>
<tr>
<td>36.6</td>
<td>8.2 × 10⁻³</td>
<td>3.54</td>
<td>0.500</td>
<td>1.0775</td>
</tr>
</tbody>
</table>

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 a screw bottle which contained distilled water. The bottles were incubated for 11–24 h at four desired temperatures in a reciprocating shaker bath. The headspace concentration of the EPICS mixture was measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was about 4.5%.

Source and Purity of Materials:
(1) Fluka AG Chemicals GmbH, greater than 98% pure by GC analysis.  
(2) Distilled water.

Estimated Errors:
Solubility: see above.  
Temperature: ±0.1 K.
Components:
(1) 1,1-dichloroethane; C₂H₃Cl₂; [75-34-3]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 298

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Henry's Law Constant (H/m² atm mol⁻¹)</th>
<th>100 x₁ (complex)</th>
<th>10³ x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>5.45 × 10⁻³</td>
<td>0.58</td>
<td>1.026</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The original method and apparatus for the determination of Henry's law constants, as described by Mackay et al., 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 thermostated, and mix overnight. 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) 100% purity available, used without further purification.
(2) Distilled and de-ionized.

Estimated Errors:
Solubility: ± 6% at dev.
Temperature: ± 0.02 K.

References:

Component:

<table>
<thead>
<tr>
<th>Original Measurements:</th>
</tr>
</thead>
</table>

Variables:
T/K = 293–303

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10⁶ x₁ (complex)</th>
<th>100 x₁ (complex)</th>
<th>10² x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>7.435 × 10⁻³</td>
<td>0.7435</td>
<td>3.613</td>
</tr>
<tr>
<td>20</td>
<td>7.377 × 10⁻³</td>
<td>0.7137</td>
<td>3.069</td>
</tr>
<tr>
<td>30</td>
<td>6.130 × 10⁻³</td>
<td>0.6130</td>
<td>1.216</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
250 cm³ bottles were filled with distilled de-ionized water and sealed. Measured volumes of 1,1-dichloroethane were injected into the bottle through each bottle septum using a microsyringe. The bottle was shaken with a vortex-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).
Component: 1,1-dichloroethane; C₂H₃Cl₂; [75-34-3]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 293–318

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^3 (x_1)</th>
<th>(10^6 w_1) (compile)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>9.09</td>
<td>0.497</td>
</tr>
<tr>
<td>35</td>
<td>8.06</td>
<td>0.441</td>
</tr>
<tr>
<td>45</td>
<td>9.52</td>
<td>0.521</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of 1,1-dichloroethane (\(\gamma^*_A\)) in water. Cells containing degassed water were submerged in a thermostatic 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.

Component: 1,1,2-trichloroethane; C₂H₂Cl₃; [77-50-5]
(3) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K = 285–346

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^3 (x_1)</th>
<th>(10^6 w_1) (compile)</th>
<th>(10^6 w_2) (compile)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11.8</td>
<td>3.83</td>
<td>0.2096</td>
<td>3.34</td>
</tr>
<tr>
<td>25.0</td>
<td>3.92</td>
<td>0.2145</td>
<td>3.40</td>
</tr>
<tr>
<td>30.8</td>
<td>3.89</td>
<td>0.2129</td>
<td>3.74</td>
</tr>
</tbody>
</table>

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 Porapack Q5 column were used for the chromatographic analyses.

Source and Purity of Materials:
(1) Source not given, contains less than 0.1% distilled material.
(2) Source not given, contains less than 0.1% distilled material.
(3) Distilled (compile).

Estimated Errors:
Solubility: ±1%.
Temperature: ± 0.1 K.
### 62. 1,1-Dichloroethane with 1,2-Dichloroethane and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$t^\circ C$</th>
<th>$10^3 x_1$</th>
<th>$100 w_1$ (complete)</th>
<th>$0^3 x_2$</th>
<th>$100 w_2$ (complete)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.5</td>
<td>2.12</td>
<td>116×$10^{-3}$</td>
<td>3.92</td>
<td>0.215</td>
</tr>
</tbody>
</table>

**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 980 gas chromatograph equipped with a flame ionization detector and an automated digital integrator. A helium carrier gas and a Porapak 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 (complete).

- **Estimated Errors:**
  - Solubility: ± 1%.
  - Temperature: ± 0.1 K.

### 63. 1,1-Dichloroethane with Calcium Chloride and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>$100 w_2$</th>
<th>$t^\circ C$</th>
<th>$a_i$</th>
<th>$p_i$/mm Hg</th>
<th>$10^3 x_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>45.54</td>
<td>25</td>
<td>0.280</td>
<td>6.65</td>
<td>1.86</td>
</tr>
<tr>
<td>39.69</td>
<td>25</td>
<td>0.099</td>
<td>4.58</td>
<td>2.42</td>
</tr>
<tr>
<td>35.77</td>
<td>25</td>
<td>0.098</td>
<td>6.53</td>
<td>2.52</td>
</tr>
<tr>
<td>31.86</td>
<td>25</td>
<td>0.097</td>
<td>14.18</td>
<td>3.54</td>
</tr>
<tr>
<td>27.44</td>
<td>25</td>
<td>0.070</td>
<td>16.63</td>
<td>4.21</td>
</tr>
<tr>
<td>18.96</td>
<td>25</td>
<td>0.085</td>
<td>20.19</td>
<td>4.74</td>
</tr>
<tr>
<td>0.0</td>
<td>25</td>
<td>1.000</td>
<td>23.76</td>
<td>5.30</td>
</tr>
<tr>
<td>0.0</td>
<td>50</td>
<td>1.000</td>
<td>92.51</td>
<td>10.87</td>
</tr>
</tbody>
</table>

- $a_i =$ water activity ($= p_i / p^*$).
- $p_i =$ 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 bath thermostat. Water analysis was done using an automatic Karl Fischer titrator apparatus. The instrument accuracy was specified to be 1%. All samples were handled with a hypodermic syringe which was weighed before and after each addition. The instrument was calibrated using synthetic mixtures of 1% water in methanol.

- **Source and Purity of Materials:**
  - (1) Distilled (complete).
  - (2) Source not given, contained less than 0.1% dissolved material.

- **Estimated Errors:**
  - Solubility: ± 1%.
  - Temperature: ± 0.1 K.
### 64. 1,1-Dichloroethane with 1,2-Dichloroethane, Calcium Chloride, and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Equivalent mixture of (3) and (4)</th>
<th>100 ( w_2 )</th>
<th>( T^\circ \text{C} )</th>
<th>( a_2 )</th>
<th>( p_1 / \text{mm Hg} )</th>
<th>( 10^5 x_1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>45.54</td>
<td>25</td>
<td>0.280</td>
<td>5.65</td>
<td>2.09</td>
</tr>
<tr>
<td></td>
<td>46.64</td>
<td>50</td>
<td>0.330</td>
<td>33.5</td>
<td>5.21</td>
</tr>
<tr>
<td></td>
<td>39.69</td>
<td>25</td>
<td>0.399</td>
<td>3.48</td>
<td>2.99</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.434</td>
<td>0.1</td>
<td>6.08</td>
<td></td>
</tr>
<tr>
<td></td>
<td>35.37</td>
<td>25</td>
<td>0.498</td>
<td>8.83</td>
<td>3.72</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.522</td>
<td>-8.3</td>
<td>8.30</td>
<td></td>
</tr>
<tr>
<td></td>
<td>31.36</td>
<td>25</td>
<td>0.597</td>
<td>11.18</td>
<td>4.63</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.615</td>
<td>5.9</td>
<td>9.26</td>
<td></td>
</tr>
<tr>
<td></td>
<td>27.44</td>
<td>25</td>
<td>0.700</td>
<td>8.63</td>
<td>5.44</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.710</td>
<td>61.7</td>
<td>10.75</td>
<td></td>
</tr>
<tr>
<td></td>
<td>18.56</td>
<td>25</td>
<td>0.850</td>
<td>21.19</td>
<td>6.57</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>0.850</td>
<td>71.6</td>
<td>12.84</td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>25</td>
<td>1.000</td>
<td>23.76</td>
<td>7.70</td>
</tr>
<tr>
<td></td>
<td>50</td>
<td>1.000</td>
<td>3.51</td>
<td>15.41</td>
<td></td>
</tr>
</tbody>
</table>

\( a_2 \) = 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 weighed 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 (compleated).

(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.
### 65. 1,1-Dichloroethane with Magnesium Sulfate and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>$10^3 c_1$ (mol dm$^{-3}$)</th>
<th>$10^3 w_1$ (compiler)</th>
<th>$10^5 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.5</td>
<td>0.315</td>
<td>3.06</td>
</tr>
</tbody>
</table>

**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 withdrawn and the concentration of the 1,1-dichloroethane was determined using a Zilni water interferometer.

**Source and Purity of Materials:**
1. Commercial reagent, fractionally distilled before use.
2. Kahlbaum chemical, certified grade.
3. Distilled.

**Estimated Errors:**
Solubility: ±2.5%.
Temperature: ±0.01 K.

---

### 66. 1,1-Dichloroethane with Potassium Chloride and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>$10^3 c_1$ (mol dm$^{-3}$)</th>
<th>$10^3 w_1$ (compiler)</th>
<th>$10^5 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.5</td>
<td>0.443</td>
<td>8.29</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A mixture of 14 to 20 cm$^3$ 1,1-dichloroethane in 500 cm$^3$ of an aqueous KC 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 withdrawn and the concentration of the 1,1-dichloroethane was determined using a Zilni water interferometer.

**Source and Purity of Materials:**
1. Commercial reagent, fractionally distilled before use.
2. Kahlbaum chemical, certified grade.
3. Distilled.

**Estimated Errors:**
Solubility: ±2%. Temperature: ±0.01 K.
### 67. 1,1-Dichloroethane with Sodium Hydroxide and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Activity (a₁)</th>
<th>Saturated Vapor Pressure (mm Hg)</th>
<th>10⁻⁵ x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>52.2</td>
<td>7.03 × 10⁻³</td>
<td>1.67</td>
<td>0.558</td>
</tr>
<tr>
<td>59.2</td>
<td>2.3 × 10⁻³</td>
<td>2.1</td>
<td>1.04</td>
</tr>
<tr>
<td>60</td>
<td>1.000</td>
<td>23.76</td>
<td>5.30</td>
</tr>
<tr>
<td>60</td>
<td>1.000</td>
<td>92.51</td>
<td>10.67</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Methods/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 to the instrument calibrated using a synthetic mixture of 1% water in methanol.

**Source and Purity of Materials:**
- (1) Distilled (complex).
- (2) Source and purity not given.
- (3) Source not given, contained less than 0.1% dissolved material.

**Estimated Error:**
- Solubility: ± 1%.
- Temperature: ± 0.1°C.

**Components:**
- (1) Water: H₂O [184-19-3]
- (2) Sodium hydroxide: NaOH [1310-73-2]
- (3) 1,1-Dichloroethane: C₂H₅Cl [107-06-2]

**Prepared By:** A. L. Horvath

---

### 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 in water (2) in 1,2-dichloroethane (1).

**Part 1.** The solubility of 1,2-dichloroethane (1) in water (2) has been studied by 28 groups of workers with reasonably consistent results. However, the experimental work of several investigators was not used because of known errors. The measured solubility of Sobkowics,1 Pajdinić,2 et al.,3 Atti et al.,4 Coca and Tinoco,5 Cox et al.,6 and Water et al.,7 are unusually higher than the solubility values calculated from the mol fraction equation and are therefore rejected. Similarly, the data of Flees et al.,8 at 35°C and Howe et al.,9 at 30°C are excluded. The data of Satoh and Nishijima,10 Leighton and Cala,11 McGhie and Grath,12 and Proulx et al.,13 are unusually lower than the sodium solubility values and are rejected. Data from the work of Barnett et al.,14 measured at 1 atm total pressure (The increasing solubility between 298 and 373 K indicates that the data were determined at a constant pressure.) Two temperatures for the separation factors of Bold,15 were not stated in his reported data and were also excluded from the regression analysis.

The remaining data from 27 observations were compiled for use in the smoothing equation. The data analysis was conducted using all the measurements of Bax,16 Gross,17 Gross and Saylor,18 Dichtl,18 Lichachowicz et al.,19 van Arkel and Das,12 McGonagle,20 Cheadle,21 Udono and Padilla,22 Kasture and Kini,23 O'Connor,24 Johnson,25 et al.,26 Antropov et al.,27 Wolfram et al.,28 McConnell et al.,29 Fears and McConnell,30 Chiu et al.,31 Bartlett et al.,32 and Bhattacharjee et al.,33 with Newkorn,34 Howe et al.,35 Bold et al.,36 and Wright et al.,37 all values within the temperature interval from 273 to 372 K, to obtain the following mass percent (1) equation:

**Equation:**

\[
\text{Solubility} = \left[100 - \frac{10^5 x_1}{1 + 10^5 x_1}\right] \times 10^{-5} \text{ mol kg}^{-1} \text{ for water (2) in 1,2-dichloroethane (1)}
\]

**Table 1. Recommended solubility of 1,2-dichloroethane (1) in water (2).**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (mol kg⁻¹)</th>
<th>10⁻⁵ x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.024</td>
<td>1.69</td>
</tr>
<tr>
<td>5</td>
<td>0.891</td>
<td>1.63</td>
</tr>
<tr>
<td>10</td>
<td>0.868</td>
<td>1.59</td>
</tr>
<tr>
<td>15</td>
<td>0.855</td>
<td>1.57</td>
</tr>
<tr>
<td>20</td>
<td>0.852</td>
<td>1.56</td>
</tr>
<tr>
<td>25</td>
<td>0.860</td>
<td>1.58</td>
</tr>
<tr>
<td>30</td>
<td>0.877</td>
<td>1.61</td>
</tr>
<tr>
<td>35</td>
<td>0.904</td>
<td>1.66</td>
</tr>
<tr>
<td>40</td>
<td>0.941</td>
<td>1.73</td>
</tr>
<tr>
<td>45</td>
<td>0.989</td>
<td>1.82</td>
</tr>
<tr>
<td>50</td>
<td>1.046</td>
<td>1.92</td>
</tr>
<tr>
<td>55</td>
<td>1.133</td>
<td>2.04</td>
</tr>
<tr>
<td>60</td>
<td>1.190</td>
<td>2.19</td>
</tr>
<tr>
<td>65</td>
<td>1.278</td>
<td>2.35</td>
</tr>
<tr>
<td>70</td>
<td>1.375</td>
<td>2.52</td>
</tr>
<tr>
<td>75</td>
<td>1.482</td>
<td>2.73</td>
</tr>
<tr>
<td>80</td>
<td>1.599</td>
<td>2.95</td>
</tr>
<tr>
<td>85</td>
<td>1.727</td>
<td>3.19</td>
</tr>
<tr>
<td>90</td>
<td>1.864</td>
<td>3.45</td>
</tr>
<tr>
<td>95</td>
<td>2.013</td>
<td>3.72</td>
</tr>
<tr>
<td>100</td>
<td>2.168</td>
<td>4.02</td>
</tr>
</tbody>
</table>

**Components:**
- (1) 1,2-Dichloroethane: C₂H₅Cl [107-06-2]
- (2) Water: H₂O [7732-18-5]
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 0.033 [100 x2] 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 McNamara, 30 Abah et al., 5 and Odberg and Hjöfeldt 31 are substantially higher than all other studies and are rejected. The data of Udovenko and Patrulina, 32 Zelnicki, 33 Chitskikh and Shipanov, 34 Sells, 35 and Azezrov et al. 36 are markedly lower than the smoothed solubility values and are also rejected. The solubility calculated from the data of Prosyanov et al. 37 are in poor agreement; providing no confidence in their values which are regarded in dubious.

The remaining data, mainly due to Coolzide, 38 Stevanovic, 39 McGovern, and Davies et al., 40 were analyzed and used for determination of the equation:

\[
\log_{10} x_2 = -7624 - 1118.4 \left( \frac{T}{7} \right)
\]

This equation represents the combined data values which give a standard deviation of 3.34 x 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>
<thead>
<tr>
<th>Temperature</th>
<th>Solubility (10^3 x2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>°C</td>
<td>K</td>
</tr>
<tr>
<td>-20</td>
<td>225.15</td>
</tr>
<tr>
<td>-15</td>
<td>228.15</td>
</tr>
<tr>
<td>-10</td>
<td>231.15</td>
</tr>
<tr>
<td>-5</td>
<td>234.15</td>
</tr>
<tr>
<td>0</td>
<td>237.15</td>
</tr>
<tr>
<td>5</td>
<td>240.15</td>
</tr>
<tr>
<td>10</td>
<td>243.15</td>
</tr>
<tr>
<td>15</td>
<td>246.15</td>
</tr>
<tr>
<td>20</td>
<td>250.15</td>
</tr>
<tr>
<td>25</td>
<td>254.15</td>
</tr>
<tr>
<td>30</td>
<td>258.15</td>
</tr>
<tr>
<td>35</td>
<td>263.15</td>
</tr>
<tr>
<td>40</td>
<td>268.15</td>
</tr>
<tr>
<td>45</td>
<td>273.15</td>
</tr>
<tr>
<td>50</td>
<td>278.15</td>
</tr>
<tr>
<td>55</td>
<td>283.15</td>
</tr>
<tr>
<td>60</td>
<td>288.15</td>
</tr>
<tr>
<td>65</td>
<td>293.15</td>
</tr>
<tr>
<td>70</td>
<td>298.15</td>
</tr>
<tr>
<td>75</td>
<td>303.15</td>
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<td>80</td>
<td>308.15</td>
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<td>85</td>
<td>313.15</td>
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<tr>
<td>90</td>
<td>318.15</td>
</tr>
<tr>
<td>95</td>
<td>323.15</td>
</tr>
<tr>
<td>100</td>
<td>328.15</td>
</tr>
<tr>
<td>105</td>
<td>333.15</td>
</tr>
<tr>
<td>110</td>
<td>338.15</td>
</tr>
</tbody>
</table>

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).

Measured values and the linear relationship between the solubility expressed as log_{10} x_2 versus 1/(T/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.
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>1000 $V_1/V_2$ (compiler)</th>
<th>100 $w_1$ (compiler)</th>
<th>$10^2 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8.0</td>
<td>0.99</td>
<td>1.82</td>
</tr>
<tr>
<td>25</td>
<td>0.865</td>
<td>0.858</td>
<td>1.58</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

A volumetric method similar to that introduced by Akstajew 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 Purities of Materials:**

1. Forchloride, Gifco, used as received.
2. Distilled (compiler).

**Estimated Errors:**

Solubility: ±2 K (compiler).

**References:**

### Components
(1) 1,2-dichloroethane; C\(_2\)H\(_4\)Cl\(_2\); [107-06-2]
(2) Water; H\(_2\)O; [7732-18-5]

### Original Measurements
F. M. Gross and J. E. Saylor, J. Am. Chem. Soc. 53, 1744 (1931)

### Variables
\(T/K = 288–303\)

### Prepared By
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(10^3 \frac{E}{E_2})</th>
<th>(100 w_1) (compiler)</th>
<th>(10^3 x_1) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>8.72</td>
<td>0.864</td>
<td>1.58</td>
</tr>
<tr>
<td>30</td>
<td>9.00</td>
<td>0.892</td>
<td>1.64</td>
</tr>
</tbody>
</table>

### Auxiliary Information

#### Method/Apparatus/Procedure:
An excess of 1,2-dichloroethane in 500 g water was shaken for 12 h in a water bath thermostated. Samples were then withdrawn and read against pure water in an interferometer made by Zeiss. A detailed description of the complete procedure is given in a Ph.D. thesis.\(^1\)

#### Source and Purity of Materials:
(1) Eastman Kodak Co., purified by fractional distillation before use.
(2) Distilled.

#### Estimated Errors:
Solubility: ±0.15%. Temperature: ±0.02 K.

### References:
\(^1\) P. M. Gross, J. Am. Chem. Soc. 81, 2362 (1929).
Components:
1,2-dichloroethane; C₂H₄Cl₂; [107-06-2]
Water; H₂O; [7732-18-5]

Variables:
T/K = 273–329

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 x₁ /x₂</th>
<th>100 w₁ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.922</td>
<td>0.914</td>
<td>1.676</td>
</tr>
<tr>
<td>20</td>
<td>0.869</td>
<td>0.862</td>
<td>1.580</td>
</tr>
<tr>
<td>30</td>
<td>0.894</td>
<td>0.886</td>
<td>1.625</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedures:
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:
1,2-dichloroethane; C₂H₄Cl₂; [107-06-2]
Water; H₂O; [7732-18-5]

Variables:
T/K = 273–329

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 x₁ /x₂</th>
<th>100 w₁ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.873</td>
<td>0.865</td>
<td>1.58</td>
</tr>
<tr>
<td>20</td>
<td>0.849</td>
<td>0.842</td>
<td>1.54</td>
</tr>
<tr>
<td>35</td>
<td>0.895</td>
<td>0.887</td>
<td>1.63</td>
</tr>
<tr>
<td>56</td>
<td>1.030</td>
<td>1.019</td>
<td>1.87</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedures:
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: C₂H₅Cl₂; [107-06-2]
(2) Water: H₂O; [7732-18-5]

Original Measurements:

Variables:
77 K = 293

Experimental Data

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>100 w₁</th>
<th>10⁴ x₁ (compiler)</th>
<th>10⁴ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.86</td>
<td>1.58</td>
<td>0.5</td>
</tr>
<tr>
<td>25</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>30</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>100 w₁</th>
<th>10⁴ x₁ (compiler)</th>
<th>10⁴ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>900×10⁻²</td>
<td>0.495</td>
</tr>
<tr>
<td>25</td>
<td>1.865×10⁻¹</td>
<td>1.025</td>
<td>1.03×10⁻²</td>
</tr>
<tr>
<td>30</td>
<td>2.165×10⁻²</td>
<td>1.190</td>
<td>1.20×10⁻²</td>
</tr>
</tbody>
</table>

Prepared By:
A. L. Horvath

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.³

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

References:
### Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>10^2 w1</th>
<th>10^2 x1 (compiler)</th>
<th>10^2 x2 (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.90</td>
<td>1.65</td>
<td>—</td>
</tr>
<tr>
<td>10</td>
<td>0.85</td>
<td>1.56</td>
<td>—</td>
</tr>
<tr>
<td>20</td>
<td>0.84</td>
<td>1.54</td>
<td>0.16</td>
</tr>
<tr>
<td>25</td>
<td>0.84</td>
<td>1.54</td>
<td>—</td>
</tr>
<tr>
<td>30</td>
<td>0.87</td>
<td>1.59</td>
<td>—</td>
</tr>
<tr>
<td>40</td>
<td>0.91</td>
<td>1.67</td>
<td>—</td>
</tr>
<tr>
<td>50</td>
<td>0.99</td>
<td>1.82</td>
<td>—</td>
</tr>
</tbody>
</table>

**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:**
- Source and Purity of Materials:
  - (1) Commercial grade, source not given.
  - (2) Distilled (compiler).
- Estimated Errors:
  - Solubility: not specified.
  - Temperature: ±0.5 K (compiler).

**Source and Purity of Materials:**
- (1) Commercial grade, source not given.
- (2) Distilled.

**Estimated Errors:**
- Solubility: ±5%.
- Temperature: ±0.5 K (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>$t^\circ C$</th>
<th>100 $w_1$</th>
<th>$10^3 x_1$ (compiler)</th>
<th>100 $w_1 M_1^{-1}$ mol g$^{-1}$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.87</td>
<td>0.60</td>
<td>8.79$\times$10$^{-3}$</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
- Source and Purity of Materials:
  - Source and purity not given.
  - Distilled (compiler).

**Estimated Errors:**
- Solubility: not specified.
- Temperature: ±0.5 °C (compiler).

---

### Experimental Data

<table>
<thead>
<tr>
<th>$t^\circ C$</th>
<th>100 $w_1$</th>
<th>$10^3 x_1$ (compiler)</th>
<th>100 $w_2$</th>
<th>$10^3 x_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.0</td>
<td>—</td>
<td>0.163</td>
<td>—</td>
<td>0.47</td>
</tr>
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<td>23.0</td>
<td>0.03774</td>
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<td>—</td>
<td>—</td>
</tr>
<tr>
<td>25.5</td>
<td>—</td>
<td>—</td>
<td>0.1136</td>
<td>—</td>
</tr>
<tr>
<td>30.0</td>
<td>0.0998</td>
<td>—</td>
<td>0.167</td>
<td>—</td>
</tr>
<tr>
<td>33.5</td>
<td>0.2399</td>
<td>—</td>
<td>0.169</td>
<td>0.62</td>
</tr>
<tr>
<td>42.0</td>
<td>—</td>
<td>—</td>
<td>0.2079</td>
<td>1.13</td>
</tr>
<tr>
<td>44.5</td>
<td>1.001</td>
<td>—</td>
<td>0.184</td>
<td>—</td>
</tr>
<tr>
<td>46.5</td>
<td>1.342</td>
<td>—</td>
<td>0.190</td>
<td>—</td>
</tr>
<tr>
<td>47.5</td>
<td>—</td>
<td>—</td>
<td>0.5448</td>
<td>1.35</td>
</tr>
<tr>
<td>53.0</td>
<td>—</td>
<td>—</td>
<td>0.2994</td>
<td>1.62</td>
</tr>
<tr>
<td>56.5</td>
<td>1.1278</td>
<td>—</td>
<td>0.207</td>
<td>—</td>
</tr>
<tr>
<td>57.0</td>
<td>—</td>
<td>—</td>
<td>0.3494</td>
<td>1.90</td>
</tr>
<tr>
<td>58.0</td>
<td>—</td>
<td>—</td>
<td>0.3889</td>
<td>1.99</td>
</tr>
<tr>
<td>67.5</td>
<td>1.906</td>
<td>—</td>
<td>0.228</td>
<td>—</td>
</tr>
<tr>
<td>69.0</td>
<td>—</td>
<td>—</td>
<td>0.5148</td>
<td>2.76</td>
</tr>
<tr>
<td>72.5</td>
<td>1.8886</td>
<td>—</td>
<td>0.255</td>
<td>—</td>
</tr>
</tbody>
</table>

---

**Method/Apparatus/Procedure:**
- Source and Purity of Materials:
  - (1) Technical grade, further purified by distillation, b.p.=81.5 °C.
  - (2) Double distilled.

**Estimated Errors:**
- Solubility: not specified.
- Temperature: ±0.5 °C (compiler).

**References:**
**Components:**
1. 1,2-dichloroethane; C₂H₃Cl₂; [107-06-2]
2. Water; H₂O; [7732-18-5]

**Variables:**
T/K = 293

**Experimental Data**

<table>
<thead>
<tr>
<th>T/°C</th>
<th>100 w₁</th>
<th>(compiler)</th>
<th>100 w₂</th>
<th>(compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.86</td>
<td>1.58</td>
<td>0.15</td>
<td>8.18</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

Method/Apparatus/Procedure:
The mutual solubility between water and 1,2-dichloroethane was determined by titration from a micro buret until turbidity appeared. The end point of the titration, when turbidity first appeared, was determined with an accuracy of 0.3%–0.5%.

Solubility: not specified.

Temperature: ±0.5 K (compiler).

References:
Components:  
(1) Water, H₂O; [7732-18-5]  
(2) 1,2-dichloroethane, C₂H₄Cl₂; [107-06-2]  

Original Measurements:  

Variables:  
7/K = 291  

Prepared By:  
Z. Macynska  

70. 1,2-Dichloroethane with Water  

Experimental Data  

<table>
<thead>
<tr>
<th>T/°C</th>
<th>c₁/µg m⁻²</th>
<th>10⁶ x₁</th>
<th>10² γ₁</th>
<th>100 w₁</th>
<th>(compiler)</th>
<th>(compiler)</th>
<th>(compiler)</th>
<th>(compiler)</th>
<th>(compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.5</td>
<td>0.120</td>
<td>6.56</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>18</td>
<td>1.3</td>
<td>2.4</td>
<td>1.31×10⁻²</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

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) Chemical washed and re-distilled before use.  

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

References:  
### Components
1. 1,2-dichloroethane; C₆H₅Cl₂ [107-96-2]
2. Water; HO [7732-18-5]

### Original Measurements

### Variables
T/K = 293

### Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 w₁</th>
<th>10⁶ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10⁶ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.67</td>
<td>1.58</td>
<td>0.15</td>
<td>8.18</td>
</tr>
</tbody>
</table>

### Auxiliary Information
- **Method/Apparatus/Procedure:**
  - Source and Purity of Materials:
    - Dow Chemical Co., used as received.
  - Distilled (compiler).

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ±0.5 K (compiler).

### Components
1. 1,2-dichloroethane; C₆H₅Cl₂ [107-96-2]
2. Water; HO [7732-18-5]

### Original Measurements

### Variables
T/K = 294

### Experimental Data

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 w₁</th>
<th>10⁶ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10⁶ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20.45</td>
<td>1.2</td>
<td>1.2</td>
<td>3.5</td>
<td>2.7</td>
</tr>
</tbody>
</table>

### Auxiliary Information
- **Method/Apparatus/Procedure:**
  - The isobestic titration method as described by Abahi et al.¹,² was used. The sets for the 1,2-dichloroethane–water–ethylalcohol ternary system was also reported.

- **Estimated Errors:**
  - Solubility: not specified.
  - Temperature: ±0.1 K.

### References
### Experimental Data

<table>
<thead>
<tr>
<th>$n^\circ C$</th>
<th>100 $w_1$</th>
<th>$D^3 x_1$ (compiler)</th>
<th>100 $w_1 M_1^+$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>9.0x10^{-3}</td>
<td>4.92</td>
<td>5.0x10^{-3}</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

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

**Estimated Errors:**

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

---

### Experimental Data

<table>
<thead>
<tr>
<th>$n^\circ C$</th>
<th>$10^{-3} \alpha$ (mol dm$^{-3}$)</th>
<th>100 $w_2$ (compiler)</th>
<th>100 $w_2 M_2^+$ (compiler)</th>
<th>$K_0$ $w_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
<td>0.0000</td>
</tr>
<tr>
<td>25</td>
<td>0.0815</td>
<td>0.0886</td>
<td>1.662x10^{-3}</td>
<td>3.182</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

- 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, H2O [7732-18-5]
(2) 1,2-dichloroethane, C2H4Cl2 [107-06-2]

Variables:
T/K  = 283–298

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>10^-3 c_i/mol dm^-3</th>
<th>100 w_i (complex)</th>
<th>10^3 x_i (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>8.12×10^-2</td>
<td>0.115</td>
<td>6.28</td>
</tr>
<tr>
<td>25</td>
<td>1.262×10^-1</td>
<td>0.182</td>
<td>9.92</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Samples of the organic-water solutions were equilibrated in water bath isotherms. The description of the static isopiestic apparatus has been reported elsewhere.1 Water solubility was determined using the Beckman Model KF-3 Aquaometer.

Source and Purity of Materials:
(1) Distilled (comple). (2) Source not given. Reagent grade, distilled in an Oldershaw column before use.

Estimated Errors:
Solubility: ±1.2×10^-2; Temperature: ±0.1 K.

References:

Source and Purity of Materials:
(1) Distilled.
(2) Source not given, redistilled before use, nD = 1.444 at 20 °C.

Estimated Errors:
Solubility: ±2.0×10^-4; Temperature: ±0.05 K.

References:
Components:
(1) Water; H₂O; [7732-18-5] 
(2) 1,2-dichloroethane; C₂H₄Cl₂ ; [107-06-2]

Original Measurements:

Variables:
T/K = 283–308

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>T/°C</th>
<th>n₁ V₁⁻¹/m I cm⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10² x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.0112±0.0010</td>
<td>0.115</td>
<td>6.30</td>
</tr>
<tr>
<td>25</td>
<td>0.1262±0.0014</td>
<td>0.182</td>
<td>9.94</td>
</tr>
<tr>
<td>35</td>
<td>0.1570±0.0016</td>
<td>0.230</td>
<td>12.49</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
The solute isopentane 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 solvents. Equilibrium was attained after a period of 6–8 h. Samples of the solution were analyzed for water with the Beckman RF-Aqua meter. The Karl Fischer reagent was standardized against crystalline sodium thiosulfate.

Source and Purity of Materials:
(1) Distilled.
(2) Certified or reagent grade, distilled through a 30 plate Glass column before use.

Estimated Errors:
Solubility; see above.
Temperature: ±0.1 K.

References:
### Experimental Data

<table>
<thead>
<tr>
<th>t (°C)</th>
<th>$10^{-3} x_1$ (complex)</th>
<th>$10^2 x_2$ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>8.06</td>
<td>0.794</td>
</tr>
</tbody>
</table>

### 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 definite volume of water. After 2-3 h, the solution became saturated and samples were taken periodically. 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:**


**Estimated Errors:**

Solubility: ± 3%.
Temperature: ± 0.5 K (complex).

### Reference

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O [7732-18-5]</td>
<td></td>
</tr>
<tr>
<td>Variables:</td>
<td>Prepared By:</td>
</tr>
<tr>
<td>T/K=293 not given and P/mmHg=530–760</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

**Experimental Data**

<table>
<thead>
<tr>
<th>p/mmHg</th>
<th>α²</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.30×10²</td>
<td>6.6×10²</td>
<td>0.590</td>
<td>1.06</td>
</tr>
<tr>
<td>6.40×10²</td>
<td>4.7×10²</td>
<td>0.973</td>
<td>1.79</td>
</tr>
<tr>
<td>7.60×10²</td>
<td>3.5×10²</td>
<td>1.551</td>
<td>2.86</td>
</tr>
</tbody>
</table>

*Separation factor, (α)=[solution/water]supersat/solution/water*<sub>actual</sub>.

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O [7732-18-5]</td>
<td></td>
</tr>
<tr>
<td>Variables:</td>
<td>Prepared By:</td>
</tr>
<tr>
<td>T/K=291–295</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

**Experimental Data**

<table>
<thead>
<tr>
<th>α°C</th>
<th>10⁴ w₁ (compiler)</th>
<th>10⁴ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>—</td>
<td>0.082</td>
</tr>
<tr>
<td>20</td>
<td>0.111</td>
<td>1.49</td>
</tr>
<tr>
<td>26</td>
<td>—</td>
<td>0.114</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The Altenjew's method of solubility determination was introduced. A fixed weight of 12-chloroethane and water was placed 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:**

### Components:
1. Water: $\text{H}_2\text{O}$ [7732-18-5]
2. 1,2-dichloroethane: $\text{C}_2\text{H}_4\text{Cl}_2$ [107-06-2]

### Original Measurements:

### Variables:
$\text{T}^\circ\text{K} = 296–352$

### Experimental Data

<table>
<thead>
<tr>
<th>$\text{C}^\circ\text{C}$</th>
<th>Distribution coefficient, $D_x$ (dimensionless)</th>
<th>100 $x_1$ (complex)</th>
<th>10$^3$ $x_1$ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>24.9</td>
<td>2.07x10$^{-2}$</td>
<td>1.14</td>
</tr>
<tr>
<td>25</td>
<td>26.7</td>
<td>2.31x10$^{-2}$</td>
<td>1.27</td>
</tr>
<tr>
<td>50</td>
<td>36.7</td>
<td>1.34x10$^{-3}$</td>
<td>7.30</td>
</tr>
<tr>
<td>65</td>
<td>46.6</td>
<td>3.12x10$^{-4}$</td>
<td>16.92</td>
</tr>
<tr>
<td>79.2</td>
<td>52.0</td>
<td>7.33x10$^{-4}$</td>
<td>38.96</td>
</tr>
</tbody>
</table>

*Gas–liquid system analysis parameter, from calibration measurements.

### Auxiliary Information

**Method/Apparatus/Procedure:**
The concentration of water in the organic-rich phase was determined radiochemically using tritium labeled water. A full description of the apparatus and methods used is given in the paper.

**Source and Purity of Materials:**
(1) Animated (complex).
(2) Source and purity not given.

**Estimated Errors:**
Solubility: not specified.
Temperature: ± 0.5 K (complex).

---

### Components:
1. L,2-dichloroethane: $\text{C}_2\text{H}_4\text{Cl}_2$ [107-06-2]
2. Water: $\text{H}_2\text{O}$ [7732-18-5]

### Original Measurements:

### Variables:
$\text{T}^\circ\text{K} = 288–373$

### Experimental Data

<table>
<thead>
<tr>
<th>$\text{C}^\circ\text{C}$</th>
<th>Distribution coefficient, $D_x$ (dimensionless)</th>
<th>100 $x_1$ (complex)</th>
<th>10$^3$ $x_1$ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>2.58x10$^3$</td>
<td>0.0128</td>
<td>2.2333</td>
</tr>
<tr>
<td>32</td>
<td>1.62x10$^3$</td>
<td>0.0488</td>
<td>0.8889</td>
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<tr>
<td>41</td>
<td>1.40x10$^3$</td>
<td>0.0835</td>
<td>0.5211</td>
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<tr>
<td>50</td>
<td>1.12x10$^3$</td>
<td>0.1505</td>
<td>2.744</td>
</tr>
<tr>
<td>60</td>
<td>9.00x10$^2$</td>
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<tr>
<td>70</td>
<td>7.80x10$^2$</td>
<td>0.449</td>
<td>8.204</td>
</tr>
<tr>
<td>80</td>
<td>6.50x10$^2$</td>
<td>0.748</td>
<td>13.705</td>
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<td>90</td>
<td>5.50x10$^2$</td>
<td>1.201</td>
<td>22.076</td>
</tr>
<tr>
<td>95.7</td>
<td>4.90x10$^2$</td>
<td>1.645</td>
<td>20.408</td>
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<tr>
<td>100</td>
<td>4.30x10$^2$</td>
<td>2.040</td>
<td>17.770</td>
</tr>
</tbody>
</table>

*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 to provide sampling of the equilibrium vapor phase. The concentrations of L,2-dichloroethane in both phases were determined using $^{36}$Cl labeled compound.

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

**Estimated Errors:**
Solubility: not specified.
Temperature: ± 0.5 K (complex).
Components:
(1) 1,2-dichloroethane; C₂H₃Cl₂; [107-06-2]
(2) Water; H₂O; [1732-31-3]

Variables:
77K = 283–353

Experimental Data
The temperature dependence of the solubility of 1,2-dichloroethane in water versus absolute temperature was expressed by the equation:

\( \log [\text{solubility}] = \frac{2070}{T} - 15360 + 0.0247[T/K], \)

where S = solubility and T = absolute temperature.

For example, the calculated solubility derived from the above equation is \(8.53 \times 10^{-1}\) moles/l 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: ±0.1 K.

Components:
(1) 1,2-dichloroethane; C₂H₃Cl₂; [107-06-2]
(2) Water; H₂O; [1732-31-3]

Variables:
77K = 293

Experimental Data

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(10^6\ \text{g}/\text{cm}^3)</th>
<th>(10^3\ \text{g}/\text{cm}^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8.80 x 10⁻³</td>
<td>0.872</td>
</tr>
</tbody>
</table>

Auxiliary Information

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; C₂H₅Cl₂ ; [107-06-2] (2) Water; H₂O; [7732-18-5]


Variables: 77K=293

Prepared By: A. I. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Tt°C</th>
<th>10^6 g₁/σ₂</th>
<th>10^2 w₁</th>
<th>10^3 x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8.80×10^5</td>
<td>0.880</td>
<td>1.84</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
Saturated solutions were prepared in a constant-temperature thermostat bath. Water samples were extracted with a pentane and an allisot of the extract taken for GLC analysis. The gas chromatograph was fitted with a 66N electron capture detector.

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

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

Auxiliary Information

Method/Apparatus/Procedure:
An excess of 5–10 g 1,2-dichloroethane was equilibrated with 100 cm³ of distilled water for 14 h in a bottle. The aqueous solution taken from the bottle was analyzed using a gas chromatograph equipped with a 66N electron capture detector. The GLC column was packed with porous polymer Chromosorb 102. 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.

Components:
(1) 1,2-dichloroethane; C₂H₄Cl₂; [107-06-2]
(2) Water; H₂O; [7732-18-5]

Original Measurements:

Variables:

Prepared By:

A. L. Horvath

Experimental Data

\[ \begin{array}{cccc}
\text{t/°C} & 10^3 f_j & 100 w_j & 100 w_j f_j \cdot 1 \text{mol g}^{-1} \\
20 & 8.1 \times 10^{-3} & 1.48 & 8.1 \times 10^{-3} \\
\end{array} \]

Auxiliary Information

Partition coefficient, \( K_j/\text{dimensionless} \)

\( 10^3 f_j \) (compiler)

\( 100 w_j \) (compiler)

\( 100 w_j f_j \cdot 1 \text{mol g}^{-1} \) (compiler)

37

11.3

0.794

1.455

4Gas-liquid chromatographic parameter, from instrument calibration.

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: \( \text{C}_2\text{H}_4\text{Cl}_2 \) [107-06-2]
(2) Water: \( \text{H}_2\text{O} \) [7732-18-5]

### Original Measurements:

### Variables:
\( T/K = 298 \)

### Prepared By:
A. J. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>( u^{\circ}C )</th>
<th>100 ( w_1 )</th>
<th>( 10^3 \ x_1 ) (compiler)</th>
<th>100 ( w_2 )</th>
<th>( 10^3 \ x_2 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.06</td>
<td>1.95</td>
<td>0.18</td>
<td>9.81</td>
</tr>
</tbody>
</table>

### 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 constant agitation using a magnetic stirrer.

**Source and Purity of Materials:**
(1) Jofran Chemical, laboratory grade reagent, further purified by distillation; middle fraction was used.
(2) Reagent grade.

**Estimated Errors:**
Solubility: not specified.
Temperature: ±0.005 K.

### Components:
(1) 1,2-dichloroethane: \( \text{C}_2\text{H}_4\text{Cl}_2 \) [107-06-2]
(2) Water: \( \text{H}_2\text{O} \) [7732-18-5]

### Original Measurements:

### Variables:
\( T/K = 298 \)

### Prepared By:
A. L. Horvath

### Experimental Data

<table>
<thead>
<tr>
<th>( u^{\circ}C )</th>
<th>100 ( w_1 )</th>
<th>( 10^3 \ x_1 ) (compiler)</th>
<th>100 ( w_2 )</th>
<th>( 10^3 \ x_2 ) (compiler)</th>
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<tr>
<td>25</td>
<td>.02</td>
<td>.02</td>
<td>0.18</td>
<td>9.81</td>
</tr>
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</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
The mutual solubility data were determined by a method described by Otterer et al.1 A 10 cm³ 1,2-dichloroethane sample was added to water from a buret and stirred 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 grade, further purified by distillation in a helix-packed column.
(2) Distilled.

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

**References:**
Components:
(1) 1,2-dichloroethane: C₂H₄Cl₂; [107-06-2]
(2) Water: H₂O; [7732-18-5]

Original Measurements:

Variables:
T/K: 293
Prepared By: A. L. Horváth

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>n₁V₁⁻¹/mol dm⁻³</th>
<th>10⁷ x₁</th>
<th>10⁷ x₁ compiler</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8.13×10⁻²</td>
<td>8.00×10⁻¹</td>
<td>1.47</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedure:
An excess of 1,2-dichloroethane was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. The equilibrium mixture was analyzed by using radioactive techniques. The ¹⁴C activity of the water sample 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: ±0.1 K.
### Experimental Data

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$10^{-3} c_1$, mol dm$^{-3}$</th>
<th>$10^5 w_1$ (compiler)</th>
<th>$10^5 s_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>$8.07 \times 10^{-3}$</td>
<td>0.795</td>
<td>1.46</td>
</tr>
</tbody>
</table>

### 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 determined 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% ad. dev.
Temperature: ±0.3 °C.
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$D_1$ (dimensionless)</th>
<th>100$w_1$ (compiler)</th>
<th>10$^3$ $x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>30.62</td>
<td>0.526</td>
<td>9.610</td>
</tr>
<tr>
<td>1.3</td>
<td>30.89</td>
<td>0.533</td>
<td>9.807</td>
</tr>
<tr>
<td>11.0</td>
<td>46.56</td>
<td>0.632</td>
<td>11.055</td>
</tr>
<tr>
<td>21.0</td>
<td>48.89</td>
<td>0.693</td>
<td>12.451</td>
</tr>
<tr>
<td>22.0</td>
<td>46.79</td>
<td>0.626</td>
<td>11.761</td>
</tr>
<tr>
<td>27.2</td>
<td>95.46</td>
<td>0.698</td>
<td>11.985</td>
</tr>
</tbody>
</table>

*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 cm³ equilibrium 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: not specified.
2. Purity: 99.9%.

**Estimated Errors:**

- Purity: ± 0.5%.
- Temperature: ± 0.5 °C.

**Source and Purity of Materials:**

- Water: H$_2$O [7732-18-5]
- 1,2-dichloroethane: C$_2$H$_4$Cl$_2$ [107-06-2]

**Prepared By:**

- A. L. Horvath

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>$x_1$ (compiler)</th>
<th>100$w_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.80</td>
<td>0.146</td>
</tr>
<tr>
<td></td>
<td></td>
<td>7.97</td>
</tr>
</tbody>
</table>
Components:  
1. 1,2-dichloroethane; C\textsubscript{2}H\textsubscript{4}Cl\textsubscript{2}; [107-06-2]  
2. Water; H\textsubscript{2}O; [7732-18-5]

Original Measurements:  

Variables:  
T/K = 303

Prepared By:  
A. J. Horvath

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>( \sigma \times V_r^{-1/2} \text{g dm}^{-3} )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10(^2) ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>3.306</td>
<td>0.3509</td>
<td>6.406</td>
</tr>
</tbody>
</table>

Auxiliary Information

Method/Apparatus/Procedural:  
Standard 1,2-dichloroethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere. The aqueous organic liquid phase was 25 cm\(^3\) and the vapor phase above the mixture was 55 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:  

Components:  
1. 1,2-dichloroethane; C\textsubscript{2}H\textsubscript{4}Cl\textsubscript{2}; [107-06-2]  
2. Water; H\textsubscript{2}O; [7732-18-5]

Original Measurements:  

Variables:  
T/K = 293

Prepared By:  
A. L. Horvath

Prepared By:  
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10(^2) ( p_i / \mu \text{g cm}^{-2} )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10(^2) ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8.490 \times 10^4</td>
<td>0.8490</td>
<td>1.556</td>
</tr>
<tr>
<td></td>
<td>9.170 \times 10^4</td>
<td>0.9170</td>
<td>1.682</td>
</tr>
<tr>
<td></td>
<td>8.420 \times 10^4</td>
<td>0.8420</td>
<td>1.544</td>
</tr>
<tr>
<td></td>
<td>8.830 \times 10^4</td>
<td>0.8830</td>
<td>1.619</td>
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</table>

Auxiliary Information

Method/Apparatus/Procedural:  
A mixture of 1 cm\(^3\) 1,2-dichloroethane and X 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 type 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, distilled before use.  
(2) Double distilled.

Estimated Errors:  
Solubility: ± 0.9%–2.3% coeff. of var.  
Temperature: ± 1.0 K.
### Experimental Data

<table>
<thead>
<tr>
<th>$t^\circ C$</th>
<th>$10^5 x_1$ (compiler)</th>
<th>$10^5 x_2$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.60</td>
<td>0.873</td>
</tr>
<tr>
<td>35</td>
<td>1.66</td>
<td>0.905</td>
</tr>
<tr>
<td>50</td>
<td>1.81</td>
<td>0.986</td>
</tr>
</tbody>
</table>

Mole fraction of 1,2-dichloroethane ($x_1$) was calculated from the activity coefficients at infinite dilution ($y_1$) using the relation $x_1 = 1/y_1$.

### Auxiliary Information

**Method/Apparatus/Procedure:**

The water–rich mixture was studied using gas–liquid chromatography in which a mixture of n-hexane 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 isopentane 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. Stated as received.
2. Double distilled water.

**Estimated Errors:**

Solubility: not specified.
Temperature: ±0.0 K.

### Source and Purity of Materials:

1. Purity grade available, used as received, stated purity greater than 99%.
2. Distilled and de-ionized.

### References:

## Components:
(1) 1,2-dichloroethane: C₂H₄Cl₂ [107-06-2]
(2) Water: H₂O [7732-18-5]

## Original Measurements:

## Variables:
T/K = 283-303

## Preparing:
A. L. Horváth

## Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10⁶ g₁ / g₂</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>1.0554×10⁶</td>
<td>1.0554</td>
<td>1.9566</td>
</tr>
<tr>
<td>20</td>
<td>8.667×10⁵</td>
<td>0.8467</td>
<td>1.5521</td>
</tr>
<tr>
<td>30</td>
<td>1.0467×10⁶</td>
<td>1.0467</td>
<td>1.9219</td>
</tr>
</tbody>
</table>

## Auxillary Information

**Method/Apparatus/Procedure:**
250 cm³ 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 microsyringe. 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: ± 0.5% (compiler).
Temperature: ± 0.5 K (compiler).

## Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10⁶ w₁ (compiler)</th>
<th>10⁶ x₁ (compiler)</th>
<th>10⁶ w₂ (compiler)</th>
<th>10⁶ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>32.55</td>
<td>---</td>
<td>---</td>
<td>0.25</td>
<td>1.36</td>
</tr>
<tr>
<td>42.55</td>
<td>---</td>
<td>---</td>
<td>0.30</td>
<td>1.65</td>
</tr>
<tr>
<td>55.05</td>
<td>---</td>
<td>---</td>
<td>0.217</td>
<td>---</td>
</tr>
<tr>
<td>56.05</td>
<td>---</td>
<td>---</td>
<td>0.47</td>
<td>2.55</td>
</tr>
<tr>
<td>62.05</td>
<td>---</td>
<td>---</td>
<td>0.55</td>
<td>2.95</td>
</tr>
<tr>
<td>66.05</td>
<td>1.37</td>
<td>0.252</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>71.25</td>
<td>1.46</td>
<td>0.269</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>74.55</td>
<td>---</td>
<td>0.73</td>
<td>3.88</td>
<td>---</td>
</tr>
<tr>
<td>78.05</td>
<td>1.56</td>
<td>0.288</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>81.35</td>
<td>1.69</td>
<td>0.312</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>90.25</td>
<td>1.85</td>
<td>0.342</td>
<td>---</td>
<td>---</td>
</tr>
<tr>
<td>92.05</td>
<td>---</td>
<td>---</td>
<td>1.08</td>
<td>4.89</td>
</tr>
<tr>
<td>98.55</td>
<td>2.11</td>
<td>0.391</td>
<td>1.24</td>
<td>6.45</td>
</tr>
<tr>
<td>107.55</td>
<td>---</td>
<td>---</td>
<td>1.54</td>
<td>7.91</td>
</tr>
</tbody>
</table>

## Auxillary Information

**Method/Apparatus/Procedure:**
Samples were prepared of different compositions 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.

**Sources and Purity of Materials:**
(1) Supplied by Lachema, Brno, designated by "Impur."
Redistilled before use, 99.9% pure.
(2) Double distilled.

**Estimated Errors:**
Solubility: ± 0.0251 std. dev.(1),
± 6.2×10⁻⁴ std. dev.(2).
Temperature: ± 0.1 K.
### Experimental Data

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>$n_1$</th>
<th>$n_2$</th>
<th>$10^4 w_1$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10</td>
<td>3.3x10^{-3}</td>
<td></td>
<td>6.00x10^{-2}</td>
<td>3.39</td>
</tr>
<tr>
<td>0</td>
<td>4.7x10^{-3}</td>
<td></td>
<td>8.55x10^{-3}</td>
<td>4.68</td>
</tr>
<tr>
<td>10</td>
<td>6.5x10^{-3}</td>
<td></td>
<td>1.18x10^{-3}</td>
<td>6.46</td>
</tr>
<tr>
<td>20</td>
<td>8.7x10^{-3}</td>
<td></td>
<td>1.58x10^{-3}</td>
<td>8.62</td>
</tr>
<tr>
<td>30</td>
<td>1.15x10^{-2}</td>
<td></td>
<td>2.09x10^{-4}</td>
<td>11.4</td>
</tr>
<tr>
<td>40</td>
<td>1.48x10^{-2}</td>
<td></td>
<td>2.69x10^{-4}</td>
<td>14.6</td>
</tr>
<tr>
<td>50</td>
<td>1.91x10^{-2}</td>
<td></td>
<td>3.47x10^{-4}</td>
<td>18.7</td>
</tr>
<tr>
<td>60</td>
<td>2.37x10^{-2}</td>
<td></td>
<td>4.30x10^{-4}</td>
<td>23.2</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

Equilibria were 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 Error:**

Solubility: ± 1%.
Temperature: ± 0.1 K.
### Components:
1. 1,2-dichloroethane; 
2. Hydrogen chloride; 
3. Water; 

### Original Measurements:

### Variables:
77K = 303–333

### 71. 1,2-Dichloroethane with Hydrogen Chloride and Water

#### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>100 w₁ (wt %)</th>
<th>100 w₁ (complex)</th>
<th>10⁴ x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>8.20</td>
<td>0.820</td>
<td>15.84</td>
</tr>
<tr>
<td>45</td>
<td>5.26</td>
<td>0.526</td>
<td>10.33</td>
</tr>
<tr>
<td>60</td>
<td>3.34</td>
<td>0.304</td>
<td>5.644</td>
</tr>
</tbody>
</table>

2. Solubility of 1,2-dichloroethane in 20 wt % HCl solution

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>1000 w₁ (complex)</th>
<th>100 w₁ (complex)</th>
<th>10⁴ x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>8.01</td>
<td>0.804</td>
<td>16.41</td>
</tr>
<tr>
<td>45</td>
<td>5.68</td>
<td>0.568</td>
<td>11.56</td>
</tr>
<tr>
<td>60</td>
<td>3.09</td>
<td>0.300</td>
<td>6.093</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**
The dynamic method used for the solubility determination consisted of the saturation of nitrogen with 1,2-dichloroethane vape which was then bubbled through a thermostatically controlled flask filled with a definite volumed water. After 2–3 h, the solution became saturated and samples were taken periodically. 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. Commercial reagent, fractionally distilled before use.
2. Kahlbaum chemical, certified grade.
3. Distilled.

**Estimated Errors:**
Solubility: ±1%, Temperature: ±0.05 K.

### References:

---

### Components:
1. 1,2-dichloroethane; 
2. Magnesium sulfate; 
3. Water; 

### Original Measurements:
P. M. Green, Z. Phys. Chem. 61, 215 (1929).

### Variables:
77K = 308

### 72. 1,2-Dichloroethane with Magnesium Sulfate and Water

#### Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>10⁻³ c₁ (mol dm⁻³)</th>
<th>100 g₁/g₂ (complex)</th>
<th>10⁵ x₂ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.5</td>
<td>0.552</td>
<td>0.549</td>
</tr>
</tbody>
</table>

### Auxiliary Information

---

**Method/Apparatus/Procedure:**
A mixture of 0 to 20 cm³ 1,2-dichloroethane in 500 cm³ of an aqueous solution of MgSO₄ was placed in a flask and immersed in a water bath thermostat. The sample container was placed in the thermostat and agitated until no free liquid droplets remained unsolubilized. One or more samples were withdrawn at 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.
73. 1,2-Dichloroethane with Potassium Chloride and Water

**Experimental Data**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>D / 100 g H₂O</th>
<th>x₁ (complex)</th>
<th>x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.5</td>
<td>0.752</td>
<td>0.746</td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
A mixture of 10 to 20 cm³ of 1,2-dichloroethane in 500 cm³ of an aqueous solution of KCl was placed in a beaker 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 spectrophotometer.

**Source and Purity of Materials:**
(1) Commercial reagent, fractionally distilled before use.
(2) Sphagnum chemical, certified grade.
(3) Jutland.

**Estimated Errors:**
Solubility: ± 1%
Temperature: ± 0.01 K.

**Components:**
(1) 1,2-Dichloroethane: C₂H₅Cl₂ • [107-06-2]
(2) Potassium chloride: KC • [7447-01-7]
(3) Water: H₂O • [7732-18-5]

**Prepared By:**
A. L. Horvath

---

**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 one paper, between 273 and 303 K.

The available solubility data of Rex, F. Ühmer,² van Arkel and Vles,² and Donahue and Barcell⁴ were used to obtain the following mass percent (1) equation:

\[ \text{Solubility} \times 10^5 = 13.248 - 8.0012 \times 10^{-5} (\text{T} / \text{K}) + 2.9546 \times 10^{-7} (\text{T} / \text{K})^2 \]

This equation, which represents the combined data points, shows a standard deviation of 1.53 x 10⁻³ 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 solubility minimum exists above 303 K, no experiments have been reported for this temperature range.

**TABLE 1. Tentative solubility of bromoethane (1) in water (2)**

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (10⁵)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.051</td>
</tr>
<tr>
<td>5</td>
<td>1.008</td>
</tr>
<tr>
<td>10</td>
<td>0.971</td>
</tr>
<tr>
<td>15</td>
<td>0.941</td>
</tr>
<tr>
<td>20</td>
<td>0.917</td>
</tr>
<tr>
<td>25</td>
<td>0.900</td>
</tr>
<tr>
<td>30</td>
<td>0.889</td>
</tr>
</tbody>
</table>

**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 Lyon⁶ and Donahue and Barcell⁴ compare 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 w₁) at 298.15 K. This value is classified as tentative. More accurate solubility determinations are required, most certainly at the higher temperatures.

**References:**
¹A. Rex, Z. Phys. Chem. 55, 155 (1906).
²F. Ühmer, Ber. 57, 510 (1924).
Components:  
(1) Bromoethane: C₂H₃Br; [74-96-4]  
(2) Water: H₂O; [7732-18-5]

Variables:  
T(°K) = 273-303

Prepared By:  
A. L. Horváth

Experimental Data

<table>
<thead>
<tr>
<th>T(°C)</th>
<th>100 w₁</th>
<th>10¹² x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.97</td>
<td>1.055</td>
</tr>
<tr>
<td>10</td>
<td>0.95</td>
<td>0.996</td>
</tr>
<tr>
<td>20</td>
<td>0.94</td>
<td>0.906</td>
</tr>
<tr>
<td>30</td>
<td>0.86</td>
<td>0.888</td>
</tr>
</tbody>
</table>

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, reagent grade, further purified before use.
(2) Distilled (compiler).

Estimated Errors:
Solubility: not specified.
Temperature: ± 0.5 K (compiler).
<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t/\degree C$</td>
</tr>
<tr>
<td>30.0</td>
</tr>
</tbody>
</table>

**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 the procedure was taken from a secondary source. 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: ±0.0x10^{-2} \text{ av. dev.}
Temperature: ±0.05 \degree C.

References:
Components:
(1) Bromoethane: C₂H₅Br, [74-91-4]
(2) Water: H₂O, [7732-18-5]

Original Measurements:

Variables:
T/K=298

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>100 w₁ M⁻¹g⁻¹</th>
<th>100 w₂ M⁻¹g⁻¹</th>
<th>10² w₁ (complex)</th>
<th>10² w₂ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>3.52×10⁻¹</td>
<td>7.05×10⁻²</td>
<td>3.81</td>
<td></td>
</tr>
</tbody>
</table>

Auxiliary Information

A mixture of water and bromoethane was placed in a glass-stopped 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

References:
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 various groups of workers over the temperature range from 273 to 313 K. The data are in very good 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)

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (g/L)</th>
<th>Solubility (mol/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.445</td>
<td>1.15</td>
</tr>
<tr>
<td>10.3</td>
<td>0.45</td>
<td>1.36</td>
</tr>
<tr>
<td>12.5</td>
<td>0.570</td>
<td>1.50</td>
</tr>
<tr>
<td>17.5</td>
<td>0.9256</td>
<td>2.02</td>
</tr>
<tr>
<td>20</td>
<td>0.789</td>
<td>2.10</td>
</tr>
<tr>
<td>24.8</td>
<td>0.9195</td>
<td>2.38</td>
</tr>
<tr>
<td>25</td>
<td>0.871</td>
<td>1.88</td>
</tr>
<tr>
<td>30</td>
<td>0.661</td>
<td>1.35</td>
</tr>
<tr>
<td>34.6</td>
<td>0.632</td>
<td>1.77</td>
</tr>
<tr>
<td>40</td>
<td>0.673</td>
<td>1.51</td>
</tr>
</tbody>
</table>

References


Experimental Data

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (g/L)</th>
<th>Solubility (mol/L)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11</td>
<td>0.2</td>
<td>7.12</td>
</tr>
</tbody>
</table>

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 CaCl2 and P2O5. 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:
Components:  
(1) Chloroethane: C₂H₅Cl [75-40-1]  
(2) Water: H₂O [7732-18-5]  

Variables:  
77 K = 286  

Experimental Data  

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>100 w₁</th>
<th>100 w₂ M⁻¹ mol g⁻¹ (complex)</th>
<th>10² x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12.5</td>
<td>0.570</td>
<td>160</td>
<td>8.83x 0⁻³</td>
</tr>
</tbody>
</table>

Auxiliary Information:  
Method/Apparatus/Procedure:  
Chloroethane was added gradually from a pipette to 100 cm³ water in a sealed beaker with continuous stirring and shaking in or oil bath. The appearance of the first cloud (nucleation) 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 (complex).

Estimated Errors:  
Solubility: not specified.  
Temperature: ±0.5 K (complex).

Components:  
(1) Chloroethane: C₂H₅Cl [75-40-1]  
(2) Water: H₂O [7732-18-5]  

Variables:  
77 K = 293–313  

Experimental Data  

<table>
<thead>
<tr>
<th>T (°C)</th>
<th>Osmotic coefficient, L/dimensionless</th>
<th>100 w₁ (complex)</th>
<th>10² x₁ (complex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.12</td>
<td>0.749</td>
<td>2.10</td>
</tr>
<tr>
<td>25</td>
<td>1.62</td>
<td>0.671</td>
<td>1.88</td>
</tr>
<tr>
<td>30</td>
<td>1.37</td>
<td>0.661</td>
<td>1.65</td>
</tr>
<tr>
<td>40</td>
<td>0.89</td>
<td>0.573</td>
<td>1.61</td>
</tr>
</tbody>
</table>

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 760 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 manometer.

Source and Purity of Materials:  
(1) Laboratory reagent, source and purity not given.  
(2) Distilled (complex).

Estimated Errors:  
Solubility: not specified.  
Temperature: ±0.5 K (complex).
<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Chloroethane, C₂H₅Cl, [75-00-3]</td>
<td>L. Sesti-Fogliani, Cl. Soc. Biol. 100, 959 (1950).</td>
</tr>
<tr>
<td>(2) Water, H₂O, [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 303</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K (°C)</td>
</tr>
<tr>
<td>30</td>
</tr>
</tbody>
</table>

**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.

<table>
<thead>
<tr>
<th>Components:</th>
<th>Original Measurements:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water, H₂O, [7732-18-5]</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Variables:</th>
<th>Prepared By:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 273</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K (°C)</td>
</tr>
<tr>
<td>0</td>
</tr>
</tbody>
</table>

**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) Chloroform: C₂H₃Cl [75-00-3]
(2) Water: H₂O [7732-18-5]

### Original Measurements:


### Variables:
\( T/K = 273 \)

### Prepared By:
A. L. Harvath

### Experimental Data

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( w_1 )</th>
<th>( 1/N \times 10^3 ) (compiler)</th>
<th>( 100 \ w_1 M_1^{-1/2} \text{mol} \ g^{-1} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.45</td>
<td>1.26</td>
<td>6.97 \times 10^{-3}</td>
</tr>
</tbody>
</table>

### 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) Chloroform: C₂H₃Cl [75-00-3]
(2) Water: H₂O [7732-18-5]

### Original Measurements:

### Variables:
\( T/K = 293 \)

### Prepared By:
A. L. Harvath

### Experimental Data

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( w_1 )</th>
<th>( 10^3 \times 1 ) (compiler)</th>
<th>( 100 \ w_1 M_1^{-1/2} \text{mol} \ g^{-1} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.57</td>
<td>1.66</td>
<td>8.83 \times 10^{-3}</td>
</tr>
</tbody>
</table>

### 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:**
Components:
(1) Iodoethane, C₂H₅I; [75-03-1]
(2) Water, H₂O; [7732-18-5]

Prepared By:
A. L. Horvath

Experimental Data

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, R/m³ atm mol⁻¹</th>
<th>CV %</th>
<th>10^2 w₁ (compiler)</th>
<th>10^2 x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.3</td>
<td>6.51×10⁻³</td>
<td>3.90</td>
<td>0.9087</td>
<td>2.554</td>
</tr>
<tr>
<td>17.5</td>
<td>8.46×10⁻³</td>
<td>3.62</td>
<td>0.9256</td>
<td>2.602</td>
</tr>
<tr>
<td>24.8</td>
<td>1.11×10⁻²</td>
<td>5.84</td>
<td>0.9195</td>
<td>2.585</td>
</tr>
<tr>
<td>34.6</td>
<td>1.55×10⁻²</td>
<td>4.64</td>
<td>0.9176</td>
<td>2.580</td>
</tr>
</tbody>
</table>

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

 Auxiliary Information

Method/Apparatus/Procedures:
A modification of the EPICS procedure was used for measuring Henry's law constants. A precise quantity of chloroethene 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 bottle 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) Speleo Inc., QC standard reagent, 0.2 mg/cm³ in methanol.
(2) Distilled.

Estimated Errors:
Solubility: See above
Temperature: ±0.1 K.

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 Ren,² Fühner,³ Gross and Sayer,⁴ and van Adel and Vlees⁵ 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 Ren.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 solubilities¹⁵ were smoothed by least squares analysis to obtain the following mass percent (w) equation:

$$w = 8.5757 - 5.6860 \times 10^{-2} (T/°C) + 9.4391 \times 10^{-4}(T/°C)^2,$$

which shows a standard deviation of 6.04×10⁻³ 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>
<thead>
<tr>
<th>Temperature</th>
<th>Solubility</th>
</tr>
</thead>
<tbody>
<tr>
<td>°C</td>
<td>K</td>
</tr>
<tr>
<td>0</td>
<td>273.10</td>
</tr>
<tr>
<td>5</td>
<td>278.11</td>
</tr>
<tr>
<td>10</td>
<td>283.11</td>
</tr>
<tr>
<td>15</td>
<td>288.11</td>
</tr>
<tr>
<td>20</td>
<td>293.11</td>
</tr>
<tr>
<td>25</td>
<td>298.11</td>
</tr>
<tr>
<td>30</td>
<td>303.11</td>
</tr>
</tbody>
</table>

References:
¹ A. Ren, Z. Phys. Chem. 58, 35 (1906).
² H. Fühner, Ber. 57, 510 (1924).
**Components:**
1. Iodoethane; C₂H₅I; [75-9-6]
2. Water; H₂O; [77-32-18-5]

**Original Measurements:**
- H. Führer, Ber. 87, 51e (1924).

**Variables:**
T/K = 273–303

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 w₁</th>
<th>10⁶ n₁</th>
<th>Experimental Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.441</td>
<td>0.439</td>
<td>5.09</td>
</tr>
<tr>
<td>10</td>
<td>0.412</td>
<td>4.78</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>0.404</td>
<td>4.65</td>
<td></td>
</tr>
<tr>
<td>30</td>
<td>0.413</td>
<td>4.79</td>
<td></td>
</tr>
</tbody>
</table>

**Auxiliary Information**

**Method/Apparatus/Procedure:**
The solubility of iodoethane in water was determined using specially designed flasks with calibrated capillary tubes. After the samples were equilibrated in a thermostatic bath at the desired temperature, the volumes and weights were determined and the solubility calculated.

**Source and Purity of Materials:**
(1) alkylated, redistilled and washed before use; b.p. = 72.3 °C.
(2) Distilled.

**Estimated Errors:**
Solubility: not specified.
Temperature: ±0.5 K (compiler).
### Experimental Data

<table>
<thead>
<tr>
<th>Method/Apparatus/Procedure:</th>
<th>Source and Purity of Materials:</th>
</tr>
</thead>
<tbody>
<tr>
<td>An excess of isooctane in 100 g water was shaken for 12 h in a water bath thermostated. Samples were then withdrawn at room temperature and pure water in an interferometer made by Zeiss. A detailed description of the complete procedure is given in a Ph.D. thesis.</td>
<td>Source and purity not given.</td>
</tr>
<tr>
<td>(1) Eastman Kodak Co., purified by fractional distillation before use.</td>
<td>(2) Distilled (compiler).</td>
</tr>
<tr>
<td>(2) Distilled.</td>
<td>Estimated Errors:</td>
</tr>
<tr>
<td>Estimated Errors:</td>
<td>Solubility: not specified.</td>
</tr>
<tr>
<td>Solubility: ±0.5.</td>
<td>Temperature: ±0.3 K (compiler).</td>
</tr>
<tr>
<td>Temperature: ±0.003 K.</td>
<td></td>
</tr>
</tbody>
</table>
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.

Acetylene dichloride (see ethene, cis-1,2-dichloro-)
Acetylene tetrabromide (see ethane, 1,1,2,2-tetrabromo-)
Acetylene tetrachloride (see ethane, 1,1,2,2-tetrachloro-)
sym-Dichloroethylene (see ethene, cis-1,2-dichloro-)
uns-Dichloroethylene (see ethene, 1,1-dichloro-)
cis-1,2-Diiodoethylene (see ethene, cis-1,2-diido-)
trans-1,2-Diiodoethylene (see ethene, trans-1,2-diido-)
Ammonium sulfate (see sulfuric acid, diammonium salt)
Ethane, 1,1,2-trichloro-1,2,2-trifluoro- + water
+ sodium chloride (aqueous) + water E406, 407–409
410–411
Ethane, 1,1,2,2-tetrachloro-1,2-difluoro- + water 432
Ethane, hexachloro- + water E433, 433–437
Ethane, 2,2-dichloro-1,1,1-trifluoro- + water E446, 446–447
Ethane, pentachloro- + water E472, 472–473, 474–476
Ethane, 1,1,2,2-tetrabromo- + water E478, 479, 480–481
Ethane, 1,2-dichloro-1,1-difluoro- + water 498
Ethane, 1,1,1,2-tetrachloro- + water E498–E499, 499, 500–502
Ethane, 1,1,2,2-tetrachloro- + water E502–E504, 504–505, 506, 507, 508, 509, 510, 511–517
Ethane, 1,1-dichloro-1-fluoro- + water 520
Ethane, 1,1,1-trichloro- + water
+ water, MQ- E521–E522, 522, 523, 524–530, 531–536
+ water, Municipal tap, PASE) E536
+ water, sea- E537
Ethane, 1,1,2-trichloro- + water E538–E539, 539–540, 541–546, 547–549
Ethane, 1,1,2-dibromo- + water E549, 550
Ethane, 1,1,2-dibromo- + water
+ magnesium chloride (aqueous) + sulfuric acid, magnesium salt (aqueous) + water 561
+ sulfuric acid, magnesium salt (aqueous) + water 562
+ sodium chloride (aqueous) + water 563
+ sodium chloride (aqueous) + magnesium chloride (aqueous) + water 564
+ sodium chloride (aqueous) + sulfuric acid, disodium salt (aqueous) + water 565
+ sulfuric acid, disodium salt (aqueous) + water 566
+ sulfuric acid, magnesium salt (aqueous) + sulfuric acid, magnesium salt (aqueous) + water 567
Ethane, 1-chloro-2-fluoro- + water 568
Ethane, 1,1-dichloro- + water E566–E567, 567–569, 570–576
+ ethane, 1,1,2-trichloro- + water 576
+ ethane, 1,2-dichloro- + water 577
+ sulfuric acid, magnesium salt (aqueous) + water 578
+ potassium chloride (aqueous) + water 579
Ethane, dichloro + water E589
+ hydrogen chloride (aqueous) + water 609
+ sulfuric acid, magnesium salt (aqueous) + water 609
+ potassium chloride (aqueous) + water 610
Ethane, bromo-
+ water

Ethane, chloro-
+ water

Ethane, iodo-
+ water

Ethene, tetrachloro-
+ water
  + water, MQ-
  + water, Municipal tap, (PASE)
  + ammonium carbonate (aqueous) + water
  + hydrogen chloride (aqueous) + water
  + hydrogen chloride (aqueous) + sodium chloride (aqueous) + water
  + nitric acid (aqueous) + ammonium nitrate (aqueous) + water
  + phosphoric acid (aqueous) + sulfuric acid (aqueous) + water
  + sodium chloride (aqueous) + water
  + sulfuric acid (aqueous) + water
  + sulfuric acid (aqueous) + sulfuric acid, diammonium salt (aqueous) + water

Ethene, trichloro-
+ water
  + water, MQ-
  + water, Municipal tap, (PASE)

Ethene, 1,1-dichloro-
+ water

Ethene, cis-1,2-dichloro-
+ water

Ethene, trans-1,2-dichloro-
+ water

Ethene, cis-1,2-diodo-
+ water

Ethene, trans-1,2-diodo-
+ water

Ethyl bromide (see ethane, bromo-)

Ethyl chloride (see ethane, chloro-)

Ethyl iodide (see ethane, iodo-)

Ethylene chlorobromide (see ethane, 1-bromo-2-chloro-)

Ethylene bromide (see ethane, 1,2-dibromo-)

Ethylene chloride (see ethane, 1,2-dichloro-)

Ethylene fluorochloride (see ethane, 1-chloro-2-fluoro-)

Ethylene chloride (see ethane, 1,1-dichloro-)

Ethylene dichloride (see ethane, 1,1-dichloro-)

Magnesium sulfate (see sulfuric acid, magnesium salt)

Methyldichloroform (see ethane, 1,1,1-trichloro-)

Sodium sulfate (see sulfuric acid, disodium salt)

Tetrachloroethylene (see ethane, tetrachloro-)

Trichloroethylene (see ethane, trichloro-)

Vinyl tribromide (see ethane, 1,1,2-tribromo-)

Vinyl trichloride (see ethane, 1,1,2-trichloride-)

Water
  + ethane, 1,2-dibromo-1,1,2,2-tetrafluoro-
  + ethane, 2-bromo-2-chloro-1,1,1-trifluoro-
  + ethane, 2,2-dichloro-1,1,1-trifluoro-
  + ethane, pentachloro-
  + ethane, 1,2 dibromo-1,2-dichloro-
  + ethane, 1,1,2,2-tetrabromo-
  + ethane, 1,1,1,2-tetrachloro-
  + ethane, 1,1,1,2,2-tetrachloro-
  + ethane, 1,2 dibromo-1-chloro-
  + ethane, 1,1,2-trichloro-
  + ethane, 1,1,1-trichloro-
  + ethane, 1,1,2-trichloro-
  + ethane, 1,2 dibromo-
  + ethane, 1,1-dichloro-
  + calcium chloride (aqueous) + ethane, 1,1-dichloro-
  + calcium chloride (aqueous) + ethane, 1,2-dichloro-
  + sodium hydroxide (aqueous) + ethane,
IUPAC-NIST SOLUBILITY DATA SERIES

79. Registry Number Index

Page numbers preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

67–72-1
71-55-6
74-96-4
75-00-3
75-03-6
75-34-3
75-35-4
76-01-7
76-12-0
76-13-1
78-74-0
79-00-5
79-01-6
79-27-6
79-34-5
106-83-4
107-04-0
107-06-2
124-73-2
127-18-4
151-67-7
156-59-2
156-60-5
306-83-2
506-87-6
590-26-1
590-27-2
598-20-9
630-20-6
683-68-1
762-50-5
1300-21-6
1310-73-2
1649-08-7
1717-00-6
3811-04-9
6484-52-2
7587-68-9
7647-01-0
7647-14-5
7664-38-2
7697-37-2
7732-18-5
757-82-6
7783-20-2
7786-30-3

80. Author Index

Ababi, V. 591
Affenstren, H. E. 508-509, 593-594
Aleksejev, S. 585
Alessi, P. 460, 552
Andrews, L. J. 518-519
Antropov, L. I. 416, 458, 596
Archer, W. L. 419, 461, 526
Aver’yan, M. G. 448
Bagasas, G. 408
Bakin, V. M. 596
Balls, P. W. 531, 537
Banerjee, S. 422, 463, 514, 529, 603
Baranaev, M. K. 589
Bar, R. S. 516, 534, 548, 574, 606
Bartell, F. E. 613
Bell, R. P. 413, 552-553
Berndt, P. 440
Bilewicz, R. 560
Blumberg, R. 480
Bobok, D. 607
Boehm, R. F. 409-411
Booth, H. S. 480, 556
Browning, J. S. 481
Call, F. 557
Calo, J. M. 423, 464, 487, 515, 530, 546, 604
Carlisle, P. J. 451
Carroll, J. 422, 435, 476, 513, 528, 544, 602
Chiao, C. T. 421, 460, 501, 512, 526, 559, 599
Chistyakov, V. M. 592
Chitwood, B. G. 414, 550, 556, 588
Christian, S. D. 508, 509, 593, 594
Coca, J. 421, 462, 528, 543, 544, 601
Cohen, J. M. 426, 436, 469, 489, 496, 535, 575, 606
Czaplinskiwicz, J. 602
Czankiewicz-Tulai, B. 602
Daley, J. F. 541
Davies, W. 587
DeLassus, P. T. 486
DeVoll, D. 470, 493, 497, 502, 517, 536, 549, 576, 608
Devos, A. 475, 500, 511, 524, 542, 570, 598
Diaz, R. M. 421, 462, 528, 543, 544, 601
Donahue, D. J. 613
Doolittle, A. K. 584
Dreisbach, R. R. 558
Druzhinin, I. G. 554, 555, 560-564
Duncan, W. A. M. 439
2000 Encyclopedia of Polymer Science and Technology 407, 432.446, 447, 498, 617
Eberius, E. 454
Eger, E. I. 439, 440
Encyclopedia of Polymer Science and Technology 484
Ehrenst, J. P. 600
Everson, H. E. 480, 556
Farukulina, I. G. 588
Ferguson, D. M. 418, 459, 485, 525, 598
Femmerl, M. 465, 532
Frid, R. M. 595, 609
Freed, V. H. 421, 460, 501, 512, 526, 559, 599
Fridenburg, A. E. 565
Fischer, H. 611, 615, 619
Furniss, B. S. 517
Gendrano, M. C. 593
Gillam, W. S. 509, 594

Severinghaus, J. W.
Shalygin, V. A.
Shamsuddinov, T. M.
Shapurova, V. V.
Shiu, W.-Y.
Shorthose, D. N.
Shostakovskii, M. F.
Simonov, V. D.
Sonin, E. V.
Soucek, B.
Staverman, A. J.
Stepanova, G. G.
Stevens, V. L.
Strowcl, H.
Stoepling, R. K.
Stringer, W.
Sukhotin, A. M.
Solomnich, B.
Surgy, J.
Svetlanov, E. B.
Takano, J.
Tan, D.
Tettamanti, K.
Tewari, Y. B.
Tokoro, R.
Tregger, Yu. A.
Treybal, R. E.
Trouillet, P.
Trueger, E.
Udovsko, V. V.
Valvani, S. C.
van Arkel, A. E.
Veith, G. D.
Valle, S. M.
Vinogradov, G. R.
Vles, E. B.
Vogel, A. J.
Wade, P.
Walraeens, R.
Warner, H. P.
Wasil, S. P.
Watanabe, L. D.
Whalley, H. K.
White, R. E.
Wibowo, A. E.
Wienker, H.
Won, K. W.
Wong, H. V.
Wright, D. A.
Wright, W. H.
Yalkowsky, S. H.
Yasuoka, T.
Yoshioka, Y.
Zel’tsov, Yu. D.
Zielinski, A. Z.