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COMMISSION ON SOLUBILITY DATA

SOLUBILITY DATA SERIES

Volume 60

HALOGENATED METHANES WITH WATER
SOLUBILITY DATA SERIES

Volume 60

HALOGENATED METHANES WITH WATER

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INTRODUCTION TO THE SOLUBILITY DATA SERIES

SOLUBILITY OF LIQUIDS IN LIQUIDS

NATURE OF THE PROJECT

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

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

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

COMPILATIONS AND EVALUATIONS

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

Compilations

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

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

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

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

Columns 1 and 2: H, alkali elements, ammonium, alkaline earth elements
Columns 3 to 12: transition elements
Columns 13 to 17: boron, carbon, nitrogen groups; chalcogenides, halogens
Column 18: noble gases
Row 1: Ce to Lu
Row 2: Th to the end of the known elements, in order of atomic number.

Organic compounds within each Hill formula are ordered in the following succession:
(a) by degree of unsaturation
(b) by order of increasing chain length in the parent hydrocarbon
(c) by order of increasing chain length of hydrocarbon branches
(d) numerically by position of unsaturation
(e) numerically by position by substitution
(f) alphabetically by IUPAC name.
Example:

**C₅H₈**
cyclopentane
2-methyl-1,3-butadiene
1,4-pentadiene
1-pentyne

**C₅H₁₀**
cyclopentane
3-methyl-1-butene
2-methyl-2-butene
1-pentene
2-pentene

**C₅H₁₂**
2,2-dimethylpropane
2-methylbutane
pentane

**C₅H₁₂O**
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

**C₆H₁₂O**
cyclohexanol
4-methyl-1-penten-3-ol
1-hexen-3-ol
4-hexen-3-ol

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

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

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

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

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

Errors in calculations, fitting equations, etc. are noted, and where possible corrected. Material inserted by the compiler is identified by the word "compiler" or by the compiler's name in parentheses or in a footnote. In addition, compiler-calculated values of mole or mass fractions are included if the original data do not use these units. If densities are reported in the original paper, conversions from concentrations to mole fractions are included, but otherwise this is done in the evaluation, with the values and sources of the densities being quoted and referenced.

Details of smoothing equations (with limits) are included if they are present in the original publication and if the temperature or pressure ranges are wide enough to justify this procedure and if the compiler finds that the equations are consistent with the data.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases graphs have been included, either to illustrate presented data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

**Method:** The apparatus and procedure are mentioned briefly. Abbreviations used in Chemical Abstracts are often used here to save space, reference being made to sources of further detail if these are cited in the original paper.

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

Estimated Error: If estimated errors were omitted by the original authors, and if relevant information is available, the compilers have attempted to estimate errors (identified by "compiler" or the compiler’s name in parentheses or in a footnote) from the internal consistency of data and type of apparatus used. Methods used by the compilers for estimating and reporting errors are based on Ku and Eisenhart (4).

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

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

Evaluations

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

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

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

Critical Evaluation:

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

The solubility of comparatively few systems is known with sufficient accuracy to enable a set of recommended values to be presented. Although many systems have been studied by at least two workers, the range of temperatures is often sufficiently different to make meaningful comparison impossible.

Occasionally, it is not clear why two groups of workers obtained very different but internally consistent sets of results at the same temperature, although both sets of results were obtained by reliable methods. In such cases, a definitive assessment may not be possible. In some cases, two or more sets of data have been classified as tentative even though the sets are mutually inconsistent.

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

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

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

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

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units (3) when the data can be converted accurately.
QUANTITIES AND UNITS USED IN COMPILATION AND EVALUATION OF SOLUBILITY DATA

Mixtures, Solutions and Solubilities

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

A solution (5, 6) describes a liquid or solid phase containing more than one substance, when for convenience one of the substances, which is called the solvent, and may itself be a mixture, is treated differently than the other substances, which are called solutes. If the sum of the mole fractions of the solutes is small compared to unity, the solution is called a dilute solution.

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

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

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

\[
x_1 = \frac{n_1}{\sum_{s=1}^{c} n_s}
\]

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

2. Ionic mole fractions of salt \(i\), \(x_{i+}, x_{i-}\):

For a mixture of \(s\) binary salts \(i\), each of which ionizes completely into \(v_s^+\) cations and \(v_s^-\) anions, with \(v_s = v_s^+ + v_s^-\), and a mixture of \(p\) non-electrolytes \(j\), of which some may be solvent components, a generalization of the definition in (8) gives:

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

\[
x'_j = \frac{x_j}{1 + \sum_{l=1}^{s} (v_{l}-1)x_{l}}, \quad j = (s+1),...,p
\]

The sum of these mole fractions is unity, so that, with \(c = s + p\).
General conversions to other units in multicomponent systems are complicated. For a three-component system containing non-electrolyte 1, electrolyte 2 and solvent 3,

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

\[ x_1 = \frac{v_2x_1'}{v_2 - (v_2 - 1)x_2} \quad x_2 = \frac{x_2'}{v_2 - (v_2 - 1)x_2} \]  \[5\]

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

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

\[ w_1 = \frac{g_1}{\sum_{s=1}^{c} g_s} \]  \[6\]

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

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

\[ m_1 = \frac{n_1}{n_2 M_2} \]  \[7\]

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

5. **Aquamolality**, **Solvomolality** of substance 1 in a mixed solvent with components 2, 3 (9), \( m_1^{(3)} \):

\[ m_1^{(3)} = m_1 \overline{M}/M_3 \]  \[8\]

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

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

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

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

\[ c_1 = [\text{formula of solute}] = \frac{n_1}{V} \]  \[10\]

SI base units: mol m\(^{-3}\). The symbol \( c_1 \) is preferred to \([\text{formula of solute}]\), 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 \( V \), \( \rho_1 \): SI base units: kg m\(^{-3}\).

\[ \rho_1 = \frac{g_1}{V} \]  \[11\]

8. **Mole ratio**, \( r_{n,12} \) (dimensionless)

\[ r_{n,12} = \frac{n_1}{n_2} \]  \[12\]
Mass ratio, symbol \( r_{g,12} \), may be defined analogously. 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, \( \rho \):

\[
\rho = \frac{g}{V} \quad [13]
\]

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

10. Relative density, \( d = \rho / \rho^0 \): the ratio of the density of a mixture at temperature \( t \), pressure \( p \) to the density of a reference substance at temperature \( t' \), pressure \( p' \). For liquid solutions, the reference substance is often water at 4°C, 1 bar. (In some cases 1 atm is used instead of 1 bar.) The term specific gravity is no longer used.

**Thermodynamics of Solubility**

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

**REFERENCES**


A.F.M. Barton  
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January, 1994
Table 1. Interconversions between Quantities Used as Measures of Solubility
\( c \)-component Systems Containing \( c - 1 \) Solutes \( i \) and Single Solvent \( c \)

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

\( \rho \) - density of solution; \( M_i \) - molar masses of \( i \). For relations for 2-component systems, set summations to 0.
PREFACE

This volume contains a comprehensive collection and critical evaluation of solubility data published prior to 1993 for halogenated methanes with water, seawater, heavy water, 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.

Table 1. Sources of Solubility Data

A. Bibliographies:

B. Secondary Sources:
Table 1. Sources of Solubility Data (continued)


C. Databases:


D. Primary Sources:

1. Journals
2. Reports
3. Brochures, leaflets
4. Patents
5. Private communications

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 (ref. 1) and TRCVP (ref. 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. (ref. 2). An illustration of the
Table 2. Conversion Formulas for Solubility Units.

<table>
<thead>
<tr>
<th>a. Henry’s Law Constant ($H$):</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Mass} % = \frac{P_{\text{vap}} \ (\text{atm}) \ M_{\text{solute}}}{H \ (\text{dimensionless}) \ d_{\text{solvent}} \ (g \ \text{cm}^{-3})} \times 10^4$</td>
</tr>
<tr>
<td>$H \ (\text{dimensionless}) = \frac{C_{\text{solute}}}{C_{\text{solvent}}} = \frac{16.04 \ P_{\text{vap}} \ (\text{mmHg}) \ M_{\text{solute}}}{T(\text{K}) \ S_{\text{solute}} \ (\text{mg} / \text{dm}^3)}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>b. Air/Water Partition Coefficient ($K_{\text{AW}}$):</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Mass} % = \frac{100 \ K_{\text{AW}} \ P_{\text{vap}}}{82.054 \ T(\text{K}) \ d_{\text{solvent}}}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>c. Distribution Ratio ($p/c$):</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(p/c) = \frac{\text{solute vapor pressure}}{\text{solute concentration}} \ (\text{mmHg}) / (\text{mmole} / \text{dm}^3)$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>d. Partition Coefficient ($K$):</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K = \frac{1}{\text{Ostwald coefficient}} = \frac{1}{L}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>e. Distribution Coefficient ($K_d$):</th>
</tr>
</thead>
<tbody>
<tr>
<td>$K_d = \text{Ostwald coefficient} = L = \frac{y_i}{x_i}$</td>
</tr>
</tbody>
</table>

difficulty of obtaining accurate conversions is shown by the following typical case.

The solubility of carbon tetrachloride ($\text{CCl}_4$) in water ($\text{H}_2\text{O}$) is 0.10 cm³/100 cm³ water at 25 °C. The solubility in mass per cent (100 $w_1$) is required. The density of pure carbon tetrachloride is 1.5834 g $\text{CCl}_4$/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

$$g \ \text{CCl}_4 / 100 \ g \ \text{H}_2\text{O} = 100 \ w_1$$

On the other hand, for solubility values larger than, say, 2 - 3 mass per cent, the differences become significant, as the following example illustrates. The solubility in water of dichloromethane ($\text{CH}_2\text{Cl}_2$) is 2.363 g/100 g water at 0°C. The mass per cent solubility, 100 $w_1$, at the same temperature is required.
If 100 g water dissolves 2.363 g CH$_2$Cl$_2$, then the total mass of the solution becomes 102.363 g. This means that 100 g aqueous solution will dissolve less CH$_2$Cl$_2$ than 100 g pure water, that is,

$$w_{1} = \frac{2.363 \text{ g CH}_2\text{Cl}_2}{102.363 \text{ g soln}}. \quad 100 = 2.3084.$$

The resulting mass per cent is 2.3084 at 0°C. Consequently, there is a 2.31 per cent reduction in the solubility relative to 100 g pure water. This is in comparison to the reduction of only 0.10 per cent in the case of the solubility of CCl$_4$ in 100 g water or 100 g aqueous solution at 25°C.

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

- Purity of the components (solute and solvents)
- Date of the experiment
- Accuracy of the method
- Reproducibility of the experiment
- Experience of the investigator(s), previous publications
- 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 per cent) 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:

- obscure or dubious - rejected data
- tentative - not recommended data
- recommended - good agreement among the published results.

A graphical presentation of the solubility data may be performed on linear, semi-logarithmic, etc. scales. The unit of solubility may be given as specific or molar scales. For practical reasons, the mass per cent 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 $\log_{10} x_{2}$ versus $1/T$. 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., solubility of water in chloroform), the normal polynomial equations were used for smoothing the solubility data.

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

The temperature dependence of the solubility of halogenated hydrocarbons in water has been correlated using normal polynomial equations over limited temperature intervals. These equations should be used only in the temperature range indicated. The equations play two major roles; to provide data users with interpolated data with good accuracy and to provide data users with acceptable data for use in computer programs, if desired. The deviation of the various experimental values from the fitted data are given as standard or average deviations.
If the experimental data cover a reasonable temperature interval, then the data and the smoothing equation are often illustrated in a figure. The graphical presentation of the reported and fitted data clearly indicates the risks involved when one attempts to extrapolate the raw experimental data. In some cases, an extrapolation is quite safe for the desired temperature (see for example, the solubility of water in halogenated hydrocarbons over moderate temperature intervals); whereas, in other cases, the risk is very high and it is not recommended. The shape of the solubility curves suggests the extrapolation and interpolation possibilities.

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

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

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

It is well recognised 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 ($\Delta_{\text{sol}}H^\text{m}$). This value is very large and varies from negative to positive values with 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 ($\Delta_{\text{sol}}C_p^\text{m}$) is required for the calculation of the minimum solubility temperature ($T_{\text{min}}$):

$$T_{\text{min}} = 298.15 \text{ K} - \frac{\Delta_{\text{sol}}H^\text{m}(298.15 \text{ K})}{\Delta_{\text{sol}}C_p^\text{m}}$$

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

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

In general, solubility depends on many parameters and is of a very complex nature. There is no simple relation established between solubility and the other properties of the pure components (solute and solvent). Despite the lack of a simple relationship, the solubility of halogenated benzenes in water at 25°C has been correlated with a reasonable success using the molar volume of the solutes (ref. 8). Similarly, the solubility of halogenated methanes in water shows a linear relationship (ref. 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 Figure 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.
Figure 1. Logarithm of Saturated Molarity versus Solute Molar Volume at 25 °C for Halogenated Methanes in Water.

Correlation equation:

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

REFERENCES:


2. TRCVP, Thermodynamic Research Center, Texas A & M University System, College Station, TX., 1989.


<table>
<thead>
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<th><strong>ORIGINAL MEASUREMENTS:</strong></th>
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<td>(1) Water; H₂O; [7732-18-5]</td>
<td>O'Connell, W. L.</td>
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<th><strong>PREPARED BY:</strong></th>
</tr>
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<td>T/K = 293</td>
<td>A. L. Horvath</td>
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**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:** Details are not available.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

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

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<th><strong>ORIGINAL MEASUREMENTS:</strong></th>
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<td>O'Connell, W. L.</td>
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<tr>
<td>T/K = 293 - 298</td>
<td>A. L. Horvath</td>
</tr>
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<td>100 g₁/g₂</td>
<td>10° x₁ (compiler)</td>
<td>100 g₂/g₁ (compiler)</td>
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<td>-</td>
<td>-</td>
<td>2.0 × 10⁻²</td>
</tr>
<tr>
<td>25</td>
<td>4.0 × 10⁻²</td>
<td>2.66</td>
<td>-</td>
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**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:** Details are not available.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
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<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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</thead>
<tbody>
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<td>(1) Tetrabromomethane (Carbon tetrabromide); CBr₄; [558-13-4]</td>
<td>Gross, P. M.; Saylor, J. H.</td>
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**VARIABLES:**  
\[ T/K = 303 \]

**PREPARED BY:**  
A. L. Horvath

**EXPERIMENTAL VALUES:**

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<tr>
<th>( t/°C )</th>
<th>( 1000 g_1/g_2 )</th>
<th>( 100 w_r ) (compiler)</th>
<th>( 10^3 x_r ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>0.24</td>
<td>2.4 x 10⁻³</td>
<td>1.30</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

An excess of tetrabromomethane in 500 g water was shaken for 12 hours in a thermostat bath. Samples were then withdrawn and read against water in an interferometer made by Zeiss (ref. 1). A detailed description of the complete procedure is given in a Ph. D. thesis (ref. 2).

**SOURCE AND PURITY OF MATERIALS:**

(1) Eastman Kodak Co., recrystallized from ethyl alcohol and petroleum ether before use.  
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: ± 8.0%.  
Temperature: ± 0.02 K.

**REFERENCES:**


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<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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<tr>
<td>(1) Tetrabromomethane (Carbon tetrabromide); CBr₄; [558-13-4]</td>
<td>van Arkel, A. E.; Vles, S. E.</td>
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**VARIABLES:**  
\[ T/K = 303 \]

**PREPARED BY:**  
A. L. Horvath

**EXPERIMENTAL VALUES:**

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<tr>
<th>( t/°C )</th>
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<th>( 100 w_r ) (compiler)</th>
<th>( 10^3 x_r ) (compiler)</th>
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<tbody>
<tr>
<td>30</td>
<td>7.0 x 10⁻⁴</td>
<td>2.32 x 10⁻²</td>
<td>1.26</td>
</tr>
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**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

No details are 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) Trichlorofluoromethane; CCl$_3$F; [75-69-4]; R-11

(2) Water; H$_2$O; [7732-18-5]

EVALUATOR:

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

January 1993.

CRITICAL EVALUATION:

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

Part 1. The solubility of trichlorofluoromethane (1) in water (2) has been studied by at least eleven different work groups with only partial agreement of results. The data of Howe et al. (ref. 1) are substantially lower than other measurements and are therefore rejected. The solubility data reported by du Pont (refs. 2 and 3), Rauws et al. (ref. 4), McConnell et al. (ref. 5), Pearson and McConnell (ref. 6), and Sukomick (ref. 7) show some consistency, while the measurements reported by Park et al. (ref. 8), Warner and Weiss (ref. 9), Wisegarver and Cline (ref. 10), Warner et al. (ref. 11), Balls (ref. 14), and Zeininger (ref. 15) are relatively high in value.

It may be assumed that the solubility data reported in the du Pont bulletins were produced in the same laboratories with similar methods and accuracy at 298.15 and 304.15 K, respectively. There appears to be no significant difference between the two data points despite the 6 K difference in temperature. Similarly, the two measurements reported by McConnell et al. and Pearson and McConnell in 1975 most likely were made in the same laboratories under much the same conditions.

There is no obvious reason to explain the difference between the lower (refs. 2, 3, 5, 6, and 7) and higher (refs. 8, 9, 10, 11, 14, and 15) sets of data. In the opinion of the evaluator, there is not enough evidence to justify rejection of measurements from either of the two data sets. Although both data sets are classified as tentative, the smoothed solubility values in mass per cent (1) for the 273 through 313 K temperature interval (Table 1) are based upon a regression equation for all data shown in Figure 1:

Solubility [100 w$_1$] = 25.0094 - 0.16263 (T/K) + 2.6547 x 10$^{-4}$ (T/K)$^2$

with a standard error of 5.0 x 10$^{-2}$ about the regression line.

A minimum solubility occurs for most halogenated hydrocarbons in water systems between 270 and 310 K (refs. 12 and 13). A minimum solubility temperature can be calculated from an enthalpy of solution at infinite dilution and a change in solute heat capacity in going from a pure liquid to an infinitely dilute aqueous solution. However, such thermodynamic data are rarely available in the literature.

Part 2. The solubility of water (2) in trichlorofluoromethane (1) has been measured by three research groups (refs. 2, 3, and 7) with only partially consistent results with the exception of the measurements of Sukomick (ref. 7). Generally, the solubility behavior of water in halogenated hydrocarbons shows a definite increase with increasing temperature. This trend has been demonstrated in a comprehensive compilation of solubility data (ref. 12). The two measurements at 294.15 and 298.15 K from the du Pont laboratories compare favorably with the recommended values, whereas the reported value of Sukomick (ref. 7) at 304.15 K is low and classified as doubtful. More accurate solubility measurements are required for more reliable values.
COMPONENTS:

(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

CRITICAL EVALUATION: (continued)

Table 1. Tentative Solubility of Trichlorofluoromethane (1) in Water (2)

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w₁</th>
<th>10⁴ x₁</th>
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<tr>
<td>0</td>
<td>0.393</td>
<td>5.18</td>
</tr>
<tr>
<td>5</td>
<td>0.312</td>
<td>4.10</td>
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<tr>
<td>10</td>
<td>0.244</td>
<td>3.21</td>
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<tr>
<td>15</td>
<td>0.189</td>
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<td>20</td>
<td>0.148</td>
<td>1.94</td>
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<td>0.103</td>
<td>1.35</td>
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<tr>
<td>40</td>
<td>0.114</td>
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Figure 1. Solubility of Trichlorofluoromethane (1) in Water (2).
<table>
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<td>A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.</td>
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CRITICAL EVALUATION: (continued)

REFERENCES:

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichlorofluoromethane; CCl₃F; du Pont de Nemours & Company, [75-69-4]; R-11

(2) Water; H₂O; [7732-18-5]

**Original Measurements:**


### VARIABLES:

\[ T/K = 298 \]

**Prepared by:**

A. L. Horvath

### EXPERIMENTAL VALUES:

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### 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 (ref. 1).

### SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.

(2) Distilled (compiler).

### ESTIMATED ERRORS:

Solubility: Not specified.

Temperature: ± 0.5 K (compiler).

### REFERENCES:


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### COMPONENTS:

(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11

(2) Water; H₂O; [7732-18-5]

**Original Measurements:**


### VARIABLES:

\[ T/K = 294 - 304 \]

**Prepared by:**

A. L. Horvath

### EXPERIMENTAL VALUES:

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<td>6.86</td>
</tr>
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<td>31</td>
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### 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 (ref. 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:

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<table>
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<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T/\text{K} = 298$</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
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</tr>
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<tbody>
<tr>
<td>$t/\degree\text{C}$</td>
<td>100 $w_i$ $10^4 x_i$</td>
</tr>
<tr>
<td>25</td>
<td>0.11</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
A calibrated bottle was filled with nitrogen, a measured quantity of water, and the organic vapor. After mixing and equilibration, the concentrations of the vapor and the liquid phases were determined by injection of the head space samples into a gas chromatograph. Trichlorofluoromethane was detected by means of a tritium foil electron capture detector.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: $\pm$ 0.5 K (compiler).

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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<tbody>
<tr>
<td>(1) Trichlorofluoromethane; CCl$_3$F; [75-69-4]; R-11</td>
<td>McConnell, G.; Ferguson, D. M.; Pearson, C. R.</td>
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<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T/\text{K} = 293$</td>
<td>A. L. Horvath</td>
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<table>
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</tr>
</thead>
<tbody>
<tr>
<td>$t/\degree\text{C}$</td>
<td>$10^6 g_i/g_2$ $100 w_i$ $10^4 x_i$</td>
</tr>
<tr>
<td>20</td>
<td>1100</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
The solubility of the trichlorofluoromethane 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: $\pm$ 0.1 K (compiler).
### Components: Original Measurements

1. Trichlorofluoromethane; CCl₃F; Pearson, C. R.; McConnell, G. [75-69-4]; R-11
2. Water; H₂O; [7732-18-5]

### Variables

\( \theta = 293 \) A. L. Horvath

### Experimental Values

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^4 w_i )</th>
<th>( 10^4 x_i ) (compiler)</th>
<th>( 100 w_i ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>1100</td>
<td>0.110</td>
<td>1.44</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **Method/Apparatus/Procedure:**
  - Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with n-pentane and an aliquot of the extract taken for gas-liquid chromatographic analysis. The gas chromatograph was fitted with a \(^{63}\text{Ni}\) electron capture detector.

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

### Estimated Errors

- Solubility: Not specified.
- Temperature: ± 0.1 K (compiler).

### Components: Original Measurements

1. Trichlorofluoromethane; CCl₃F; Zeininger, H. [75-69-4]; R-11
2. Water; H₂O; [7732-18-5]

### Variables

\( \theta = 273 - 313 \) A. L. Horvath

### Experimental Values

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 100 w_i ) (compiler)</th>
<th>( 10^4 x_i ) (compiler)</th>
<th>( 100 w_i M_i ) g⁻¹/mol g⁻¹</th>
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</thead>
<tbody>
<tr>
<td>0</td>
<td>0.37</td>
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<td>2.69 \times 10⁻³</td>
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<tr>
<td>10</td>
<td>0.25</td>
<td>3.29</td>
<td>1.82 \times 10⁻³</td>
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<td>20</td>
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<td>2.10</td>
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<tr>
<td>40</td>
<td>0.070</td>
<td>0.919</td>
<td>5.10 \times 10⁻⁴</td>
</tr>
</tbody>
</table>

### Auxiliary Information

- **Method/Apparatus/Procedure:**
  - The organic compound was condensed into a degassed liquid water sample up to saturation at which two phases appeared. After shaking the mixture for several hours, equilibrium was achieved and the respective phases were analysed in a gas chromatograph.
  - The original report is not obtainable; therefore, the details were taken from Junge (ref. 1).

### Source and Purify of Materials

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

### Estimated Errors

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

### References

COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11

(2) Water; H₂O; [7732-18-5]

Balls, P. W.


VARIABLES:

T/K = 283 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t/°C</th>
<th>Henry's law constant, ( H/\text{dimensionless} )</th>
<th>100 ( w_r ) (compiler)</th>
<th>10^4 ( x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>2.60 ± 0.12</td>
<td>0.137</td>
<td>1.79</td>
</tr>
<tr>
<td>15</td>
<td>3.10 ± 0.18</td>
<td>0.136</td>
<td>1.79</td>
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<tr>
<td>20</td>
<td>3.40 ± 0.21</td>
<td>0.147</td>
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</tr>
<tr>
<td>25</td>
<td>3.60 ± 0.22</td>
<td>0.163</td>
<td>2.14</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method involved repeated equilibrations of nitrogen with a liquid water sample containing the trichlorofluoromethane. Each sample was shaken vigorously at the required temperature in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph. The experiments were performed at least three times at 10, 15, 20, and 25 °C; each experiment involved about six equilibrations.

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.

(2) Distilled.

ESTIMATED ERRORS:

Solubility: See above.

Temperature: ± 0.5 K (compiler).

REFERENCES:


COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11

(2) Water; H₂O; [7732-18-5]

Park, T.; Rettich, T. R.; Battino, R.; Peterson, D.; Wilhelm, E.


VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t/°C</th>
<th>Bunsen coefficient, ( \alpha/\text{dimensionless} )</th>
<th>100 ( w_r ) (compiler)</th>
<th>10^4 ( x_i ) (compiler)</th>
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<tbody>
<tr>
<td>10</td>
<td>0.2491</td>
<td>0.1602</td>
<td>2.104</td>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The Bunsen coefficient was measured in a Scholander microgasometric apparatus which was contained in an air bath. After the distilled water was degassed, the trichlorofluoromethane sample was introduced into the apparatus. About 2 hours were required to reach equilibrium conditions. The procedure for the calculation of the Bunsen coefficient is described by Douglas (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) Matheson Gas Co., minimum purity 99.9 mole percent.

(2) Distilled (reverse osmosis), passed through ion-exchange columns.

ESTIMATED ERRORS:

Solubility: ± 1.7 std. dev.

Temperature: ± 0.05 K.

REFERENCES:

### COMPONENTS

| (1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11 |
| (2) Water; H₂O; [7732-18-5] |

### ORIGINAL MEASUREMENTS

Wisegarver, D. P.; Cline, J. D.  

### VARIABLES

| T/K = 298 |

### EXPERIMENTAL VALUES

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<td>(mol dm⁻³ atm⁻¹)</td>
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<table>
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<td>0.158</td>
<td>2.08</td>
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### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The equilibration took place in a 2 liter flask rotating in a constant temperature bath for 20 hours. The analysis of CCl₃F was carried out using a Hewlett-Packard 59Ni electron capture detector mounted in a gas chromatograph. Peak areas were quantified by a HP 3388A integrator and compared to the detector response of a standard sample.

**SOURCE AND PURITY OF MATERIALS:**

(1) AIRCO, Inc., used as received.  
(2) Distilled.

**ESTIMATED ERRORS:**

| Solubility: | ± 2.0 % |
| Temperature: | ± 0.05 K |

### COMPONENTS

| (1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11 |
| (2) Water; H₂O; [7732-18-5] |

### ORIGINAL MEASUREMENTS

Warner, M. J.; Weiss, R. F.  

### VARIABLES

| T/K = 274 - 313.95 |

### EXPERIMENTAL VALUES

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<table>
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(continued)

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The equilibration of a dilute mixture of trichlorofluoromethane gas with water took place in an equilibration chamber at various temperatures. The concentrations in both the gas and the liquid phases were measured by gas chromatography using a Shimadzu 60Ni electron capture detector set in a constant current operating mode.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

| Solubility: | ± 1.5 % |
| Temperature: | ± 0.02 K |

(continued)
### COMPONENTS:

1. Trichlorofluoromethane; CCl₃F; Warner, M. J.; Weiss, R. F.  

2. Water; H₂O; 

### ORIGINAL MEASUREMENTS:

Warner, M. J.; Weiss, R. F.  

### VARIABLES:

\[ T/K = 274 - 313.95 \]

### EXPERIMENTAL VALUES:

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<td>40.80</td>
<td>0.6060</td>
<td>0.0839</td>
<td>1.10</td>
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</tbody>
</table>

### PREPARED BY:

A. L. Horvath
COMPONENTS:
(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Warner, H. P.; Cohen, J. M.; Ireland, J. C.

VARIABLES:
77K = 298

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, ( H_m ) ( \text{m}^3 \text{atm} \text{mol}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>5.83 \times 10^2</td>
</tr>
</tbody>
</table>

100 \( w_f \) (compiler) 10^4 \( x_f \) (compiler)

0.1969 2.586

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The original method and apparatus for the determination of Henry's law constants are described in Mackay et al. (ref. 1). The general procedure was to add an excess of the organic compound to distilled deionized water and stir the mixture overnight. A portion of this solution was returned to a stripping vessel. The solute was stripped isothermally from the solution at a known gas flow rate. The Henry's law constant was calculated from a log of the concentration versus time plot. The experimental data points are averages of two or more replicates.

SOURCE AND PURITY OF MATERIALS:
(1) Purest quality available and used without further purification; stated purity > 99 %.
(2) Distilled deionized.

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

REFERENCES:

COMPONENTS:
(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Howe, G. B.; Mullins, M. E.; Rogers, T. N.

VARIABLES:
77K = 283 - 303

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

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<tr>
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<tr>
<td>30</td>
<td>262</td>
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<td>3.437</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
250 ml bottles were filled with distilled deionized water and sealed. Measured volumes of trichlorofluoromethane were injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for 1 hour 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 a calibration plot to establish concentrations.

SOURCE AND PURITY OF MATERIALS:
(1) Probably a commercial reagent, at least 99 % purity, used as received.
(2) Distilled deionized.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
<table>
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<th>ORIGINAL MEASUREMENTS:</th>
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<td>(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11</td>
<td>Sukornick, B.</td>
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<table>
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<tr>
<td>T/K = 298</td>
<td>A. L. Horvath</td>
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<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>wᵢ</td>
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<tr>
<td>25</td>
<td>9.50 × 10⁻²</td>
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<td>Temperature:</td>
<td>± 1 K (compiler).</td>
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<th>COMPONENTS:</th>
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<tbody>
<tr>
<td>(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11</td>
<td>Zeininger, H.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 276 - 313</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>wᵢ</td>
</tr>
<tr>
<td>3</td>
<td>0.19</td>
</tr>
<tr>
<td>10</td>
<td>0.12</td>
</tr>
<tr>
<td>20</td>
<td>0.09</td>
</tr>
<tr>
<td>40</td>
<td>0.05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
<td>SOURCE AND PURITY OF MATERIALS:</td>
</tr>
<tr>
<td>Degassed liquid trichlorofluoromethane samples were introduced into degassed seawater samples up to saturation at which point two phases appeared. After shaking a sample for several hours equilibrium was achieved and the respective phases were analysed with a gas liquid chromatograph.</td>
<td>(1) Source and purity not given.</td>
</tr>
<tr>
<td>The original report is not obtainable; therefore, the details were taken from Junge (ref. 1).</td>
<td>(2) North Atlantic surface water, salinity not given.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ESTIMATED ERRORS:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility:</td>
<td>Not specified.</td>
</tr>
<tr>
<td>Temperature:</td>
<td>± 1 K (compiler).</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>REFERENCES:</th>
<th></th>
</tr>
</thead>
</table>
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
(2) Seawater
Balls, P. W.

VARIABLES: PREPARED BY:
7∕TK = 283 - 298
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>Henry’s law constant, H/dimensionless</th>
<th>100 w, (compiler)</th>
<th>10^4 x₀ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>2.82 ± 0.13</td>
<td>0.130</td>
<td>1.71</td>
</tr>
<tr>
<td>15</td>
<td>3.38 ± 0.17</td>
<td>0.129</td>
<td>1.70</td>
</tr>
<tr>
<td>20</td>
<td>3.95 ± 0.30</td>
<td>0.130</td>
<td>1.71</td>
</tr>
<tr>
<td>25</td>
<td>4.15 ± 0.06</td>
<td>0.145</td>
<td>1.90</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The equilibration occurred in a 2 liter flask rotating in a constant temperature water bath for 20 hours. The analysis of CCl₃F was carried out using a Hewlett-Packard 33Ni electron capture detector mounted in a gas chromatograph. Peak areas were quantified by a HP 3388A integrator and compared to the detector response of a standard sample.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Salinity = 20 %.

ESTIMATED ERRORS:
Solubility: ± 2.0 %.
Temperature: ± 0.5 K (compiler).

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
(2) Seawater
Wisegarver, D. P.; Cline, J. D.

VARIABLES: PREPARED BY:
7∕TK = 273 - 305
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>Bunsen coefficient, α/dimensionless</th>
<th>t°C</th>
<th>Bunsen coefficient, α/dimensionless</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.603 ± 0.024 (33)</td>
<td>5.3</td>
<td>0.448 ± 0.005 (11)</td>
</tr>
<tr>
<td>2.6</td>
<td>0.517 ± 0.010 (8)</td>
<td>5.4</td>
<td>0.460 ± 0.010 (7)</td>
</tr>
<tr>
<td>3.5</td>
<td>0.493 ± 0.008 (7)</td>
<td>7.0</td>
<td>0.402 ± 0.004 (14)</td>
</tr>
<tr>
<td>5.2</td>
<td>0.451 ± 0.007 (6)</td>
<td>7.2</td>
<td>0.415 ± 0.012 (9)</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The method involved repeated equilibrations of nitrogen with a water sample containing trichlorofluoromethane. The sample was shaken vigorously at the required temperature in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph. The experiments were performed at least three times at 10, 15, 20, and 25 °C with each experiment involving about six equilibrations.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Salinity = 20 %.

ESTIMATED ERRORS:
Solubility: See above.
Temperature: ± 0.5 K (compiler).

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
(2) Seawater
### COMPONENTS:
1. Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
2. Seawater

### ORIGINAL MEASUREMENTS:
Wisegarver, D. P.; Cline, J. D.

### VARIABLES:
*T/K* = 273 - 305

### EXPERIMENTAL VALUES: (continued)

<table>
<thead>
<tr>
<th><em>t</em>/°C</th>
<th>Bunsen coefficient, <em>a</em>/dimensionless</th>
</tr>
</thead>
<tbody>
<tr>
<td>7.4</td>
<td>0.411 ± 0.001 (6)</td>
</tr>
<tr>
<td>7.9</td>
<td>0.391 ± 0.003 (5)</td>
</tr>
<tr>
<td>10.0</td>
<td>0.331 ± 0.005 (6)</td>
</tr>
<tr>
<td>10.2</td>
<td>0.343 ± 0.004 (10)</td>
</tr>
<tr>
<td>10.4</td>
<td>0.344 ± 0.002 (7)</td>
</tr>
<tr>
<td>10.5</td>
<td>0.352 ± 0.004 (10)</td>
</tr>
<tr>
<td>12.3</td>
<td>0.313 ± 0.003 (9)</td>
</tr>
<tr>
<td>15.0</td>
<td>0.276 ± 0.007 (10)</td>
</tr>
<tr>
<td>15.1</td>
<td>0.274 ± 0.003 (9)</td>
</tr>
<tr>
<td>15.2</td>
<td>0.274 ± 0.001 (8)</td>
</tr>
</tbody>
</table>

The standard deviations are followed by the number of observations in parantheses.

### COMPONENTS:
1. Trichlorofluoromethane; CCl₃F; [75-69-4]; R-11
2. Seawater

### ORIGINAL MEASUREMENTS:
Warner, M. J.; Weiss, R. F.

### VARIABLES:
*T/K* = 272 - 313

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th><em>t</em>/°C</th>
<th>10^2 <em>c</em>/mol dm⁻³ atm⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>-0.77</td>
<td>2.8152</td>
</tr>
<tr>
<td>-0.77</td>
<td>2.7588</td>
</tr>
<tr>
<td>-0.52</td>
<td>2.7263</td>
</tr>
<tr>
<td>-0.52</td>
<td>2.6985</td>
</tr>
<tr>
<td>-0.45</td>
<td>2.7107</td>
</tr>
<tr>
<td>-0.43</td>
<td>2.7065</td>
</tr>
<tr>
<td>-0.37</td>
<td>2.7110</td>
</tr>
<tr>
<td>-0.37</td>
<td>2.7056</td>
</tr>
<tr>
<td>4.79</td>
<td>1.9706</td>
</tr>
<tr>
<td>4.79</td>
<td>1.9446</td>
</tr>
</tbody>
</table>

### METHOD/APPARATUS/PROCEDURE:
Equilibration of a dilute mixture of trichlorofluoromethane gas with seawater occurred in an equilibration chamber at various temperatures. Both gas and liquid phase concentrations were measured by gas chromatography using a Shimadzu 63Ni electron capture detector operating in a constant current mode.

### SOURCE AND PURITY OF MATERIALS:
1. Source and purity not given.
2. Surface water collected at La Jolla.
   Salinity = 35.807 ± 0.006 × 10⁻³.

### ESTIMATED ERRORS:
Solubility: ± 1.5 %.
Temperature: ± 0.02 K.
COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichlorofluoromethane; CCl$_3$F; [75-69-4]; R-11

(2) Seawater

Warner, M. J.; Weiss, R. F.


VARIABLES:

$T/K = 272 - 313$

Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

<table>
<thead>
<tr>
<th>$t/\degree C$</th>
<th>$10^3 c_i P_i^{-1}$/atm mol dm$^3$</th>
<th>$t/\degree C$</th>
<th>$10^3 c_i P_i^{-1}$/atm mol dm$^3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.19</td>
<td>1.5404</td>
<td>29.55</td>
<td>1.6182</td>
</tr>
<tr>
<td>20.43</td>
<td>0.8648</td>
<td>29.55</td>
<td>0.6042</td>
</tr>
<tr>
<td>20.44</td>
<td>0.8868</td>
<td>29.55</td>
<td>0.6037</td>
</tr>
<tr>
<td>20.44</td>
<td>0.8792</td>
<td>29.55</td>
<td>0.6002</td>
</tr>
<tr>
<td>20.44</td>
<td>0.8749</td>
<td>39.90</td>
<td>0.4280</td>
</tr>
<tr>
<td>20.44</td>
<td>0.8788</td>
<td>39.91</td>
<td>0.4301</td>
</tr>
<tr>
<td>20.44</td>
<td>0.8780</td>
<td>39.93</td>
<td>0.4299</td>
</tr>
<tr>
<td>29.53</td>
<td>0.6085</td>
<td>39.93</td>
<td>0.4357</td>
</tr>
<tr>
<td>29.53</td>
<td>0.6031</td>
<td>39.93</td>
<td>0.4281</td>
</tr>
</tbody>
</table>
CRITICAL EVALUATION:

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

**Part 1.** The solubility of tetrachloromethane (1) in water (2) has been studied by 41 workers. The experimental data of most investigators in the 273 to 303 K temperature interval are sufficiently reliable to use in a smoothing equation. Even though a number of measurements above 308 K were reported, the solubility values in this temperature range are rather uncertain and are classified as doubtful.

The experimental work of several workers was not used for the smoothing equation for a variety of reasons. The measured solubility of Booth and Everson (refs. 1 and 2) and of Karger et al. (ref. 3) are markedly higher than the solubility values calculated from the smoothing equation. The measurements by Powell (ref. 4), Tettamanti et al. (ref. 5), Svetlanov et al. (ref. 6), Antropov et al. (ref. 7), Simonov et al. (ref. 8), Sato and Nakijima (ref. 9), Coca et al. (ref. 10), Balls (ref. 11), Yoshioka et al. (ref. 12), Howe et al. (ref. 13), and Wright et al. (ref. 14) are all several per cents lower than the smoothed solubility values and have also been rejected. The solubilities calculated from the distribution coefficients of Prosyanov et al. (ref. 15) are in very poor agreement, giving little confidence in their values which were regarded as dubious.

The remaining data from 26 laboratories were compiled or used for the smoothing equation. The data are also shown in Figure 1. The fitting equation obtained for mass per cent (1) is given by:

\[
\text{Solubility [100 w,]} = 3.4653 - 0.0230285 (T/K) + 3.91621 \times 10^{-4} (T/K)^2
\]

The equation represents the combined data points which yield a standard deviation of 5.8 x 10^{-3} in the 273 to 308 K temperature range.

The curve obtained from the smoothing equation shows a distinct minimum at 294 K, as seen in Figure 1. The existence of the minimum solubility is discussed in the Preface.

The recommended solubility values at 5 K intervals for tetrachloromethane (1) in water (2) are presented in Table 1.

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w,</th>
<th>10^4 x,</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.0970</td>
<td>1.137</td>
</tr>
<tr>
<td>5</td>
<td>0.0898</td>
<td>1.053</td>
</tr>
<tr>
<td>10</td>
<td>0.0846</td>
<td>0.9916</td>
</tr>
<tr>
<td>15</td>
<td>0.0813</td>
<td>0.9529</td>
</tr>
<tr>
<td>20</td>
<td>0.0800</td>
<td>0.9376</td>
</tr>
<tr>
<td>25</td>
<td>0.0813</td>
<td>0.9529</td>
</tr>
<tr>
<td>30</td>
<td>0.0832</td>
<td>0.9752</td>
</tr>
<tr>
<td>35</td>
<td>0.0878</td>
<td>1.029</td>
</tr>
</tbody>
</table>

(continued next page)
CRITICAL EVALUATION: (continued)

Figure 1. Solubility of Tetrachloromethane (1) in Water (2).

Part 2. The solubility of water (2) in tetrachloromethane (1) has been reported by 37 laboratories since 1921. The solubility measurements cover the 273 to 373 K temperature range, see Figure 2. However, the data available above 323 K originate from only two investigators (refs. 16 and 17). The recommended solubility values are limited to the 283 to 307 K temperature interval.

Although data from all the workers show a general increase in solubility with temperature, the extent of the increase is variable above 313 K.

The data of Bell (ref. 18), Niini (ref. 19), and Fox and Martin (ref. 20) are substantially lower than all other studies and they have been rejected. The data of Eberius (ref. 21), Zielinski (ref. 22), Grigsby (ref. 23), Goldman (ref. 24), Ohtsuka and Kazama (ref. 25), and Kleeberg et al. (ref. 26) are significantly higher than the likely solubility and were also rejected. The remaining data mainly due to Clifford (ref. 27), Rosenbaum and Walton (ref. 28), Staverman (ref. 29), Hutchison and Lyon (ref. 30), McGovern (ref. 31), Donahue and Bartell (ref. 32), Rotariu et al. (ref. 33), Greinacher et al. (ref. 34), Desnoyer (ref. 35), Tettamanti et al. (ref. 5), Johnson et al. (refs. 36 and 37), Johnson (ref. 38), Christian et al. (ref. 39), Högfeldt and Fredlund (ref. 41), Simonov et al. (refs. 8, 41 and 42), Glasoe and Schultz (ref. 43), Antropov et al. (ref. 7), Kirchnerova (ref. 44), Kirchnerova and Cave (ref. 45), Coca et al. (ref. 10), Ksiazczak and Buchowski (ref. 46), Wu (ref. 17), and Orlandini et al. (ref. 47) are in good agreement, especially the values given in (refs. 31, 43, and 17).

The correlating equation for the combined mass per cent solubilities of water in tetrachloromethane between 283 and 308 K is as follows:

\[
\text{Solubility [100 \, w_{\text{w}}} = 0.301104 - 2.348078 \times 10^3 \, (T/K) + 4.607143 \times 10^4 \, (T/K)^2
\]

This equation yielded a standard deviation of 1.5 \times 10^3 in the 273 to 308 K temperature range.

(continued next page)
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
January 1993.

CRITICAL EVALUATION: (continued)

The recommended mass per cent solubility values at 5 K intervals for water in tetrachloromethane are presented in the Table 2.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Solubility (100 w₂)</th>
<th>Solubility (10⁴ x₂)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.00558</td>
<td>4.762</td>
</tr>
<tr>
<td>15</td>
<td>0.00699</td>
<td>5.965</td>
</tr>
<tr>
<td>20</td>
<td>0.00864</td>
<td>7.372</td>
</tr>
<tr>
<td>25</td>
<td>0.01051</td>
<td>8.967</td>
</tr>
<tr>
<td>30</td>
<td>0.01261</td>
<td>10.757</td>
</tr>
<tr>
<td>35</td>
<td>0.01495</td>
<td>12.750</td>
</tr>
</tbody>
</table>

Figure 2. Solubility of Water (2) in Tetrachloromethane (1).

REFERENCES:
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>EVALUATOR:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.</td>
</tr>
</tbody>
</table>

**CRITICAL EVALUATION: (continued)**

**REFERENCES:**


(continued next page)
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
January 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:
36. Ibid., 1966, 77.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CC14; [56-23-5]</td>
<td>Rex, A.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 273 - 303</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
<td>100 g/g</td>
</tr>
<tr>
<td></td>
<td>(compiler)</td>
</tr>
<tr>
<td></td>
<td>100 w,</td>
</tr>
<tr>
<td></td>
<td>(compiler)</td>
</tr>
<tr>
<td></td>
<td>10^4 x,</td>
</tr>
<tr>
<td></td>
<td>(compiler)</td>
</tr>
<tr>
<td>0</td>
<td>9.7 x 10^2</td>
</tr>
<tr>
<td>10</td>
<td>8.3 x 10^2</td>
</tr>
<tr>
<td>20</td>
<td>8.0 x 10^2</td>
</tr>
<tr>
<td>30</td>
<td>8.5 x 10^2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
</table>

METHOD/APPARATUS/PROCEDURE:
The solubility of tetrachloromethane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostatic bath, their volumes and weights were determined and the solubility was calculated.

SOURCE AND PURITY OF MATERIALS:
(1) Kahlbaum, redistilled and washed before use; b. p. = 76.7°C.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).

REFERENCES:

---

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Water; H2O; [7732-18-5]</td>
<td>Clifford, C. W.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 297 - 302</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
<td>100 w,</td>
</tr>
<tr>
<td></td>
<td>(compiler)</td>
</tr>
<tr>
<td></td>
<td>10^4 x,</td>
</tr>
<tr>
<td></td>
<td>(compiler)</td>
</tr>
<tr>
<td>24.0</td>
<td>1.0 x 10^2</td>
</tr>
<tr>
<td>28.5</td>
<td>1.3 x 10^2</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
</table>

METHOD/APPARATUS/PROCEDURE:
The calcium chloride method was used for the determination of water in the samples. The moisture was abstracted from the samples by air and absorbed in two calcium chloride tubes. The two tubes were weighted before and after desorption. For further details, see (ref. 1).

SOURCE AND PURITY OF MATERIALS:
(1) Distilled (compiler).
(2) Technical grade, used after distilling over CaCl2.

ESTIMATED ERRORS:
Solubility: about 1 mg.
Temperature: ± 0.5 K (compiler).

REFERENCES:
**COMPONENTS:**

(1) Tetrachloromethane (carbon tetrachloride); CCl₄ [56-23-5]
(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Gross, P. M.

**VARIABLES:**

77K = 298

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g₁/g₂</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>7.7 × 10⁻²</td>
<td>7.7 × 10⁻²</td>
<td>9.02</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

A weighted amount of tetrachloromethane was mixed with 1000 g water in a bottle and immersed in a water thermostat. The bottle was placed on a shaker until no more droplets of the liquid remained undissolved. The concentration of the tetrachloromethane in water was determined by using a Zeiss water interferometer. One or more samples were syphoned out for the determination of the solubility. The German translation is also published (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

(1) Kahlbaum's sulfur-free analytical reagent, used as received.
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: ± 5 %.
Temperature: ± 0.01 K.

**REFERENCES:**


**COMPONENTS:**

(1) Water; H₂O; [7732-18-5]
(2) Tetrachloromethane (carbon tetrachloride); CCl₄ [56-23-5]

**ORIGINAL MEASUREMENTS:**

Rosenbaum, C. K.; Walton, J. H.

**VARIABLES:**

77K = 283 - 323

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g₁/g₂</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>7.11 × 10⁻³</td>
<td>7.11 × 10⁻⁴</td>
<td>0.607</td>
</tr>
<tr>
<td>20</td>
<td>8.44 × 10⁻³</td>
<td>8.44 × 10⁻⁴</td>
<td>0.720</td>
</tr>
</tbody>
</table>

(continued)

**METHOD/APPARATUS/PROCEDURE:**

Tetrachloromethane was saturated with water in a flask using continuous shaking, followed by standing for a day or more to establish equilibrium. Samples were withdrawn from the solution and introduced into a bulb containing CaH₂. The complete apparatus was placed in a water bath. The evolved hydrogen was measured volumetrically after three days. Two to four determinations were carried out at each temperature. For more details, see (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled.
(2) Reagent grade, free from impurities, b. p. = 76.8°C.

**ESTIMATED ERRORS:**

Solubility: ± 0.001 % H₂O.
Temperature: ± 0.2 K (compiler).

**REFERENCES:**

COMPONENTS:
(1) Water; H$_2$O; [7732-18-5]
(2) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

ORIGINAL MEASUREMENTS:
Rosenbaum, C. K.; Walton, J. H.

VARIABLES:
$T/K = 283 - 323$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES: (continued)

<table>
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<th>$t/^\circ C$</th>
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</tr>
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<tbody>
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<td>30</td>
<td>$1.09 \times 10^{-2}$</td>
<td>$1.09 \times 10^{-2}$</td>
</tr>
<tr>
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<td>$1.52 \times 10^{-2}$</td>
<td>$1.52 \times 10^{-2}$</td>
</tr>
<tr>
<td>50</td>
<td>$2.37 \times 10^{-2}$</td>
<td>$2.37 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]
(2) Water; H$_2$O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Gross, P. M.; Saylor, J. H.

VARIABLES:
$T/K = 288 - 303$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<th>$1000 \ g_i/\ell_2$</th>
<th>$100 \ w_i$ (compiler)</th>
<th>$10^5 \ x_i$ (compiler)</th>
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</thead>
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<td>15</td>
<td>0.77</td>
<td>$7.7 \times 10^{-2}$</td>
<td>9.02</td>
</tr>
<tr>
<td>30</td>
<td>0.81</td>
<td>$8.1 \times 10^{-2}$</td>
<td>9.49</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An excess of tetrachloromethane in 500 g water was shaken for 12 hours in a thermostat. Samples were then withdrawn and read against water using an interferometer made by Zeiss (ref. 1). A detailed description of the complete procedure is given in a Ph. D. thesis (ref. 2).

SOURCE AND PURITY OF MATERIALS:
(1) Eastman Kodak Co., shaken with H$_2$SO$_4$ and NaOH solution, dried and fractionated before use.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: ± 2.5 %;
Temperature: ± 0.02 K.

REFERENCES:
(2) Saylor, J. H. _Ph. D. Thesis_, Duke University, Durham, **1930**.
### COMPONENTS:

1. Water; \( \text{H}_2\text{O} \); [7732-18-5]
2. Tetrachloromethane (carbon tetrachloride); \( \text{CCl}_4 \); [56-23-5]

### ORIGINAL MEASUREMENTS:

Bell, R. P.


### VARIABLES:

\( T/\text{K} = 288 - 298 \)

### EXPERIMENTAL VALUES:

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<th>( 100 w_x ) (compiler)</th>
<th>( 10^4 x_l ) (compiler)</th>
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</thead>
<tbody>
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<td>15</td>
<td>( 6.35 \times 10^{-2} )</td>
<td>( 3.96 \times 10^3 )</td>
<td>( 3.38 )</td>
</tr>
<tr>
<td>20</td>
<td>( 7.67 \times 10^{-2} )</td>
<td>( 4.81 \times 10^3 )</td>
<td>( 4.10 )</td>
</tr>
<tr>
<td>25</td>
<td>( 9.35 \times 10^{-2} )</td>
<td>( 5.90 \times 10^3 )</td>
<td>( 5.03 )</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

An about 1 to 5 ratio of water/tetrachloromethane mixture was rotated in a thermostat for 12 hours. After the equilibrium was attained, samples were taken and filtered through cottonwool. The determination of the water content was based upon the reaction with \( \alpha \)-naphthoxydichlorophosphine. The evolved HCl was absorbed in water and titrated with NaOH solution (ref. 1). Two to three successive determinations were carried out with the tetrachloromethane.

#### SOURCE AND PURITY OF MATERIALS:

1. Distilled (compiler).
2. Merck reagent, analytical grade, redistilled before use.

#### ESTIMATED ERRORS:

Solubility: \( \pm 4.4 \% \) mean.

Temperature: \( \pm 0.02 \text{ K} \).

#### REFERENCES:


### COMPONENTS:

1. Tetrachloromethane (carbon tetrachloride); \( \text{CCl}_4 \); [56-23-5]
2. Water; \( \text{H}_2\text{O} \); [7732-18-5]

### ORIGINAL MEASUREMENTS:

van Arkel, A. E.; Vles, S. E.


### VARIABLES:

\( T/\text{K} = 303 \)

### EXPERIMENTAL VALUES:

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<th>( t/°C )</th>
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<th>( 100 \text{ w}_x M_l^{-1}/\text{mol g}^{-1} ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>30</td>
<td>0.955</td>
<td>( 8.15 \times 10^2 )</td>
<td>( 5.3 \times 10^4 )</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: \( \pm 0.5 \text{ K} \) (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

**VARIABLES:**

\[ T/K = 293 \]

**EXPERIMENTAL VALUES:**

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</thead>
<tbody>
<tr>
<td>20</td>
<td>( 8.32 )</td>
<td>( 5.0 \times 10^{-3} )</td>
</tr>
</tbody>
</table>

** Auxilliary Information**

**METHOD/APPARATUS/PROCEDURE:**

The change caused by the addition of tetrachloromethane was determined by both the density and refractive index methods. The measurements of the refraction and density of the saturated solution were carried out by the conventional methods, that is by the use of a refractometer and a dilatometer, respectively.

**SOURCE AND PURITY OF MATERIALS:**

(1) Kahlbaum, analytical grade, \( d_4 = 1.59413 \) at \( 20^\circ C \) and \( n_0 = 1.4608 \) at \( 20^\circ C \).
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: \( \pm 20 \% \).
Temperature: \( \pm 0.5 \) K (compiler).

### COMPONENTS:

(1) Water; H₂O; [7732-18-5]
(2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]

**VARIABLES:**

\[ T/K = 291 \]

**EXPERIMENTAL VALUES:**

<table>
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<th>( 10^4 x_1 ) (compiler)</th>
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<tbody>
<tr>
<td>18.3</td>
<td>( 6.9 \times 10^{-3} )</td>
<td>( 6.9 \times 10^{-3} )</td>
</tr>
</tbody>
</table>

** Auxilliary Information**

**METHOD/APPARATUS/PROCEDURE:**

A grating spectrometer was used to observe the infrared absorption spectrum of water in the saturated tetrachloromethane solution. The absorption cells were constructed from fluorite plates. The gradual removal of water was revealed by the diminution of the infrared absorption, and a comparison was made using the measured weight of water collected.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: \( \pm 0.2 \) K (compiler).
### Component Information

**COMPONENTS:**

1. Water; H₂O; [7732-18-5]
2. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]

**ORIGINAL MEASUREMENTS:**

- Staverman, A. J.  

**PREPARED BY:**

- A. L. Horvath

**VARIABLES:**

- **T/K = 273 - 303**

**EXPERIMENTAL VALUES:**

<table>
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<tr>
<th>T/K (°C)</th>
<th>100 wₓ</th>
<th>10⁴ xₓ (compiler)</th>
<th>10⁴ wₓMₓ⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.50 × 10²</td>
<td>42.8</td>
<td>2.77 × 10⁴</td>
</tr>
<tr>
<td>25</td>
<td>1.16 × 10²</td>
<td>99.1</td>
<td>6.44 × 10⁴</td>
</tr>
<tr>
<td>30</td>
<td>1.58 × 10²</td>
<td>135.0</td>
<td>8.77 × 10⁴</td>
</tr>
</tbody>
</table>

### Method/Apparatus/Procedure

Tetrachloromethane was shaken with water for about 12 hours in a liquid paraffin thermostat bath. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were done in duplicates. The results were averages of two measurements at each temperature. A full description of the method used is given in a Ph. D. thesis (ref. 1).

### Source and Purity of Materials

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

### Estimated Errors

- Solubility: Not specified.
- Temperature: ± 0.5 K (compiled).

### References


---

### Component Information

**COMPONENTS:**

1. Water; H₂O; [7732-18-5]
2. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]

**ORIGINAL MEASUREMENTS:**

- Hutchison, C. A.; Lyon, A. M.  
  *Columbia University Report A-745, July 1, 1943.*

**PREPARED BY:**

- A. L. Horvath

**VARIABLES:**

- **T/K = 298**

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>T/K (°C)</th>
<th>100 wₓMₓ⁻¹/mol g⁻¹</th>
<th>100 wₓ</th>
<th>10⁴ xₓ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>5.43 × 10⁻⁴</td>
<td>9.78 × 10⁻⁴</td>
<td>8.34</td>
</tr>
</tbody>
</table>

### Method/Apparatus/Procedure

A 1 to 15 volume ratio mixture of water and tetrachloromethane was introduced into an equilibrium flask and then lowered into a waterbath thermostat. The assembly was shaken mechanically for about 90 minutes 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 description of procedure was taken from a secondary source (ref. 1). The original university report is no longer available.

### Source and Purity of Materials

1. Distilled.
2. Source is not known. Purified and dried before use.

### Estimated Errors

- Solubility: ± 0.1 × 10⁻⁴ avg. dev.
- Temperature: ± 0.05 K.

### References

**COMPONENTS:**

(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

McGovern, E. W.


**VARIABLES:**

\[ T/K = 273 - 303 \]

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
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<th>( t/°C )</th>
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<th>10⁴ ( x_1 ) (compiler)</th>
<th>100 ( w_2 )</th>
<th>10⁴ ( x_2 ) (compiler)</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>9.8 × 10⁻²</td>
<td>1.15</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>10</td>
<td>8.4 × 10⁻²</td>
<td>0.984</td>
<td>0.65 × 10⁻²</td>
<td>5.55</td>
</tr>
<tr>
<td>20</td>
<td>8.0 × 10⁻²</td>
<td>0.938</td>
<td>0.92 × 10⁻²</td>
<td>7.85</td>
</tr>
<tr>
<td>25</td>
<td>8.0 × 10⁻²</td>
<td>0.938</td>
<td>1.30 × 10⁻²</td>
<td>11.09</td>
</tr>
<tr>
<td>30</td>
<td>8.0 × 10⁻²</td>
<td>0.938</td>
<td>1.35 × 10⁻²</td>
<td>11.52</td>
</tr>
</tbody>
</table>

Solubility data as a function of temperature were presented in graphical form except the tabulated data point at 25°C.

**AUXILIARY INFORMATION**

**METHOD APPARATUS PROCEDURE:**

Details are not available.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source not given, commercial grade.
(2) Distilled (compiler).

**ESTIMATED ERRORS:**

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

---

**COMPONENTS:**

(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Powell, J. F.


**VARIABLES:**

\[ T/K = 293 - 310 \]

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
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<th>( t/°C )</th>
<th>( L/dimensionless )</th>
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<tbody>
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<td>8.05 × 10⁻²</td>
<td>9.44</td>
</tr>
<tr>
<td>37</td>
<td>0.45</td>
<td>6.82 × 10⁻²</td>
<td>7.99</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD APPARATUS PROCEDURE:**

A tetrachloromethane - air mixture was bubbled through 50 cm³ distilled water contained in a gas absorption bottle with a sintered glass plate. Equilibrium was reached in 3/4 hour with a gas flow of 50 cm³/min. The saturated solution was transferred to a measuring cylinder and shaken with toluene. The toluene extraction was allowed to settle and then analyzed for tetrachloromethane by the addition of pyridine and alkali; see (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 0.5 K (compiled).

**REFERENCES:**

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Booth, H. S.; Everson, H. E.

VARIABLES:
\[ T/K = 298 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<th>( 100 \ w_r ) (compiler)</th>
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<tbody>
<tr>
<td>25.0</td>
<td>0.10</td>
<td>0.159</td>
<td>1.86</td>
</tr>
<tr>
<td>60</td>
<td>0.10</td>
<td>0.159</td>
<td>1.86</td>
</tr>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The equilibrium was established through repeated shaking and centrifuging of a tetrachloromethane and water mixture in a stopped Goetz tube and returning the tube to a constant temperature water bath. The difference between the total amount of tetrachloromethane which was added and the amount which remained in excess was taken as the amount of solute dissolved in the known volume of water. The determination of the excess amount of solute added is described by Hanslick in his Ph. D. thesis (ref. 1).

SOURCE AND PURITY OF MATERIALS:
(1) Commercial reagent, C. P. grade, used as received.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.1 K (compiler).

REFERENCES:

---

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Booth, H. S.; Everson, H. E.

VARIABLES:
\[ T/K = 298 - 333 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

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<tr>
<td>60</td>
<td>0.10</td>
<td>0.159</td>
<td>1.86</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The solute-solvent mixture in a solubility tube was gently rotated while the tube was immersed in a constant temperature bath. The difference between the total amount of solute and the amount remaining in excess was taken as the amount of solute dissolved in the known volume of solvent. The volumetric determination is described elsewhere (ref. 1).

SOURCE AND PURITY OF MATERIALS:
(1) Commercial reagent, C. P. grade, used as received.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:
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<td>Chitwood, B. G.</td>
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<td>A. L. Horvath</td>
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<td>25</td>
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**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: \(\pm 0.5 \degree K\) (compiler).

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<td>Donahue, D. J.; Bartell, F. E.</td>
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<td>25</td>
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**METHOD/APPARATUS/PROCEDURE:**
A mixture of water and tetrachloromethane was placed in a glass stoppered flask and was shaken intermittently for at least three days in a water bath held at constant temperature. The organic phase was analyzed for water content by the Karl Fischer method and the aqueous phase was analyzed by using an interferometer.

**SOURCE AND PURITY OF MATERIALS:**
(1) Reagent grade, purified by fractional distillation.
(2) Purified by distillation.

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: \(\pm 0.1 \degree K\).
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<td>T/K = 298</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
</tr>
<tr>
<td>25</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The solute-solvent mixture was rocked for 24 hours in a water bath. Samples were removed from the organic-rich phase with a special, turned-up tip pipet. The liquid was exposed only to dry nitrogen during its removal and analysis with a Karl Fischer reagent. The result is the mean value of five determinations.

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled (compiler).

(2) Source and purity not given.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 0.01 K.

---

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Water; H₂O; [7732-18-5]</td>
<td>Eberius, E.</td>
</tr>
</tbody>
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<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>
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<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
</tr>
<tr>
<td>20</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

A 50 g tetrachloromethane sample was shaken with pure water in a 100 ml Erlenmeyer flask. The two phases were separated when equilibrium had been established. 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: Not specified.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
</table>

<table>
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<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
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</thead>
<tbody>
<tr>
<td>T/K = 293</td>
<td>A. L. Horvath</td>
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<table>
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<th>EXPERIMENTAL VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
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<tr>
<td>------</td>
</tr>
<tr>
<td>20</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
A saturated solution of water and tetrachloroethylene was prepared and the water content of the organic phase was determined by the Karl Fischer titration method.

**SOURCE AND PURITY OF MATERIALS:**
(1) Spectroscopic grade.
(2) Source not given, purified and dried before use.

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
**COMPONENTS:**

1. Water; H₂O; [7732-18-5]
2. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]

**ORIGINAL MEASUREMENTS:**

Desnoyer, M.


**VARIABLES:**

\( T/K = 299 \)

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 100 , w_i )</th>
<th>( 10^4 , x_i )</th>
<th>( 10^4 , w_i/M_i \cdot \text{mol} \cdot \text{l} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>26</td>
<td>( 1.01 \times 10^{-2} )</td>
<td>8.62</td>
<td>5.61</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The saturation of tetrachloromethane with water took place at room temperature under vigorous stirring. The concentration of water in the organic-rich phase was determined by infrared spectrometry.

**SOURCE AND PURITY OF MATERIALS:**

1. Distilled.
2. Commercial reagent, washed and dried before use.

**ESTIMATED ERRORS:**

Solubility: ± 4 %.
Temperature: ± 0.5 K (compiler).

**REFERENCES:**

<table>
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<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>Tettamanti, K.; Nogradi, M.; Sawinsky, J.</td>
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<th>PREPARED BY:</th>
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<td>T/K = 293</td>
<td>Z. Maczynska</td>
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<table>
<thead>
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<th></th>
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</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>100 ( w_1 )</td>
</tr>
<tr>
<td>20</td>
<td>7.0 ( \times 10^{-2} )</td>
</tr>
</tbody>
</table>

The reported values were graphically smoothed.

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

Turbidimetric titrations were used for both the aqueous and the organic phases. Tetrachloromethane or water was weighed into a stoppered flask with an accuracy of 0.01 g. The temperature was maintained constant in an ultrathermostat. First, the organic solvent was titrated with water from a microburet until the appearance of turbidity. Then, the water was titrated with the organic solvent until the appearance of turbidity.

#### SOURCE AND PURITY OF MATERIALS:

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

#### ESTIMATED ERRORS:

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

---

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>Liu, J.-L.; Huang, T.-C.</td>
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<td>T/K = 288 - 298</td>
<td>A. L. Horvath</td>
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<tbody>
<tr>
<td>( t/°C )</td>
<td>1000 ( g_1/g_2 )</td>
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<td>20</td>
<td>0.748</td>
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<td>25</td>
<td>0.762</td>
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### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of distilled water. The flask was rotated in a thermostat bath until the equilibrium was established. The optical densities of different concentrations of tetrachloromethane in water were measured using water as the reference liquid. Duplicate experiments were made and the results averaged. The absorption spectrum of the tetrachloromethane in water was determined by using a Hilger spectrophotometer.

#### SOURCE AND PURITY OF MATERIALS:

(1) Peking Chemical Factory, further purified by washing with H₂SO₄, NaOH, and water, dried over CaCl₂, and fractionated.
(2) Distilled.

#### ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
### COMPONENTS:

<table>
<thead>
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<th>Original Measurements</th>
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<td>Johnson, J. R.; Christian, S. D.; Affsprung, H. E.</td>
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### VARIABLES:

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<tbody>
<tr>
<td>A. L. Horvath</td>
</tr>
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### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/\text{C}$</th>
<th>$c/\text{mol m}^{-3}$</th>
<th>$10^4 x_i$ (compiler)</th>
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<tbody>
<tr>
<td>25.0</td>
<td>8.7</td>
<td>$9.89 \times 10^3$</td>
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### SOURCE AND PURITY OF MATERIALS:

<table>
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<th>Method/Apparatus/Procedure</th>
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<tr>
<td>(2) Source not given. Purified by distillation in an Oldershaw column before use.</td>
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</table>

### REFERENCES:

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<th>Source and purity of materials</th>
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<tbody>
<tr>
<td>References</td>
</tr>
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</table>
**COMPONENTS:**

(1) Tetrachloromethane (carbon tetrachloride); \( \text{CCl}_4; [56-23-5] \)

(2) Water; \( \text{H}_2\text{O}; [7732-18-5] \)

**ORIGINAL MEASUREMENTS:**

Johnson, J. R.  

**VARIABLES:**

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

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>( t/\text{C} )</th>
<th>( c_t/\text{mol m}^3 )</th>
<th>( 100 \ w_t/\text{(compiler)} )</th>
<th>( c_t/\text{mol m}^3 )</th>
<th>( 100 \ w_t/\text{(compiler)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>5.1</td>
<td>7.8 \times 10^3</td>
<td>8.7</td>
<td>9.89 \times 10^3</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The equilibrium between tetrachloromethane and water took place in a well-stirred water bath. The experimental samples were allowed to equilibrate for two or more days. Water analyses were made with a Beckman Aquameter using a Karl Fischer reagent. The solubility of tetrachloromethane in water was measured by using a vapor pressure measuring device. Full details are available in the thesis.

**SOURCE AND PURITY OF MATERIALS:**

(1) Allied Chemical Corp., purified by distillation before use.

(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: ± 4%.

Temperature: ± 0.1 K.

**COMPONENTS:**

(1) Water; \( \text{H}_2\text{O}; [7732-18-5] \)

(2) Tetrachloromethane (carbon tetrachloride); \( \text{CCl}_4; [56-23-5] \)

**ORIGINAL MEASUREMENTS:**

Grigsby, R. D.  

**VARIABLES:**

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

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
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<th>( c_t/\text{mol m}^3 )</th>
<th>( 100 \ w_t/\text{(compiler)} )</th>
<th>( 10^3 \ x_t/\text{(compiler)} )</th>
<th>Method used:</th>
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<tr>
<td>25</td>
<td>9.8</td>
<td>1.8 \times 10^2</td>
<td>1.53</td>
<td>coulometric</td>
</tr>
<tr>
<td>25</td>
<td>8.8</td>
<td>1.6 \times 10^2</td>
<td>1.36</td>
<td>total pressure</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

Two methods were used for the water concentration in tetrachloromethane determination. After equilibration in a thermostated closed system, samples were withdrawn and analyzed for total water content using a coulometric Karl Fischer titrator. In the second method, the total pressure of the saturated solution was measured in a liquid-vapor equilibrium still apparatus. Full details are described in the Ph. D. thesis; see also (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled.

(2) Fischer reagent, refluxed with Hg and redistilled before use.

**ESTIMATED ERRORS:**

Solubility: ± 12%.

Temperature: ± 0.1 K.

**REFERENCES:**

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Water; H₂O; [7732-18-5]
2. Tetrachloromethane (carbon tetrachloride); CC₄; [56-23-5]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>T/°C</th>
<th>n₁/V₂/mol m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>5.9 ± 0.2</td>
<td>6.64 × 10⁻³</td>
<td>5.66</td>
</tr>
<tr>
<td>25</td>
<td>8.7 ± 0.3</td>
<td>9.89 × 10⁻³</td>
<td>8.44</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The solute isopiestic method was used without modification. The apparatus employed consisted of a closed vessel divided into two compartments, one for water and the other for the organic solvent. Equilibrium was attained often for a period of 6 to 8 hours. The solution was analyzed for water with the Beckman KF-3 Aquameter. The Karl Fisher reagent was standardized against crystalline sodium tartarate dihydrate.

**SOURCE AND PURITY OF MATERIALS:**

1. Distilled.
2. Source not given, certified or reagent grade, distilled through a 30 plate Oldershaw column before use.

### ESTIMATED ERRORS:

**Solubility:** Not specified.

**Temperature:** ± 0.1 K.
COMPONENTS: ORIGINAL MEASUREMENTS:
(2) Tetrachloromethane (carbon tetrachloride); \( \text{CCl}_4 \); [56-23-5]

VARIABLES: PREPARED BY:
\( T/K = 303 - 323 \) A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/\degree C )</th>
<th>100 ( w_i )</th>
<th>10^3 ( x_i ) (compiler)</th>
<th>100 ( w_iM_i^{-1}/\text{mol g}^{-1} ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>30</td>
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<td>1.15</td>
<td>7.49 \times 10^{-4}</td>
</tr>
<tr>
<td>50</td>
<td>3.05 \times 10^{-2}</td>
<td>2.60</td>
<td>1.69 \times 10^{-3}</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

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

SOURCE AND PURITY OF MATERIALS:
(1) Distilled (compiler).
(2) Source not given. Chemically pure grade, dried and redistilled before use.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( \pm 0.5 \) K (compiler).

REFERENCES:
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Water; H$_2$O; [7732-18-5]
Simonov, V. D.; et al.  

(2) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

VARIABLES:
$T/K = 288 - 299$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES: (continued)

$$
\begin{array}{cccccc}
\text{t}^\circ \text{C} & 100 \text{ w}_1 & 10^4 \text{ x}_1 \\
& \text{Aexeev} & \text{Fischer} & \text{Spectroscopy} & \text{Aexeev} & \text{Fischer} & \text{Spectroscopy} \\
18 & 7.00 \times 10^{-3} & 7.20 \times 10^{-3} & 7.10 \times 10^{-3} & 5.974 & 6.144 & 6.059 \\
22 & 8.85 \times 10^{-3} & 8.90 \times 10^{-3} & 8.90 \times 10^{-3} & 7.551 & 7.594 & 7.594 \\
24 & 9.12 \times 10^{-3} & - & 10.10 \times 10^{-3} & 7.782 & - & 8.617 \\
26 & 10.70 \times 10^{-3} & 10.60 \times 10^{-3} & - & 9.129 & 9.043 & - \\
\end{array}
$$

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]
Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

(2) Water; H$_2$O; [7732-18-5]

VARIABLES:
$T/K = 288 - 333$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

$$
\begin{array}{cccc}
\text{t}^\circ \text{C} & 1000 \text{ g}_1/\text{g}_2 & 100 \text{ w}_2 & 10^3 \text{ x}_1 \\
& & (\text{compiler}) & (\text{compiler}) \\
15 & 0.81 & 8.1 \times 10^{-2} & 9.49 \\
30 & 0.45 & 4.5 \times 10^{-2} & 5.27 \\
45 & 0.25 & 2.5 \times 10^{-2} & 2.93 \\
60 & 0.14 & 1.4 \times 10^{-2} & 1.64 \\
\end{array}
$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The dynamic method used for the solubility determination consisted of the saturation of nitrogen with tetrachloromethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of water. After 2 - 3 hours, the solution became saturated and samples were taken periodically (ref. 1). The concentration of the tetrachloromethane in water was determined by GLC. Some 3 - 5 measurements were taken at each temperature.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: ± 15 %.
Temperature: ± 0.05 K.

REFERENCES:
### COMPONENTS: ORIGINAL MEASUREMENTS:

| (1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5] |
| (2) Water; H₂O; [7732-18-5] |

| ORIGINAL MEASUREMENTS: |
| Karger, B. L.; Chatterjee, A. K.; King, J. W. |


### VARIABLES: PREPARED BY:

| TIK = 286 |
| A. L. Horvath |

### EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t°C</th>
<th>Partition coefficient¹, $K_p$/dimensionless</th>
<th>100 $w_i$ (compiler)</th>
<th>$10^4 x_i$ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>12.5</td>
<td>1.9</td>
<td>0.106</td>
<td>1.24</td>
</tr>
</tbody>
</table>

¹ Gas-liquid chromatographic parameter, from instrument calibration. The solubility was calculated from the partition coefficient and the vapor pressure.

### AUXILIARY INFORMATION

### SOURCE AND PURITY OF MATERIALS:

| METHOD/APPARATUS/PROCEDURE: |
| Gas-liquid chromatography was used for the determination of the partition of tetrachloromethane with thin layers of water coated on Porasil D. Helium carrier. The gas was presaturated with water at the column temperature. The eluents were detected with an F. & N. flame ionization detector. The partition coefficient ($K_p$) was obtained from the slope of the straight line plot of $V_m/A_k$ vs. $V_s/A_k$. |

| SOURCE AND PURITY OF MATERIALS: |
| (1) J. T. Baker Chemical Co., reagent grade, used as received. |
| (2) Distilled (compiler). |

| ESTIMATED ERRORS: |
| Solubility: Not specified. |
| Temperature: ± 0.05 K (compiler). |

### COMPONENTS: ORIGINAL MEASUREMENTS:

| (1) Water; H₂O; [7732-18-5] |
| (2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5] |

| ORIGINAL MEASUREMENTS: |
| Glasoe, P. K.; Schultz, S. D. |


### VARIABLES: PREPARED BY:

| TIK = 288 - 318 |
| A. L. Horvath |

### EXPERIMENTAL VALUES:

<table>
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<th>t°C</th>
<th>$c_i$/mol m⁻³</th>
<th>100 $w_i$ (compiler)</th>
<th>$10^4 x_i$ (compiler)</th>
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<tr>
<td>15</td>
<td>6.2 ± 0.1</td>
<td>6.97 × 10⁻³</td>
<td>5.95</td>
</tr>
<tr>
<td>25</td>
<td>8.6 ± 0.3</td>
<td>9.78 × 10⁻³</td>
<td>8.35</td>
</tr>
<tr>
<td>30</td>
<td>9.3 ± 0.3</td>
<td>1.06 × 10⁻²</td>
<td>9.08</td>
</tr>
<tr>
<td>35</td>
<td>11.4 ± 0.3</td>
<td>1.31 × 10⁻²</td>
<td>11.2</td>
</tr>
<tr>
<td>45</td>
<td>15.6 ± 0.8</td>
<td>1.82 × 10⁻²</td>
<td>15.5</td>
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### AUXILIARY INFORMATION

### SOURCE AND PURITY OF MATERIALS:

| METHOD/APPARATUS/PROCEDURE: |
| The saturation of tetrachloromethane with water occurred in a closed system, protected from atmospheric moisture; the saturating vessel was placed in a constant temperature water bath. The concentration of water in tetrachloromethane was measured using the Karl Fischer titration method with a "dead stop" end-point determination (ref. 1). Fifteen observations were made at each temperature. |

| SOURCE AND PURITY OF MATERIALS: |
| (1) Distilled. |
| (2) Source not given. Reagent grade, purified by distillation before use. |

| ESTIMATED ERRORS: |
| Solubility: See above. |
| Temperature: ± 0.1 K (compiler). |

### REFERENCES:

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Antropov, L. I.; Pogulyai, V. E.; Simonov, V. D.; Shamsutdinov, T. M.

VARIABLES:
T/K = 288 - 299

EXPERIMENTAL VALUES:

<table>
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<th>10⁴ x₁ (compiler)</th>
<th>100 w₂ (compiler)</th>
<th>10⁴ x₂ (compiler)</th>
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<td>6.76 x 10⁻³</td>
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<td></td>
<td>-</td>
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<td>18</td>
<td>-</td>
<td>7.10 x 10⁻³</td>
<td>6.12</td>
<td>-</td>
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<td>20</td>
<td>7.95 x 10⁻³</td>
<td>9.31</td>
<td>-</td>
<td>-</td>
</tr>
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<td>-</td>
<td>8.30 x 10⁻³</td>
<td>7.08</td>
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<tr>
<td>26</td>
<td>9.76 x 10⁻³</td>
<td>11.43</td>
<td>1.20 x 10⁻²</td>
<td>10.24</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Alexejev’s synthetic solubility determination method was used (ref. 1). A fixed weight of tetrachloromethane 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 not given. Chemically pure grade.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1.0 K (compiler).

REFERENCES:

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Distribution coefficient₁, D₁/dimensionless (compiler)</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>29200</td>
<td>0.00439</td>
<td>0.514</td>
</tr>
</tbody>
</table>

₁ Gas-liquid system analysis parameter, from calibration measurements.
The solubility was calculated from the distribution coefficient and the vapor pressure.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The vapor-liquid equilibrium was measured by using a modification of the Rayleigh distillation method. An inert carrier gas was used for the removal of the vapor phase from the equilibration vessel. The analysis for tetrachloromethane in the water phase was accomplished radiometrically by using ³⁵Cl labeled compounds.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1.0 K (compiler).

REFERENCES:
(1) Prosyanov, N. N.; Shalygin, V. A.; Zel’venskii, Ya. D.
COMPONENTS: Original Measurements:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

Variables:

PREPARED BY:
A. L. Horvath

Experimental Values: (continued)

<table>
<thead>
<tr>
<th>t/C</th>
<th>Distribution coefficient, Dᵣ/dimensionless</th>
<th>10⁰ wᵣ (compiler)</th>
<th>10⁵ xᵣ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50.1</td>
<td>9670</td>
<td>0.0364</td>
<td>4.26</td>
</tr>
<tr>
<td>70.0</td>
<td>4100</td>
<td>0.1687</td>
<td>19.79</td>
</tr>
<tr>
<td>90.0</td>
<td>1960</td>
<td>0.637</td>
<td>75.01</td>
</tr>
<tr>
<td>96.2</td>
<td>1500</td>
<td>0.983</td>
<td>116.09</td>
</tr>
<tr>
<td>100.0</td>
<td>1380</td>
<td>1.179</td>
<td>139.52</td>
</tr>
</tbody>
</table>

¹ Gas-liquid system analysis parameter, from calibration measurements.
The solubility was calculated from the distribution coefficient and the vapor pressure.

COMPONENTS:
(1) Water; H₂O; [7732-18-5]
(2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]

ORIGINAL MEASUREMENTS:
Prosyannov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D.

PREPARED BY:
A. L. Horvath

Experimental Values:

\[ \log_{10} \alpha = \frac{733.92}{T(K)} - 0.0161 \]

where \( \alpha \) = Distribution Coefficient

At the normal boiling point of CCl₄, 349.79 K, \( \alpha = 120 \), the activity coefficient, \( \gamma_1 = 296 \), and the mole fraction of (1) at saturation, \( x_1 = 3.378 \times 10^{-2} \) (compiler).

Auxiliary Information

Method/Apparatus/Procedure:
The water concentration in the organic-rich phase was determined by a radiometric method using tritium labeled water.
The experimental procedure is described in more detail elsewhere (ref. 1).

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

Estimated Errors:
Solubility: Not specified.
Temperature: ± 1.0 K (compiler).

References:
### COMPONENTS: ORIGINAL MEASUREMENTS:

|----------------------------|--------------|

### VARIABLES:

T/K = 283 - 313

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>cᵢ/mol m³</th>
<th>10⁵ wᵢ (compiler)</th>
<th>10⁷ xᵢ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>5.23</td>
<td>0.942 × 10⁻²</td>
<td>8.04</td>
</tr>
<tr>
<td>15</td>
<td>6.05</td>
<td>1.09 × 10⁻²</td>
<td>9.30</td>
</tr>
<tr>
<td>20</td>
<td>7.47</td>
<td>1.34 × 10⁻²</td>
<td>11.4</td>
</tr>
<tr>
<td>25</td>
<td>8.87</td>
<td>1.60 × 10⁻²</td>
<td>13.6</td>
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<tr>
<td>30</td>
<td>10.35</td>
<td>1.86 × 10⁻²</td>
<td>15.8</td>
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<tr>
<td>35</td>
<td>12.38</td>
<td>2.23 × 10⁻²</td>
<td>19.0</td>
</tr>
<tr>
<td>40</td>
<td>14.33</td>
<td>2.58 × 10⁻²</td>
<td>22.0</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Tetrachloromethane was equilibrated with an excess of water in a vessel under rotation in a water bath for 1 hour. Aliquots of the water saturated organic solvent were taken for analysis with calibrated Hamilton syringes. The analyses were performed with an Aquatest II automatic Karl Fischer titrator. During the analyses, the coulometer current generated by the instrument was checked with an accurate milliammeter.

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled.
(2) Source not given. Certified grade, dried with CaCl₂ and distilled under dry nitrogen, density = 1.5826 g/cc at 25°C.

**ESTIMATED ERRORS:**

Solubility: ± 0.18 std. dev.
Temperature: ± 0.02 K.

### REFERENCES:

(1) Simonov, V. D.; Shamsudinov, T. M; Pogulyai, V. E.; Popova, L. N.
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
T/K = 293

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁴ g/g₂</th>
<th>10⁴ x₁</th>
<th>10⁴ x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>7.85</td>
<td>7.85 × 10⁻²</td>
<td>9.19</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The solubility of tetrachloromethane 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: ± 0.3 K (compiler).

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
T/K = 293

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁶ w₁</th>
<th>10⁴ x₁</th>
<th>10⁴ x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>785</td>
<td>7.85 × 10⁻²</td>
<td>9.20</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Saturated solutions were prepared in a constant temperature thermostat bath. Water samples were extracted with n-pentane and an aliquot of the extract taken for GLC analysis. The gas chromatograph was fitted with a 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 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

<table>
<thead>
<tr>
<th>(1) Water; H₂O; [7732-18-5]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
</tr>
</tbody>
</table>

**Kirchnerova, J.**


### VARIABLES:

| T/°K = 298 |

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c_i/mol m⁻³</th>
<th>100 w_i (compiler)</th>
<th>10⁴ x_i (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>8.7</td>
<td>9.96 × 10⁻³</td>
<td>8.50</td>
</tr>
</tbody>
</table>

### SOURCE AND PURITY OF MATERIALS:

**METHOD/APPARATUS/PROCEDURE:**

Binary mixtures containing 50 ml tetrachloromethane were isopiestically equilibrated with water in an equilibration vessel which was submerged in a waterbath. The equilibrium concentration of water in the binary mixtures was then determined by a Karl Fischer titration method. The apparatus included a Zeromatic II potentiometer with the dead-stop end-point indication. The determinations were made at least in duplicate.

**REFERENCES:**


---

**COMPONENTS: ORIGINAL MEASUREMENTS:**

<table>
<thead>
<tr>
<th>(1) Water; H₂O; [7732-18-5]</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
</tr>
</tbody>
</table>

**Kirchnerova, J.**

**Cave, G. C. B.**


### VARIABLES:

| T/°K = 298 |

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c_i/mol m⁻³</th>
<th>10⁴ x_i (compiler)</th>
<th>100 w_i (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>8.7</td>
<td>8.5</td>
<td>9.96 × 10⁻³</td>
</tr>
</tbody>
</table>

### SOURCE AND PURITY OF MATERIALS:

**METHOD/APPARATUS/PROCEDURE:**

A bottle containing a mixture of 50 ml tetrachloromethane and 6 ml water was submerged into a water thermostat bath for two days. The concentration of water in the organic phase was determined by a conventional Karl Fischer deadstop backtitration. The determination was carried out in triplicate. A detailed description of the complete procedure is given in a Ph. D. thesis (ref. 1).
### COMPONENTS: ORIGINAL MEASUREMENTS:

<table>
<thead>
<tr>
<th>Number</th>
<th>Description</th>
<th>Author(s)</th>
</tr>
</thead>
</table>
| 1      | Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5] | Sato, A.; Nakijima, T.  
*Arch. Envir. Health* 1979, 34, 69-75. |
| 2      | Water; H₂O; [7732-18-5]              |                                    |

### VARIABLES:

<table>
<thead>
<tr>
<th>TIK</th>
<th>Preparer</th>
</tr>
</thead>
<tbody>
<tr>
<td>310</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>Distribution coefficient¹, $D_j$/dimensionless</th>
<th>100 $w_j$ (compiler)</th>
<th>10⁵ $x_j$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>0.25</td>
<td>3.78 × 10⁻²</td>
<td>4.43</td>
</tr>
</tbody>
</table>

¹ Water-air system analysis parameter, from calibration measurements.

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

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

#### SOURCE AND PURITY OF MATERIALS:

<table>
<thead>
<tr>
<th>Number</th>
<th>Description</th>
<th>Preparer</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Source and purity not given.</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Distilled.</td>
<td></td>
</tr>
</tbody>
</table>

#### ESTIMATED ERRORS:

<table>
<thead>
<tr>
<th>Solubility:</th>
<th>± 0.04 std. dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature:</td>
<td>± 0.3 K (compiler).</td>
</tr>
</tbody>
</table>

### COMPONENTS: ORIGINAL MEASUREMENTS:

<table>
<thead>
<tr>
<th>Number</th>
<th>Description</th>
<th>Author(s)</th>
</tr>
</thead>
</table>
| 1      | Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5] | Freed, V. H.; Chiou, C. T.; Schmedding, D.; Kohnert, R.  
*Environ. Health Perspect.* 1979, 30, 75-80. |
| 2      | Water; H₂O; [7732-18-5]              |                                    |

### VARIABLES:

<table>
<thead>
<tr>
<th>TIK</th>
<th>Preparer</th>
</tr>
</thead>
<tbody>
<tr>
<td>298</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>$10^4 w_j$</th>
<th>100 $w_j$ (compiler)</th>
<th>10⁵ $x_j$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>800</td>
<td>8.0 × 10⁻³</td>
<td>9.38</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

A known volume of water was mixed with tetrachloromethane in Erlenmeyer flasks. The flasks, with their contents magnetically stirred, were immersed in a water bath. Samples were removed for analyses at regular intervals. All samples were analyzed by gas-liquid chromatography using an electron capture detector. The reported solubility is the average of five consecutive samples with less than 5% variation.

#### SOURCE AND PURITY OF MATERIALS:

<table>
<thead>
<tr>
<th>Number</th>
<th>Description</th>
<th>Preparer</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Source not given. Analytical standard grade, purity is greater than 95 %</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>Distilled and run through a resin column.</td>
<td></td>
</tr>
</tbody>
</table>

#### ESTIMATED ERRORS:

<table>
<thead>
<tr>
<th>Solubility:</th>
<th>Not specified.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature:</td>
<td>± 0.5 K.</td>
</tr>
</tbody>
</table>
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Aref’eva, R. P.; Korenman, I. M.; Gorokhov, A. A.

VARIABLES:
T/K = 293

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>8₁ V₂⁻¹/kg m³</th>
<th>10⁴ x₁</th>
<th>10⁴ x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.87 ± 0.03</td>
<td>8.72 × 10⁻²</td>
<td>1.02</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Equal quantities of diphenylthiocarbazone were added to aqueous solutions with different amounts of tetrachloromethane in several flasks. The contents of the flasks were shaken for 5 minutes and left to stand for 1 hour. The mixtures were then filtered through a paper filter and then concentration measurements were made by spectrophotometry. The turning point on the graph of optical density versus tetrachloromethane concentration was taken as the measurement.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: See above.
Temperature: ± 1 K (compiler).

REFERENCES:
### COMPONENTS:
- (1) Water; H₂O; [7732-18-5]
- (2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]

### ORIGINAL MEASUREMENTS:
Ksiaczak, A.; Buchowski, H.  

### VARIABLES:
- T/K = 323

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁴ x₁</th>
<th>10⁻⁰ w₁ (compiler)</th>
<th>10⁻⁰ w₂M₁⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>50</td>
<td>21</td>
<td>2.46 × 10⁻²</td>
<td>1.365 × 10⁻³</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:
The difference between the vapor pressures of the aqueous solution and the dry tetrachloromethane as a function of the ratio of vapor and liquid volumes was measured in an apparatus consisting of 3 tubes with mercury and a pressure adjusting device. The difference between the mercury levels in the middle tube and the reference tube gave the vapor pressure of the reference liquid. The solubility was calculated from the slope of 1/ΔP versus V/V₁.

#### SOURCE AND PURITY OF MATERIALS:
- (1) Purified by repeated distillation.
- (2) Source not given. Purified and dried before use.

#### ESTIMATED ERRORS:
- Solubility: Not specified.
- Temperature: ± 0.05 K.

### COMPONENTS:
- (1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
- (2) Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:
Balls, P. W.  

### VARIABLES:
- T/K = 283 - 298

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, H/m³ atm mol⁻¹</th>
<th>10⁰ w₁ (compiler)</th>
<th>10⁵ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.75 ± 0.06</td>
<td>6.54 × 10⁻²</td>
<td>7.66</td>
</tr>
<tr>
<td>15</td>
<td>0.90 ± 0.07</td>
<td>6.84 × 10⁻²</td>
<td>8.02</td>
</tr>
<tr>
<td>20</td>
<td>1.05 ± 0.07</td>
<td>7.28 × 10⁻²</td>
<td>8.53</td>
</tr>
<tr>
<td>25</td>
<td>1.30 ± 0.10</td>
<td>7.24 × 10⁻²</td>
<td>8.48</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:
The measurements involved repeated equilibra-
tions of nitrogen with a water sample containing tetrachloromethane. The mixture was shaken vigorously at the required temperature in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph for analysis. The experiments were performed at least three times at 10, 15, 20, and 25°C. Each run at constant temperature involved about six equilibra-
tions.

#### SOURCE AND PURITY OF MATERIALS:
- (1) Source and purity not given.
- (2) Distilled.

#### ESTIMATED ERRORS:
- Solubility: See above.
- Temperature: ± 0.5 K (compiler).
<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 = 298</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>c/mol m³</td>
</tr>
<tr>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>25</td>
<td>4.92</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
</tr>
<tr>
<td>An excess of tetrachloromethane was added to a stainless steel tube containing water and then the tube was sealed. It was allowed to equilibrate during shaking for a 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.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) New England Nuclear, used as received.</td>
</tr>
<tr>
<td>(2) Distilled.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ESTIMATED ERRORS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility: ± 2.5 % std. dev.</td>
</tr>
<tr>
<td>Temperature: ± 0.3 K.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
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</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 VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>nᵢVᵢ/mol m³</td>
</tr>
<tr>
<td>------</td>
<td>----------</td>
</tr>
<tr>
<td>20</td>
<td>5.01</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
</tr>
<tr>
<td>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 mixture was analyzed by using radioactive techniques. The ¹⁴C activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Source and purity not given.</td>
</tr>
<tr>
<td>(2) Distilled.</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.</td>
</tr>
</tbody>
</table>
## COMPONENTS:

1. Water; H$_2$O; [7732-18-5]
2. Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

## ORIGINAL MEASUREMENTS:

Wu, X.


## VARIABLES:

T/$\mathbf{K}$ = 278 - 348

## PREPARED BY:

A. L. Horvath

## EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/\mathbf{^\circ C}$</th>
<th>$10^6 w_t$</th>
<th>$100 w_t$ (compiler)</th>
<th>$10^4 x_t$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>42</td>
<td>$0.42 \times 10^2$</td>
<td>3.59</td>
</tr>
<tr>
<td>10</td>
<td>46</td>
<td>$0.46 \times 10^2$</td>
<td>3.93</td>
</tr>
<tr>
<td>15</td>
<td>67</td>
<td>$0.67 \times 10^2$</td>
<td>5.72</td>
</tr>
<tr>
<td>20</td>
<td>92</td>
<td>$0.92 \times 10^2$</td>
<td>7.85</td>
</tr>
<tr>
<td>25</td>
<td>109</td>
<td>$1.09 \times 10^2$</td>
<td>9.30</td>
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<tr>
<td>30</td>
<td>123</td>
<td>$1.23 \times 10^2$</td>
<td>10.5</td>
</tr>
<tr>
<td>35</td>
<td>144</td>
<td>$1.44 \times 10^2$</td>
<td>12.3</td>
</tr>
<tr>
<td>40</td>
<td>190</td>
<td>$1.90 \times 10^2$</td>
<td>16.2</td>
</tr>
<tr>
<td>45</td>
<td>201</td>
<td>$2.01 \times 10^2$</td>
<td>17.1</td>
</tr>
<tr>
<td>50</td>
<td>232</td>
<td>$2.32 \times 10^2$</td>
<td>19.8</td>
</tr>
<tr>
<td>55</td>
<td>250</td>
<td>$2.50 \times 10^2$</td>
<td>21.3</td>
</tr>
<tr>
<td>60</td>
<td>299</td>
<td>$2.99 \times 10^2$</td>
<td>25.5</td>
</tr>
<tr>
<td>65</td>
<td>324</td>
<td>$3.24 \times 10^2$</td>
<td>27.6</td>
</tr>
<tr>
<td>70</td>
<td>380</td>
<td>$3.80 \times 10^2$</td>
<td>32.4</td>
</tr>
<tr>
<td>75</td>
<td>408</td>
<td>$4.08 \times 10^2$</td>
<td>34.7</td>
</tr>
</tbody>
</table>

## AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

A known amount of water was added to dried tetrachloromethane to make a series of standard samples for preparing calibration curves and obtaining the saturated solutions at each temperature. The determination of the water content of the tetrachloromethane was made with an RM-250 NMR spectrometer (radiation frequency 250 MHz). The water peak amplitude was the mean of four readings taken at a particular temperature.

### SOURCE AND PURITY OF MATERIALS:

1. Distilled.
2. Source not given. Grade 2 purity, washed with KOH and H$_2$SO$_4$ solutions and distilled water before dried on molecular sieve.

### ESTIMATED ERRORS:

Solubility: ± 28 std. dev.
Temperature: ± 1 - 2 K.
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

(2) Water; H$_2$O; [7732-18-5]

### VARIABLES:

$T/K = 274 - 300$

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>Distribution coefficient $D_t$/dimensionless</th>
<th>$10^4 w_1$ (compiler)</th>
<th>$10^4 x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0</td>
<td>412.1</td>
<td>9.611 $\times 10^{-2}$</td>
<td>1.127</td>
</tr>
<tr>
<td>1.3</td>
<td>412.4</td>
<td>9.866 $\times 10^{-2}$</td>
<td>1.157</td>
</tr>
<tr>
<td>11.0</td>
<td>719.5</td>
<td>9.238 $\times 10^{-2}$</td>
<td>1.083</td>
</tr>
<tr>
<td>13.0</td>
<td>859.5</td>
<td>8.533 $\times 10^{-2}$</td>
<td>1.000</td>
</tr>
<tr>
<td>21.0</td>
<td>1280.3</td>
<td>8.358 $\times 10^{-2}$</td>
<td>0.9796</td>
</tr>
<tr>
<td>22.0</td>
<td>1319.4</td>
<td>8.488 $\times 10^{-2}$</td>
<td>0.9948</td>
</tr>
<tr>
<td>27.2</td>
<td>1571.4</td>
<td>8.899 $\times 10^{-2}$</td>
<td>1.043</td>
</tr>
</tbody>
</table>

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

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A 5 $\mu$L tetrachloromethane sample was injected into a 2.3 liter equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 minutes, 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 tetrachloromethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

### SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.

(2) Distilled.

### ESTIMATED ERRORS:

Solubility: $\pm$ 3.4 %.

Temperature: $\pm$ 0.5 K.

### COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

(2) Water; H$_2$O; [7732-18-5]

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

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

### SOURCE AND PURITY OF MATERIALS:

Mackay, D.; et al.


### ESTIMATED ERRORS:

Solubility: Not specified.

Temperature: $\pm$ 1.0 K.
### COMPONENTS: ORIGNAL MEASUREMENTS:

1. Water; H₂O; [7732-18-5]  
   - Ohtsuka, K.; Kazama, K.  

2. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]  
   - Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S.  

### VARIABLES: PREPARED BY:

- $T/K = 298$
- $A. L. Horvath$

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$g_i V_i/\text{kg m}^3$</th>
<th>$100 w_i$ (compiler)</th>
<th>$10^3 x_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.22</td>
<td>1.4 x 10⁻²</td>
<td>1.19</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**  
Water was added gradually to 50 ml tetra-chloromethane in a flask which was then lowered into a thermostat bath. The flask was shaken vigorously until the first cloud (turbidity) appeared. The sample water content was determined by the Karl Fischer titration method.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

- Solubility: Not specified.
- Temperature: $± 0.5 K$ (compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]  
   - Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S.  

2. Water; H₂O; [7732-18-5]  

### VARIABLES: PREPARED BY:

- $T/K = 278 - 306$
- $A. L. Horvath$

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>Henry's law constant, $H$/dimensionless</th>
<th>$100 w_i$ (compiler)</th>
<th>$10^3 x_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.4864</td>
<td>8.006 x 10⁻²</td>
<td>9.383</td>
</tr>
<tr>
<td>10</td>
<td>0.5854</td>
<td>8.420 x 10⁻²</td>
<td>9.869</td>
</tr>
<tr>
<td>15</td>
<td>0.7000</td>
<td>8.823 x 10⁻²</td>
<td>10.34</td>
</tr>
<tr>
<td>20</td>
<td>0.8200</td>
<td>9.206 x 10⁻²</td>
<td>10.79</td>
</tr>
<tr>
<td>25</td>
<td>0.9831</td>
<td>9.584 x 10⁻²</td>
<td>11.23</td>
</tr>
<tr>
<td>33</td>
<td>1.2696</td>
<td>1.0554 x 10⁻¹</td>
<td>12.37</td>
</tr>
</tbody>
</table>

The Henry's law constant ($H$) was derived from the best-fit lines of van't Hoff plots:

$$\log_e H = - \frac{2918}{T(K)} + 9.77$$

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**  
The multiple equilibration technique was used to measure the Henry's law constant as described by McAuliffe (ref. 1). A known volume of water in a syringe was shaken with a known volume of pure tetrachloromethane. After equilibration of the sample, 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 specified.
2. Distilled.

**ESTIMATED ERRORS:**

- Solubility: $± 5.5$ % std. dev.
- Temperature: $± 0.2$ K.

**REFERENCES:**

**COMPONENTS:**

1. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]  
2. Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**
Orlandini, M.; Fermeglia, M.; Kikic, I.; Alessi, P.  

**VARIABLES:**

T/K = 293

**PREPARED BY:**
A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10⁴ x₁</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₂</th>
<th>100 w₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.9</td>
<td>7.68 × 10⁻²</td>
<td>7.1</td>
<td>8.322 × 10⁻³</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

A mixture of water and tetrachloromethane was agitated overnight and left at equilibrium for 24 hours. Three samples were withdrawn from each phase with a syringe and analyzed by gas chromatography. The gas chromatograph (Erba ATc/l) was equipped with a Shimadzu Chromatopac E-1A integrator. A stainless column packed with 100-120 mesh Chromosorb W DMCD coated with heptadecane nitrile was used for analysis.

**SOURCE AND PURITY OF MATERIALS:**

1. Fluka reagent, purified by distillation before use.  
2. Distilled (compiler).

**ESTIMATED ERRORS:**

Solubility: ± 0.1%  
Temperature: ± 0.1 K.

---

**COMPONENTS:**

1. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]  
2. Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**
Munz, C. D.  

**VARIABLES:**

T/K = 283 - 303

**PREPARED BY:**
A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's Law Constant, H/dimensionless</th>
<th>ρ/μg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.609</td>
<td>0.810</td>
<td>8.10 × 10⁻²</td>
<td>9.493</td>
</tr>
<tr>
<td>20</td>
<td>0.980</td>
<td>0.784</td>
<td>7.84 × 10⁻²</td>
<td>9.188</td>
</tr>
<tr>
<td>30</td>
<td>1.530</td>
<td>0.755</td>
<td>7.55 × 10⁻²</td>
<td>8.848</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 dimensionless Henry's law constant. A known volume of liquid and gas was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected directly into a gas chromatograph, the liquid samples were pre-concentrated by liquid-liquid extraction before analysis. The experiments were carried out in duplicates.

**SOURCE AND PURITY OF MATERIALS:**

1. Aldrich Chemicals Co., WI, > 99.5 % pure.  
2. Distilled and deionized.

**ESTIMATED ERRORS:**

Solubility: ± 1.28 × 10⁻² std. dev.  
Temperature: ± 0.5 K.
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Yoshioka, Y.; Ose, Y.; Sato, T.  

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

\[
\begin{array}{ccc}
\text{t/°C} & \rho/\text{kg m}^{-3} & 10^6 \nu_i \quad 10^3 x_i \\
20 & 2.6 \times 10^{-3} & 100 \nu_i \quad \text{(compiler)} \\
& & 2.6 \times 10^{-4} \quad 3.04 \quad \text{(compiler)} \\
\end{array}
\]

\(^1\) Cited value is in error (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A supersaturated solution of tetrachloromethane in water was agitated for two hours at 20°C. After storing for 2 hours the water phase was filtered through Whatman no. 2 filter paper before analysis. The concentration of tetrachloromethane in water was determined by gas chromatography or by ultraviolet spectroscopy.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1.0 K.

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Lo, J. M.; Tseng, C. L.; Yang, J. Y.  

VARIABLES:
T/K = 298

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

\[
\begin{array}{ccc}
\text{t/°C} & \nu_i & 10^4 x_i & 100 \nu_i M_i^{-1}/\text{mol g}^{-1} \\
25 & 8.0 \times 10^{-2} & 9.38 & 5.20 \times 10^{-4} \\
\end{array}
\]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A 5 ml tetrachloromethane sample containing a labeled complex, cobalt(III) pyrrolidinecarbodithioate, was placed together with 1000 ml water into a separation funnel. After rigorous shaking of the funnel for 5 minutes the mixture was left for 30 minutes before separation of the two phases. Samples were withdrawn for activity measurement using a NaI (TI) scintillation detector. Several factors were adjusted to obtain accurate measurements.

SOURCE AND PURITY OF MATERIALS:
(1) E. Merck Co., used as received.
(2) Demineralized and then boiled at reduced pressure.

ESTIMATED ERRORS:
Solubility: ± 0.7 \times 10^{-2} \text{ std. dev.}
Temperature: ± 1.0 K (compiler).
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Water; H₂O; [7732-18-5]


VARIABLES:

T/K = 283 - 308

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry’s Law Constant, ( H/m^3 ) atm mol⁻¹</th>
<th>CV₁ %</th>
<th>100 ( w_r ) (compiler)</th>
<th>10⁴ ( x_r ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10.0</td>
<td>1.32 × 10⁻²</td>
<td>5.15</td>
<td>8.64 × 10⁻²</td>
<td>1.013</td>
</tr>
<tr>
<td>17.5</td>
<td>2.11 × 10⁻²</td>
<td>4.20</td>
<td>7.79 × 10⁻²</td>
<td>0.912</td>
</tr>
<tr>
<td>24.8</td>
<td>3.04 × 10⁻²</td>
<td>3.92</td>
<td>7.62 × 10⁻²</td>
<td>0.893</td>
</tr>
<tr>
<td>34.6</td>
<td>4.60 × 10⁻²</td>
<td>3.42</td>
<td>7.73 × 10⁻²</td>
<td>0.906</td>
</tr>
</tbody>
</table>

¹ 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 tetrachloromethane was injected into serum bottles which contained distilled water. The bottles were incubated for 18 - 24 hours at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was approximately 4.3 %.

SOURCE AND PURITY OF MATERIALS:
(1) J. T. Baker reagent, analytical grade. Used as received.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: See above.
Temperature: ± 0.1 K.

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Water; H₂O; [7732-18-5]
(2) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]


VARIABLES:

T/K = 298

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c/mol m⁻³</th>
<th>100 ( w_r ) (compiler)</th>
<th>10⁴ ( x_r ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>9.3</td>
<td>1.68 × 10⁻²</td>
<td>1.43</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Samples of solutions of different composition were prepared by mixing the pure components at room temperature. The samples were incubated for 24 hours or longer before the water concentration was determined by Karl Fischer titration.

SOURCE AND PURITY OF MATERIALS:
(1) Distilled.
(2) Source and purity not specified.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1.0 K.
### COMPONENTS:
1. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:
- Warner, H. P.; Cohen, J. M.; Ireland, J. C.

### VARIABLES:
- \( T/K = 298 \)

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( \text{Henry’s law constant, } H/m^2 \text{ atm mol}^{-1} )</th>
<th>( 100 , w_x )</th>
<th>( 10^3 , x_x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>3.02 \times 10^{-2}</td>
<td>7.61 \times 10^{-2}</td>
<td>8.92</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The original method and apparatus for the determination of Henry's law constant, as described by Mackay et al. (ref. 1), was used. The general procedure was to add an excess quantity of tetrachloromethane to distilled deionized water, place the sample in a thermostat bath, and provide overnight mixing. A portion of this solution was returned to the stripping vessel. Tetrachloromethane 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. Source not given. Purest quality available was used without further purification. Stated purity > 99%.
2. Distilled and deionized.

**ESTIMATED ERRORS:**

- Solubility: \( \pm 6\% \) std. dev.
- Temperature: \( \pm 0.05 \) K.

**REFERENCES:**


---

### COMPONENTS:
1. Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:
- Howe, G. B.; Mullins, M. E.; Rogers, T. N.

### VARIABLES:
- \( T/K = 283 - 303 \)

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^4 , w_x )</th>
<th>( 100 , w_x )</th>
<th>( 10^3 , x_x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>104</td>
<td>1.04 \times 10^{-2}</td>
<td>1.218</td>
</tr>
<tr>
<td>20</td>
<td>146</td>
<td>1.46 \times 10^{-2}</td>
<td>1.710</td>
</tr>
<tr>
<td>30</td>
<td>105</td>
<td>1.05 \times 10^{-2}</td>
<td>1.230</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

250 ml bottles were filled with distilled and deionized water and sealed. A measured volume of tetrachloromethane was injected into the bottles through each septum using a microliter syringe. Tetrachloromethane was in excess of the anticipated solubility limit. The bottles were shaken for one hour with a wristaction shaker and allowed to equilibrate for about 3 weeks. Samples were then injected into a gas chromatograph equipped with a CarPack column and a FID detector. The GC response was compared with calibration plots.

**SOURCE AND PURITY OF MATERIALS:**

1. Source not given. Probably a commercial reagent, at least 99% purity. Used as received.
2. Distilled and deionized.

**ESTIMATED ERRORS:**

- Solubility: Not specified.
- Temperature: \( \pm 0.5 \) K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Tetrachloromethane (carbon tetrachloride); Vogel, A. I., rev. by Furniss, B. S.; et al.  

2. Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 298 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^2 \gamma \gamma )</th>
<th>( 10^4 \gamma )</th>
<th>( 100 \gamma )</th>
<th>( 100 \gamma_{M} / \text{mol g}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>8.0 × 10⁻²</td>
<td>9.38</td>
<td>5.2 × 10⁻⁴</td>
<td></td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The solubility determination was carried out in small test tubes (e.g. 100x12 mm) to permit vigorous shaking of the tetrachloromethane and water mixtures. During the experiments, 0.20 ml tetrachloromethane was added to 3.0 ml of water and agitated. The concentration of tetrachloromethane in water was analyzed by passing the sample through a chromatographic column.

**SOURCE AND PURITY OF MATERIALS:**

2. Distilled.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 1.0 K (compiler).

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Tetrachloromethane (carbon tetrachloride); Wright, D. A.; Sandler, S. I.; DeVoll, D.  

2. Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 293 - 313 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( \gamma )</th>
<th>( 10^4 \gamma )</th>
<th>( 100 \gamma )</th>
<th>( 100 \gamma_{M} / \text{mol g}^{-1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>12.200 ± 250</td>
<td>8.20</td>
<td>7.00 × 10⁻²</td>
<td>4.55 × 10⁻⁴</td>
</tr>
<tr>
<td>30</td>
<td>13.100 ± 100</td>
<td>7.63</td>
<td>6.31 × 10⁻²</td>
<td>4.23 × 10⁻⁴</td>
</tr>
<tr>
<td>40</td>
<td>13.100 ± 300</td>
<td>7.63</td>
<td>6.51 × 10⁻²</td>
<td>4.23 × 10⁻⁴</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 tetrachloromethane (\( \gamma \)) in water. Cells containing degassed water were submerged in a thermostated water bath. Tetrachloromethane was injected into the mixture cells and a magnetic stirrer was turned on. 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: See above.

Temperature: ± 0.05 K.
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) MQ-Water
Munz, C. D.

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

\[
\begin{array}{ccc}
T/°C & \text{Henry’s law constant,} & 100 \, w_i \\
      & H/dimensionless & (\text{compiler}) & 10^3 \, x_i \\
      & & (\text{compiler}) \\
20  & 0.980 & 7.80 \times 10^{-2} & 9.145 \\
\end{array}
\]

AUXILIARY INFORMATION

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

SOURCE AND PURITY OF MATERIALS:
(1) Aldrich Chemicals Co., WI, > 99.5 % pure.
(2) 0.25 mg total organic carbon per liter and 0.75 mg COD per liter.

ESTIMATED ERRORS:
Solubility: \( \pm 0.1 \times 10^{-3} \) std. dev.
Temperature: \( \pm 0.5 \) K.

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Municipal tap water (PASE)
Munz, C. D.

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

\[
\begin{array}{ccc}
T/°C & \text{Henry’s law constant,} & 100 \, w_i \\
      & H/dimensionless & (\text{compiler}) & 10^3 \, x_i \\
      & & (\text{compiler}) \\
20  & 0.958 & 7.996 \times 10^{-2} & 9.372 \\
\end{array}
\]

AUXILIARY INFORMATION

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

SOURCE AND PURITY OF MATERIALS:
(1) Aldrich Chemicals Co., WI, > 99.5 % pure.
(2) 10 mg total organic carbon per liter and 40 mg COD per liter.

ESTIMATED ERRORS:
Solubility: \( \pm 1.7 \times 10^{-2} \) std. dev.
Temperature: \( \pm 0.5 \) K.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>Liss, P. S.; Slater, P. G.</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 VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>Henry’s law constant¹, H/dimensionless</td>
</tr>
<tr>
<td>20</td>
<td>1.08</td>
</tr>
</tbody>
</table>

¹ Obtained from (mass(1) cm³(air)/mass(1) cm³(seawater)).

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>METHOD/APPARATUS/PROCEDURE:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Source and purity not given.</td>
</tr>
<tr>
<td>Samples from Atlantic.</td>
</tr>
</tbody>
</table>

<table>
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<th>ESTIMATED ERRORS:</th>
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<tbody>
<tr>
<td>Salinity: Not specified.</td>
</tr>
<tr>
<td>Temperature: ± 0.5 K (compiler).</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>REFERENCES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Lovelock, J. E. <em>Personal communication.</em></td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>Balls, P. W.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 283 - 298</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>Henry’s law constant, H/dimensionless</td>
</tr>
<tr>
<td>10</td>
<td>0.82 ± 0.01</td>
</tr>
<tr>
<td>15</td>
<td>0.95 ± 0.10</td>
</tr>
<tr>
<td>20</td>
<td>1.21 ± 0.04</td>
</tr>
<tr>
<td>25</td>
<td>1.43 ± 0.05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
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</table>

<table>
<thead>
<tr>
<th>METHOD/APPARATUS/PROCEDURE:</th>
</tr>
</thead>
<tbody>
<tr>
<td>The method involved repeated equilibrations of nitrogen with a water sample containing tetrachloromethane. The sample was shaken vigorously at the required temperature in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph. The experiments were performed at least three times at 10, 15, 20, and 25°C, each experiment involving about six equilibrations.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Source and purity not given.</td>
</tr>
<tr>
<td>(2) Salinity = 20 %.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ESTIMATED ERRORS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility: See above.</td>
</tr>
<tr>
<td>Temperature: ± 0.5 K (compiler).</td>
</tr>
</tbody>
</table>
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Seawater

ORIGINAL MEASUREMENTS:
Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S. 

VARIABLES:

\[ T/K = 278 - 306 \]

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, ( H/dimensionless )</th>
<th>100 ( w_t ) (compiler)</th>
<th>10⁵ ( x_t ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>0.7100</td>
<td>5.596 \times 10^{-2}</td>
<td>6.557</td>
</tr>
<tr>
<td>10</td>
<td>0.8716</td>
<td>5.759 \times 10^{-2}</td>
<td>6.748</td>
</tr>
<tr>
<td>15</td>
<td>1.0624</td>
<td>5.911 \times 10^{-2}</td>
<td>6.927</td>
</tr>
<tr>
<td>20</td>
<td>1.2863</td>
<td>6.049 \times 10^{-2}</td>
<td>7.088</td>
</tr>
<tr>
<td>25</td>
<td>1.5473</td>
<td>6.180 \times 10^{-2}</td>
<td>7.242</td>
</tr>
<tr>
<td>33</td>
<td>2.0536</td>
<td>6.625 \times 10^{-2}</td>
<td>7.763</td>
</tr>
</tbody>
</table>

The Henry's law constants \( H \) were derived from the best-fit lines of van't Hoff plots:

\[
\log_e H = - \frac{3230}{T(K)} + 11.27
\]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The multiple equilibrium technique was used to measure the Henry's law constant \( (H) \) as described by McAuliffe (ref. 1). A known volume of seawater in a syringe was shaken with a known volume of tetrachloromethane. After equilibration, the headspace was separated and analyzed for tetrachloromethane. A gas chromatograph with an electron capture detector was used for the analysis.

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.
(2) Samples from 48° N to 65° S in the Atlantic in late 1981.

ESTIMATED ERRORS:

Solubility: ± 5.5 % std. dev.
Temperature: ± 0.2 K.

REFERENCES:

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Calcium chloride; CaCl₂; [10043-52-4]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Liu, J.-L.; Huang, T.-C.
*Scientia Sinica (Peking)* 1961, 10, 700-10.

VARIABLES:

<table>
<thead>
<tr>
<th>rijk</th>
<th>Concentration</th>
</tr>
</thead>
</table>

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>cₐ/mol dm⁻³</th>
<th>ρ/µg m⁻³</th>
<th>100 wₐ (compiler)</th>
<th>10⁻⁵ xₐ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.205</td>
<td>0.652</td>
<td>6.41 × 10⁻¹</td>
<td>7.66</td>
</tr>
<tr>
<td></td>
<td>0.280</td>
<td>0.598</td>
<td>5.85 × 10⁻¹</td>
<td>7.03</td>
</tr>
<tr>
<td></td>
<td>0.333</td>
<td>0.565</td>
<td>5.49 × 10⁻¹</td>
<td>6.64</td>
</tr>
<tr>
<td></td>
<td>0.581</td>
<td>0.452</td>
<td>4.29 × 10⁻¹</td>
<td>5.31</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of aqueous solution. The flask was rotated in a thermostat bath until equilibrium was established. The optical densities of different concentration of tetrachloromethane in the aqueous solutions were measured using water as the reference liquid. Duplicate experiments were made and the results averaged. The absorption spectra of tetrachloromethane in aqueous calcium chloride solutions were determined using a Hilger spectrophotometer.

SOURCE AND PURITY OF MATERIALS:
(1) Peking Chemical Factory, further purified by washing with H₂SO₄, NaOH and water; dried over CaCl₂ and fractionated.
(2) Peking Chemical Factory, recrystallized twice before use.
(3) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Hydrogen chloride; HCl; [7647-01-0]
(3) Water; H₂O; [7732-18-5]

VARIABLES:
\( T/K = 288 - 333 \)
Concentration

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>Concentration of HCl, ( 100 , \text{w}_2 )</th>
<th>( t/°C )</th>
<th>1000 ( w_i )</th>
<th>100 ( w_i ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>15</td>
<td>1.00</td>
<td>1.00 × 10¹</td>
<td>12.35</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>0.55</td>
<td>5.5 × 10²</td>
<td>6.79</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>0.30</td>
<td>3.0 × 10²</td>
<td>3.70</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>0.18</td>
<td>1.8 × 10²</td>
<td>2.22</td>
</tr>
<tr>
<td>20</td>
<td>15</td>
<td>1.25</td>
<td>1.25 × 10¹</td>
<td>16.31</td>
</tr>
<tr>
<td></td>
<td>30</td>
<td>0.74</td>
<td>7.4 × 10²</td>
<td>9.65</td>
</tr>
<tr>
<td></td>
<td>45</td>
<td>0.40</td>
<td>4.0 × 10²</td>
<td>5.21</td>
</tr>
<tr>
<td></td>
<td>60</td>
<td>0.23</td>
<td>2.3 × 10²</td>
<td>3.00</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The dynamic method was used for the determination of solubility. It involved the saturation of nitrogen with tetrachloromethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of the aqueous solution. After 2 - 3 hours the solution became saturated and samples were taken periodically (ref. 1). The concentration of tetrachloromethane in the aqueous solution was determined by gas chromatography. On average 3 - 5 measurements were taken at each temperature.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled (compiler)

ESTIMATED ERRORS:
Solubility: ± 15 %.
Temperature: ± 0.05 K.

REFERENCES:
(1) Treger, Yu. A.; Flid, R. M.; Spector, S. S. 
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Lithium chloride; LiCl; [7447-41-8]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Liu, J.-L.; Huang, T.-C.
Scienit Sinica (Peking) 1961, 10, 700-10.

VARIABLES:
\[ T/K = 293 \]
Concentration

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( c_r \text{mol dm}^{-3} )</th>
<th>( \rho_r/\text{kg m}^{-3} )</th>
<th>( 100 \text{ ( w_1 )} ) (compiler)</th>
<th>( 10^5 x_l ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.1867</td>
<td>0.717</td>
<td>7.13 ( \times 10^{-2} )</td>
<td>8.389</td>
</tr>
<tr>
<td></td>
<td>0.3496</td>
<td>0.696</td>
<td>6.86 ( \times 10^{-2} )</td>
<td>8.108</td>
</tr>
<tr>
<td></td>
<td>0.4352</td>
<td>0.676</td>
<td>6.69 ( \times 10^{-2} )</td>
<td>7.924</td>
</tr>
<tr>
<td></td>
<td>0.7015</td>
<td>0.644</td>
<td>6.33 ( \times 10^{-2} )</td>
<td>7.541</td>
</tr>
<tr>
<td></td>
<td>0.9765</td>
<td>0.609</td>
<td>5.94 ( \times 10^{-2} )</td>
<td>7.130</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of aqueous solution. The flask was rotated in a thermostatic bath until the equilibrium was established. The optical densities of different concentrations of tetrachloromethane in the aqueous solution were measured using water as the reference liquid. Duplicate experiments were done and the results averaged. The absorption spectra of tetrachloromethane in aqueous lithium chloride solutions were determined using a Hilger spectrophotometer.

PREPARED BY:
A. L. Horvath

SOURCE AND PURITY OF MATERIALS:
(1) Peking Chemical Factory, further purified by washing with \( \text{H}_2\text{SO}_4 \), NaOH and water; dried over CaCl₂ and fractionated.
(2) Merck reagent, mixed with HCl and re-crystallized.
(3) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( \pm 0.5 \text{ K} \) (compiler).
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Magnesium sulfate; MgSO₄; [7487-88-9]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Gross, P. M.

VARIABLES:
T/K = 298
One concentration

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c₀/mol dm⁻³</th>
<th>100 p₀/g</th>
<th>100 w₀ (compiler)</th>
<th>10⁴ x₀ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.5</td>
<td>4.8 × 10⁻²</td>
<td>4.8 × 10⁻²</td>
<td>5.93</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A mixture of 10 to 20 ml tetrachloromethane in 500 ml of an aqueous solution of MgSO₄ was placed in a water thermostat bath. The sample container was placed on a shaker and agitated until no more liquid droplets remained undissolved. One or more samples were syphoned out and the concentration of tetrachloromethane was determined using a Zeiss water interferometer.

SOURCE AND PURITY OF MATERIALS:
(1) Source not given. Commercial reagent, fractionally distilled before use.
(2) Kahlbaum chemical, certified grade.
(3) Distilled.

ESTIMATED ERRORS:
Solubility: ± 5 %.
Temperature: ± 0.01 K.

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Magnesium sulfate; MgSO₄; [7487-88-9]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Liu, J.-L.; Huang, T.-C.
Scienza Sinica (Peking) 1961, 10, 700-10.

VARIABLES:
T/K = 298
Concentration

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c₀/mol dm⁻³</th>
<th>ρ₀/kg m⁻³</th>
<th>100 w₀ (compiler)</th>
<th>10⁴ x₀ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.199</td>
<td>0.637</td>
<td>6.21 × 10⁻²</td>
<td>7.429</td>
</tr>
<tr>
<td></td>
<td>0.318</td>
<td>0.572</td>
<td>5.50 × 10⁻²</td>
<td>6.662</td>
</tr>
<tr>
<td></td>
<td>0.433</td>
<td>0.522</td>
<td>4.97 × 10⁻²</td>
<td>6.094</td>
</tr>
<tr>
<td></td>
<td>0.537</td>
<td>0.487</td>
<td>4.58 × 10⁻²</td>
<td>5.679</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of aqueous solution. The flask was rotated in a thermostat bath until equilibrium was established. The optical densities of different concentration of tetrachloromethane in the aqueous solutions were measured using water as the reference liquid. Duplicate experiments were made and the results averaged. The absorption spectra of tetrachloromethane in aqueous magnesium sulfate solutions were determined using a Hilger spectrophotometer.

SOURCE AND PURITY OF MATERIALS:
(1) Peking Chemical Factory, further purified by washing with H₂SO₄, NaOH and water; dried over CaCl₂ and fractionated.
(2) Peking Chemical Factory, recrystallized twice before use.
(3) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
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<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>Gross, P. M.</td>
</tr>
<tr>
<td>(3) 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>
<tr>
<td>One concentration</td>
<td></td>
</tr>
</tbody>
</table>

<table>
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<tr>
<th>EXPERIMENTAL VALUES:</th>
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<tbody>
<tr>
<td>t/°C</td>
<td>c_i/mol dm⁻³</td>
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<tr>
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<td>---</td>
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<table>
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<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
<td>SOURCE AND PURITY OF MATERIALS:</td>
</tr>
<tr>
<td>An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of aqueous solution. The flask was rotated in a thermostat bath until equilibrium was established. The optical densities of different concentration of tetrachloromethane in the aqueous solutions were measured using water as the reference liquid. Duplicate experiments were made and the results averaged. The absorption spectra of tetrachloromethane in aqueous potassium chloride solutions were determined using a Hilger spectrophotometer.</td>
<td>(1) Source not given. Commercial reagent, fractionally distilled before use.</td>
</tr>
<tr>
<td></td>
<td>(2) Kahlbaum chemical, certified grade.</td>
</tr>
<tr>
<td></td>
<td>(3) Distilled.</td>
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<td>Solubility: ± 5 %.</td>
<td>Temperature: ± 0.01 K.</td>
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<tr>
<td>(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]</td>
<td>Liu, J.-L.; Huang, T.-C.</td>
</tr>
<tr>
<td>(3) Water; H₂O; [7732-18-5]</td>
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<table>
<thead>
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<th>VARIABLES:</th>
<th>PREPARED BY:</th>
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</thead>
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<tr>
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<td>A. L. Horvath</td>
</tr>
<tr>
<td>Concentration</td>
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<td>c_i/mol dm⁻³</td>
</tr>
<tr>
<td>---</td>
<td>---</td>
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<tr>
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<table>
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<tbody>
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<td>SOURCE AND PURITY OF MATERIALS:</td>
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<td></td>
<td>(1) Peking Chemical Factory, further purified by washing with H₂SO₄,NaOH and water; dried over CaCl₂ and fractionated.</td>
</tr>
<tr>
<td></td>
<td>(2) Peking Chemical Factory, recrystallized twice before use.</td>
</tr>
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<td>(3) Distilled.</td>
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<table>
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<td>Temperature: ± 0.5 K (compiler).</td>
</tr>
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<td></td>
</tr>
</tbody>
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### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Potassium hydroxide; KOH; [1310-58-3]
(3) Water; H₂O; [7732-18-5]

### VARIABLES:

T/K = 333
One concentration

### EXPERIMENTAL VALUES:

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<th>ρ_j/kg m⁻³</th>
<th>100 w_j (compiler)</th>
<th>10⁶ x_j (compiler)</th>
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</thead>
<tbody>
<tr>
<td>60</td>
<td>1.0</td>
<td>0.2</td>
<td>1.98 × 10⁻²</td>
<td>2.41</td>
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</tbody>
</table>

### SOURCE AND PURITY OF MATERIALS:

(1) Prepared in the authors' laboratory; purified by fractional distillation before use.
(2) Source and purity not given.
(3) Distilled.

### ESTIMATED ERRORS:

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

---

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Potassium sulfate; K₂SO₄; [7778-80-5]
(3) Water; H₂O; [7732-18-5]

### VARIABLES:

T/K = 298
Concentration

### EXPERIMENTAL VALUES:

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<th>100 w_j (compiler)</th>
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</thead>
<tbody>
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<tr>
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<td>0.3150</td>
<td>0.544</td>
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<td></td>
<td>0.3518</td>
<td>0.507</td>
<td>4.84 × 10⁻²</td>
<td>6.001</td>
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</table>

### SOURCE AND PURITY OF MATERIALS:

(1) Prepared in the authors' laboratory; purified by fractional distillation before use.
(2) Source and purity not given.
(3) Distilled.

### ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Potassium sulfate; K₂SO₄; [7778-80-5]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Liu, J.-L.; Huang, T.-C.
*Scientia Sinica (Peking)* 1961, 10, 700-10.

VARIABLES:

\[ T/K = 298 \]
Concentration

EXPERIMENTAL VALUES: (continued)

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<tr>
<th>( t/°C )</th>
<th>( c_s/\text{mol dm}^{-3} )</th>
<th>( \rho_s/\text{kg m}^{-3} )</th>
<th>100 ( w_s ) (compiler)</th>
<th>10⁵ ( x_s ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>25</td>
<td>0.4516</td>
<td>0.464</td>
<td>4.37 \times 10^{-2}</td>
<td>5.509</td>
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<tr>
<td></td>
<td>0.5177</td>
<td>0.430</td>
<td>4.02 \times 10^{-2}</td>
<td>5.124</td>
</tr>
<tr>
<td></td>
<td>0.6034</td>
<td>0.388</td>
<td>3.60 \times 10^{-2}</td>
<td>4.657</td>
</tr>
</tbody>
</table>

COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Liu, J.-L.; Huang, T.-C.
*Scientia Sinica (Peking)* 1961, 10, 700-10.

VARIABLES:

\[ T/K = 298 \]
Concentration

EXPERIMENTAL VALUES:

<table>
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<th>( t/°C )</th>
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<th>( \rho_s/\text{kg m}^{-3} )</th>
<th>100 ( w_s ) (compiler)</th>
<th>10⁵ ( x_s ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.2549</td>
<td>0.690</td>
<td>6.84 \times 10^{-2}</td>
<td>8.099</td>
</tr>
<tr>
<td></td>
<td>0.5025</td>
<td>0.642</td>
<td>6.30 \times 10^{-2}</td>
<td>7.536</td>
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<tr>
<td></td>
<td>0.6375</td>
<td>0.616</td>
<td>6.01 \times 10^{-2}</td>
<td>7.229</td>
</tr>
<tr>
<td></td>
<td>0.8383</td>
<td>0.578</td>
<td>5.58 \times 10^{-2}</td>
<td>6.768</td>
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<tr>
<td></td>
<td>0.9623</td>
<td>0.553</td>
<td>5.32 \times 10^{-2}</td>
<td>6.486</td>
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<td></td>
<td>1.0250</td>
<td>0.541</td>
<td>5.19 \times 10^{-2}</td>
<td>6.344</td>
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</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of aqueous solution. The flask was rotated in a thermostat bath until equilibrium was established. The optical densities of different concentration of tetrachloromethane in the aqueous solutions were measured using water as the reference liquid. Duplicate experiments were made and the results averaged. The absorption spectra of tetrachloromethane in aqueous sodium chloride solutions were determined using a Hilger spectrophotometer.

SOURCE AND PURITY OF MATERIALS:
(1) Peking Chemical Factory, further purified by washing with H₂SO₄, NaOH and water; dried over CaCl₂ and fractionated.
(2) Peking Chemical Factory, analytical grade.
(3) Distilled.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl₄; [56-23-5]
(2) Sodium sulfate; Na₂SO₄; [7757-82-6]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Liu, J.-L.; Huang, T.-C.
*Scientia Sinica (Peking)* 1961, 10, 700-10.

VARIABLES:
\( T/k = 298 \)
Concentration

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( c_y / \text{mol dm}^{-3} )</th>
<th>( \rho_y / \text{kg m}^{-3} )</th>
<th>( 100 \omega_y ) (compiler)</th>
<th>( 10^3 \chi_y ) (compiler)</th>
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<tbody>
<tr>
<td>25</td>
<td>0.130</td>
<td>0.657</td>
<td>( 6.47 \times 10^2 )</td>
<td>7.706</td>
</tr>
<tr>
<td>0.230</td>
<td>0.593</td>
<td>( 5.76 \times 10^2 )</td>
<td>6.948</td>
<td></td>
</tr>
<tr>
<td>0.380</td>
<td>0.491</td>
<td>( 4.69 \times 10^2 )</td>
<td>5.767</td>
<td></td>
</tr>
<tr>
<td>0.464</td>
<td>0.450</td>
<td>( 4.26 \times 10^2 )</td>
<td>5.296</td>
<td></td>
</tr>
<tr>
<td>0.564</td>
<td>0.401</td>
<td>( 3.75 \times 10^2 )</td>
<td>4.726</td>
<td></td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An accurate amount of tetrachloromethane was transferred into an Erlenmeyer flask containing a weighed amount of aqueous solution. The flask was rotated in a thermostat bath until equilibrium was established. The optical densities of different concentration of tetrachloromethane in the aqueous solutions were measured using water as the reference liquid. Duplicate experiments were made and the results averaged. The absorption spectra of tetrachloromethane in aqueous sodium sulfate solutions were determined using a Hilger spectrophotometer.

SOURCE AND PURITY OF MATERIALS:
(1) Peking Chemical Factory, further purified by washing with H₂SO₄, NaOH and water; dried over CaCl₂ and fractionated.
(2) Peking Chemical Factory, recrystallized twice before use.
(3) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( \pm 0.5 \) K (compiler).
COMPONENTS:

(1) Water-$d_2$; D$_2$O; [7789-20-0]
(2) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

ORIGINAl MEASUREMENTS:

Hutchison, C. A.; Lyon, A. M.
_Columbia University Report A-745, July 1, 1943._

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$100 w_i M_i/mol g$</th>
<th>$100 w_i$ (compiler)</th>
<th>$10^4 x_i$ (compiler)</th>
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<tbody>
<tr>
<td>25</td>
<td>$4.78 \times 10^{-4}$</td>
<td>$9.57 \times 10^{-3}$</td>
<td>7.34</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 1 to 15 volume ratio mixture of heavy water and tetrachloromethane was introduced into an equilibration flask and then lowered into the water thermostat bath. The assembly was shaken mechanically for about 90 minutes at constant temperature. The amount of heavy water in the organic phase was determined by a modified Karl Fischer titration method. The determinations were done in triplicate. The description was taken from a secondary source (ref. 1). The original report is not available from Columbia University.

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.
(2) Source not given. Purified and dried before use.

ESTIMATED ERRORS:

Solubility: $\pm 0.1 \times 10^{-3}$ avg. dev.  
Temperature: $\pm 0.05$ K.

REFERENCES:


COMPONENTS:

(1) Water-$d_2$; D$_2$O; [7789-20-0]
(2) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$10^3 g_i/g_2$</th>
<th>$100 w_i$ (compiler)</th>
<th>$10^4 x_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>9</td>
<td>$0.9 \times 10^{-2}$</td>
<td>6.9</td>
</tr>
</tbody>
</table>

The isotope dilution technique was used. It involved the mixing of about 100 cm$^3$ tetrachloromethane with 1 cm$^3$ heavy water in a volumetric flask which was then inserted into a constant temperature bath. The mixture was agitated for 15 minutes to ensure the equilibrium between the two phases. The radioactivity of the samples were determined by a liquid scintillation counting procedure.

SOURCE AND PURITY OF MATERIALS:

(1) Received from pile EL 3 of Saclay, contained traces of tritium.
(2) Source not given, commercial grade.

ESTIMATED ERRORS:

Solubility: $\pm 0.4 \times 10^{-3}$ g.
Temperature: $\pm 1$ K (compiler).
**COMPONENTS:**

(1) Water-$d_2$; D$_2$O; [7789-20-0]

(2) Tetrachloromethane (carbon tetrachloride); CCl$_4$; [56-23-5]

**VARIABLES:**

$\frac{T}{K} = 288 - 308$

**EXPERIMENTAL VALUES:**

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<th>$t/°C$</th>
<th>$c_t$/mol m$^{-3}$</th>
<th>$100 w_t$ (compiler)</th>
<th>$10^4 x_t$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>5.7 ± 0.1</td>
<td>0.713 × 10$^2$</td>
<td>5.47</td>
</tr>
<tr>
<td>25</td>
<td>7.5 ± 0.2</td>
<td>0.949 × 10$^2$</td>
<td>7.28</td>
</tr>
<tr>
<td>30</td>
<td>8.4 ± 0.3</td>
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<td>8.21</td>
</tr>
<tr>
<td>35</td>
<td>10.3 ± 0.3</td>
<td>1.32 × 10$^2$</td>
<td>10.13</td>
</tr>
</tbody>
</table>

**ORIGINAL MEASUREMENTS:**

Glasoe, P. K.; Schultz, S. D.


**PREPARED BY:**

A. L. Horvath

**ORIGINAL MEASUREMENTS:**

Glasoe, P. K.; Schultz, S. D.


**PREPARED BY:**

A. L. Horvath

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The saturation of heavy water with tetrachloromethane was done in a closed system, protected from atmospheric moisture, and placed in a constant temperature water bath. The solubility of heavy water in tetrachloromethane was measured using the Karl Fischer titration method with a "dead stop" end-point determination (ref. 1). 15 Trials were done at each temperature.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source not given, 99.8 % pure, used as received.

(2) Source not given. Reagent grade, purified by distillation before use.

**ESTIMATED ERRORS:**

Solubility: See above.

Temperature: ± 0.1 K (compiler).

**REFERENCES:**

COMPONENTS:
(1) Bromodichloromethane; CHBrCl₂; [75-27-4]
(2) Water; H₂O; [77-32-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
January 1993.

CRITICAL EVALUATION:

All the available solubility data for bromodichloromethane (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 values are the more reliable. Further studies will be necessary before even tentative values can be assigned. Even so, it may be observed that the solubility trend for halogenated hydrocarbon - water systems, as presented in the Preface, provided some support for the mass per cent (1) value, 100 \( w_i \), of 1.618 at 298.15 K (ref. 1).

Table 1. Reported Solubility of Bromodichloromethane (1) in Water (2)

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Reported Solubility 100 ( w_i )</th>
<th>10^3 ( x_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.099 (ref. 4)</td>
<td>2.352 (ref. 4)</td>
</tr>
<tr>
<td>24.85</td>
<td>1.821 (ref. 5)</td>
<td>2.035 (ref. 5)</td>
</tr>
<tr>
<td>25</td>
<td>1.618 (ref. 1)</td>
<td>1.805 (ref. 1)</td>
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<tr>
<td>30</td>
<td>0.3023 (ref. 2), 0.2972 (ref. 3)</td>
<td>0.3333 (ref. 2), 0.3277 (ref. 3)</td>
</tr>
</tbody>
</table>

REFERENCES:

3. Ibid., 1984, 284, 105.
<table>
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<tr>
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<th>ORIGINAL MEASUREMENTS:</th>
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<tr>
<td>(1) Bromodichloromethane; CHBrCl₂; [75-27-4]</td>
<td>Symons, J. M.; et al.</td>
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<th>VARIABLES:</th>
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<tr>
<td>77K = 298</td>
<td>A. L. Horvath</td>
</tr>
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<thead>
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<th>EXPERIMENTAL VALUES:</th>
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<tr>
<td>t/°C</td>
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<th>METHOD/APPARATUS/PROCEDURE:</th>
<th>SOURCE AND PURITY OF MATERIALS:</th>
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<tr>
<td>(2) Cincinnati tap water.</td>
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<td>Temperature: $\pm 0.5$ K.</td>
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<tr>
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<tbody>
<tr>
<td>(1) Bromodichloromethane; CHBrCl₂; [75-27-4]</td>
<td>McNally, M. E.; Grob, R. L.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>77K = 303</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>30</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>METHOD/APPARATUS/PROCEDURE:</th>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard solutions were prepared in 100 ml flasks. They were shaken for 5 minutes and then allowed to equilibrate in a constant temperature bath held at 30°C for 24 hours. Samples were pipetted in headspace vials, sealed, thermostated and then examined by the gas chromatographic head space analysis technique. An F. &amp; M. Model 402 gas chromatograph equipped with dual columns and dual flame-ionization detectors was used.</td>
<td>(1) Chemical Service, West Chester, PA., purest grade available.</td>
</tr>
<tr>
<td>(2) Distilled and run through two Barnstead purification cartridges.</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ESTIMATED ERRORS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility: $\pm 150$ ppm std. dev.</td>
</tr>
<tr>
<td>Temperature: $\pm 0.5$ K (compiler).</td>
</tr>
<tr>
<td>COMPONENTS:</td>
</tr>
<tr>
<td>------------</td>
</tr>
<tr>
<td>(1) Bromodichloromethane; CHBrCl₂; [75-27-4]</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>
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<tr>
<th>EXPERIMENTAL VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>30</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

Standard bromodichloromethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere (ref. 1). The aqueous organic liquid phase was 25 ml and the vapor phase above the mixture was 35 ml. 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 5 measurements.

**SOURCE AND PURITY OF MATERIALS:**

(1) Chemical Service, West Chester, P.A., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

**ESTIMATED ERRORS:**

Solubility: ± 7.12 % std. dev.
Temperature: ± 0.5 K (compiler).

**REFERENCES:**


<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Bromodichloromethane; CHBrCl₂; [75-27-4]</td>
<td>Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.</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 VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>-------</td>
</tr>
<tr>
<td>20</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow was maintained. Samples of the solution being stripped were taken for analysis. After extraction of the sample, the extracts were analyzed by a gas chromatograph equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: ± 0.2 × $10^3$ std. dev.
Temperature: ± 0.1 K.

**REFERENCES:**

COMPONENTS:
(1) Bromodichloromethane; CHBrCl₂; [75-27-4]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Warner, H. P.; Cohen, J. M.; Ireland, J. C.

VARIABLES:

\[ T/k = 298 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m³ atm mol⁻¹ )</th>
<th>( 100 w_r ) (compiler)</th>
<th>( 10^3 x_r ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>2.12 ( \times 10^3 )</td>
<td>1.821</td>
<td>2.036</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The original method and apparatus for the determination of Henry's law constants, described by Mackay et al. (ref. 1), were used. The general procedure was to add an excess quantity of bromodichloromethane to distilled deionized water and mix the system overnight. A portion of the solution was returned to the stripping vessel. Bromodichloromethane 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) Source not given. Purest quality available and was used without further purification, stated purity > 99 %.
(2) Distilled and deionized.

ESTIMATED ERRORS:
Solubility: \( \pm 6 \% \) std. dev.
Temperature: \( \pm 0.05 \) K.

REFERENCES:

COMPONENTS:
(1) Bromodichloromethane; CHBrCl₂; [75-27-4]
(2) Milang water

ORIGINAL MEASUREMENTS:

VARIABLES:

\[ T/k = 293 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m³ atm mol⁻¹ )</th>
<th>( 100 w_r ) (compiler)</th>
<th>( 10^3 x_r ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.6 ( \times 10^3 )</td>
<td>2.099</td>
<td>2.353</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow was maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) \( pH = 8.4, 700 \) mg salt/dm³, 140 mg CaCO₃/dm³, 13 mg organic carbon/dm³, 110 mg suspended solid/dm³.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( \pm 0.1 \) K.

REFERENCES:
### Components

1. Bromodichloromethane; CHBrCl₂; [75-27-4]
2. Myponga water

### Original Measurements

Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.

### Variables

\[ T/K = 293 \]

### Experimental Values

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 100 \ \rho )</th>
<th>( 10^3 \chi )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 1.5 \times 10^{-3} )</td>
<td>2.239</td>
<td>2.515</td>
</tr>
</tbody>
</table>

#### Auxiliary Information

**Method/Apparatus/Procedure:**

The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed using a gas chromatograph equipped with a capillary column.

### Source and Purity of Materials

1. Source and purity not given.
2. \( \rho = 7.6, 570 \text{ mg salt/dm}^3, 60 \text{ mg CaCO}_3/dm^3, 10 \text{ mg organic carbon/dm}^3 \).

### Estimated Errors

Solubility: Not specified.
Temperature: ± 0.1 K.

### References

COMPONENTS:
(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]
(2) Water; H₂O; [7732-18-5]

CRITICAL EVALUATION:

All the available solubility data for dibromochloromethane (1) in water (2) are summarized in Table 1. The data are in very poor agreement. Considerable discrepancies exist even between the two solubility values reported by the same workers, compare (ref. 2) and (ref. 3). In the absence of further independent studies, it is not possible to determine which value is the more reliable. Additional investigations will be necessary before even tentative values can be assigned. Even so, it may be noted that the solubility trend for halogenated hydrocarbon - water systems, as presented in the Preface, provided some support for the mass per cent (1) value, 100 w₁, of 0.8124 at 298.15 K (ref. 1).

Table 1. Reported Solubility of Dibromochloromethane (1) in Water (2)

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w₁</th>
<th>10⁴ x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.3040 (ref. 6)</td>
<td>2.637 (ref. 6)</td>
</tr>
<tr>
<td>20</td>
<td>0.6320 (ref. 4),</td>
<td>5.498 (ref. 4),</td>
</tr>
<tr>
<td></td>
<td>0.2375 (ref. 6)</td>
<td>2.059 (ref. 6)</td>
</tr>
<tr>
<td>24.85</td>
<td>1.423 (ref. 5)</td>
<td>12.470 (ref. 5)</td>
</tr>
<tr>
<td>25</td>
<td>0.8124 (ref. 1)</td>
<td>7.079 (ref. 1)</td>
</tr>
<tr>
<td>30</td>
<td>0.1049 (ref. 2),</td>
<td>0.9082 (ref. 2),</td>
</tr>
<tr>
<td></td>
<td>0.2514 (ref. 3)</td>
<td>2.179 (ref. 3)</td>
</tr>
<tr>
<td></td>
<td>0.3132 (ref. 6)</td>
<td>2.7168 (ref. 6)</td>
</tr>
</tbody>
</table>

REFERENCES:

3. Ibid., 1984, 284, 105.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]</td>
<td>Symons, J. M. <em>et al.</em></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 VALUES:</th>
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<tbody>
<tr>
<td>t/°C</td>
<td>Henry’s law constant</td>
</tr>
<tr>
<td></td>
<td>$H/\text{dimensionless}$</td>
</tr>
<tr>
<td>25</td>
<td>$3.5 \times 10^2$</td>
</tr>
<tr>
<td></td>
<td>$100 , w_i$ (compiler)</td>
</tr>
<tr>
<td></td>
<td>$10^4 , x_i$ (compiler)</td>
</tr>
<tr>
<td></td>
<td>0.8124</td>
</tr>
<tr>
<td></td>
<td>7.080</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
Details are given elsewhere (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**
(1) Source and purity not given.
(2) Cincinnati tap water.

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: $\pm 0.5 \, \text{K}$.

**REFERENCES:**

---

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]</td>
<td>McNally, M. E.; Grob, R. L.</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>
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<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>$10^6 , w_i$</td>
</tr>
<tr>
<td>30</td>
<td>1049.9</td>
</tr>
<tr>
<td></td>
<td>$100 , w_i$ (compiler)</td>
</tr>
<tr>
<td></td>
<td>$10^5 , x_i$ (compiler)</td>
</tr>
<tr>
<td></td>
<td>0.1049</td>
</tr>
<tr>
<td></td>
<td>9.081</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
Standard solutions were prepared in 100 cm³ flasks. They were shaken for 5 minutes and then allowed to equilibrate in a constant-temperature bath held at 30°C for 24 hours. Samples were pipetted into headspace vials, sealed, thermostated, and then examined by the gas chromatographic head space analysis technique. An F. & M. Model 402 gas chromatograph equipped with dual columns and dual flame ionization detectors was used.

**SOURCE AND PURITY OF MATERIALS:**
(1) Chemical Service, West Chester, PA., USA., purest grade available as received.
(2) Distilled and run through two Barnstead purification cartridges.

**ESTIMATED ERRORS:**
Solubility: $\pm 36.4 \, \text{ppm std. dev.}$
Temperature: $\pm 0.5 \, \text{K}$ (compiler).
## COMPONENTS: ORIGINAL MEASUREMENTS:

<table>
<thead>
<tr>
<th>Components</th>
<th>Original Measurements</th>
</tr>
</thead>
</table>
| (1) Dibromochloromethane; CHBr₂Cl; [124-48-1] | McNally, M. E.; Grob, R. L.  
*J. Chromatogr. 1984, 284, 105-16.* |
| (2) Water; H₂O; [7732-18-5] | |

## VARIABLES:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
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<tr>
<td>T/K</td>
<td>303</td>
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## EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t°C</th>
<th>8V₁/g m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>30</td>
<td>2509</td>
<td>0.2514</td>
<td>2.179</td>
</tr>
</tbody>
</table>

## AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

Standard dibromochloromethane solutions of increasing concentration were prepared in volumetric flasks as described elsewhere (ref. 1). The aqueous organic liquid phase was 25 ml and the vapor phase above the mixture was 35 ml. 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 5 measurements.

### SOURCE AND PURITY OF MATERIALS:

<table>
<thead>
<tr>
<th>Source and Purity</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>Chemical Service, West Chester, PA., USA, purest grade available.</td>
</tr>
<tr>
<td>(2)</td>
<td>Distilled and run through two Barnstead purification cartridges.</td>
</tr>
</tbody>
</table>

### ESTIMATED ERRORS:

| Solubility | ± 3.47 % std. dev. |
| Temperature | ± 0.5 K (compiler) |

### REFERENCES:

(1) McNally, M. E.; Grob, R. L. *J. Chromatogr. 1984, 284, 105-16.*

---

## COMPONENTS: ORIGINAL MEASUREMENTS:

<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:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K</td>
<td>293</td>
</tr>
</tbody>
</table>

## EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>Henry's law constant, H/m² atm mol⁻¹</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8.7 × 10⁻⁴</td>
<td>0.6320</td>
<td>5.498</td>
</tr>
</tbody>
</table>

## AUXILIARY INFORMATION

### METHOD/APPARATUS/PROCEDURE:

The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

### SOURCE AND PURITY OF MATERIALS:

<table>
<thead>
<tr>
<th>Source and Purity</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1)</td>
<td>Source and purity not given.</td>
</tr>
<tr>
<td>(2)</td>
<td>Distilled and deionized.</td>
</tr>
</tbody>
</table>

### ESTIMATED ERRORS:

| Solubility | ± 0.2 × 10⁻⁴ std. dev. |
| Temperature | ± 0.1 K |

### REFERENCES:

COMPONENTS:  
(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]  
(2) Water; H₂O; [7732-18-5]  

ORIGINAL MEASUREMENTS:  
Warner, H. P.; Cohen, J. M.; Ireland, J. C.  

VARIABLES:  
T/K = 298

EXPERIMENTAL VALUES:  
\[ t/°C \quad \text{Henry's law constant,}\  
\frac{H/m² \text{ atm mol}^1}{100 w_i} \quad 10^3 x_i \]  

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^4 w_i (compiler)</th>
<th>10^3 x_i (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>7.83 \times 10^{-4}</td>
<td>1.423</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:  
The original method and apparatus for the determination of Henry's law constants, described by Mackay _et al._ (ref. 1), were used. The general procedure was to add an excess quantity of dibromochloromethane to distilled deionized water and mix the system overnight. A portion of the solution was returned to the stripping vessel. Dibromochloromethane was stripped isothermally from the solution at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

SOURCE AND PURITY OF MATERIALS:  
(1) Purest quality available, > 99 % pure, used as received.  
(2) Distilled and deionized.

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

REFERENCES:  

COMPONENTS:  
(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]  
(2) Water; H₂O; [7732-18-5]

VARIABLES:  
T/K = 283 - 303

EXPERIMENTAL VALUES:  
\[ t/°C \quad 10^4 w_i \quad 100 w_i (compiler) \quad 10^3 x_i (compiler) \]  

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^4 w_i</th>
<th>100 w_i (compiler)</th>
<th>10^3 x_i (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3040</td>
<td>0.3040</td>
<td>2.6368</td>
</tr>
<tr>
<td>20</td>
<td>2375</td>
<td>0.2375</td>
<td>2.0587</td>
</tr>
<tr>
<td>30</td>
<td>3132</td>
<td>0.3132</td>
<td>2.7168</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:  
250 cm³ bottles were filled with distilled deionized water and sealed. A measured volume of dibromochloromethane was injected into the bottles through each bottle septum using a microliter syringe. The solute was in excess of the anticipated solubility limit. The bottles were shaken for one hour 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 response was compared with the calibration plot.

SOURCE AND PURITY OF MATERIALS:  
(1) Probably a commercial reagent, at least 99 % purity, used as received.  
(2) Distilled and deionized.

ESTIMATED ERRORS:  
Solubility: Not specified.  
Temperature: ± 0.5 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]

(2) Milang water

Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.


### VARIABLES:

\[ T/K = 293 \]

PREPARED BY:

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry’s law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 10^4 w_j ) (compiler)</th>
<th>( 10^4 x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 8.5 \times 10^4 )</td>
<td>0.6469</td>
<td>5.632</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source and purity not given.

(2) pH = 8.4, 700 mg salt/dm³, 140 mg CaCO₃/dm³, 10 mg organic carbon/dm³, 110 mg suspended solid/dm³.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 0.1 K.

**REFERENCES:**


---

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]

(2) Myponga water

Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.


### VARIABLES:

\[ T/K = 293 \]

PREPARED BY:

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry’s law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 10^4 w_j ) (compiler)</th>
<th>( 10^4 x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 8.0 \times 10^4 )</td>
<td>0.6873</td>
<td>5.984</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source and purity not given.

(2) pH = 7.6, 370 mg salt/dm³, 60 mg CaCO₃/dm³, 10 mg organic carbon/dm³.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 0.1 K.

**REFERENCES:**

COMPONENTS:
(1) Dibromochloromethane; CHBr₂Cl; [124-48-1]
(2) Myponga water + humic acid

VARIABLES:
\( T/K = 293 \)

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/m^3 \text{ atm mol}^{-1} )</th>
<th>100 ( w_0 )</th>
<th>( 10^4 x_i )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 7.7 \times 10^4 )</td>
<td>0.7141</td>
<td>6.2191</td>
</tr>
</tbody>
</table>

ORIGINAL MEASUREMENTS:
Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.

PREPARED BY:
A. L. Horvath

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) pH = 7.9, 20 mg humic acid/dm³, 370 mg salt/dm³, 68 mg CaCO₃/dm³, 17 mg organic carbon/dm³.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:
(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P.
COMPONENTS:
(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
February 1993.

CRITICAL EVALUATION:
The tribromomethane (1) and water (2) binary system is discussed in two parts; part 1 is tribromomethane (1) in water (2) and part 2 is water (2) in tribromomethane (1).

Part 1. All the available data for the solubility of tribromomethane (1) in water (2) were considered acceptable for use in the smoothing equation except the following reported values. The datum of Squire and Caines (ref. 1) is rejected because of the lack of details on the purity of the sample, method of the experimental work, and significant deviation from other measurements. The approximate value of Booth and Everson (ref. 2) is also rejected because it is significantly lower than later studies. The datum of McNally and Grob (ref. 3) is rejected because the reported solubility is rather higher than other determinations. The data of Wright et al. (ref. 4) are contrary to the general trend of the temperature dependence of the solubilities in water (formation of maximum) and are rejected.

The remaining data, mainly at 298 K, are in reasonable agreement although further studies are required before any values can be recommended without qualification.

The tentative solubility values in mass per cent for tribromomethane (1) in water (2) over the 283 to 303 K temperature range were used to obtain the following equation:

\[
\text{Solubility \ [100 \ w_f\]} = 2.371 - 0.01517 \ (T/K) + 2.7808 \times 10^{-3} \ (T/K)^2
\]

This regression equation was established using the combined data from (refs. 5 - 12), which yielded a standard deviation of 1.6 x 10⁻².

The tentative solubility values in mass per cent at 5 K intervals for tribromomethane (1) in water (2) are presented in the Table 1.

The curve obtained from the smoothing equation is shown in Figure 1. It should be noted that the solubility minimum, which is discussed in the Preface, appearing in the 283 to 303 K temperature interval is not pronounced.

![Figure 1. Solubility of Tribromomethane (1) in Water (2).](image-url)
COMPONENTS:

(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

February 1993.

CRITICAL EVALUATION: (continued)

Table 1. Tentative Solubility of Tribromomethane (1) in Water (2)

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Temperature K</th>
<th>Solubility 100 w₁</th>
<th>10⁴ x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.305</td>
<td>2.18</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.309</td>
<td>2.21</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.314</td>
<td>2.24</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.320</td>
<td>2.29</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.328</td>
<td>2.34</td>
</tr>
</tbody>
</table>

Part 2. The only datum available for the solubility of water (2) in tribromomethane (1) is that of Mackay et al. (ref. 9); therefore, no Critical Evaluation is possible. The interested reader is referred to the relevant Compilation Sheet for the experimental solubility.

REFERENCES:

1. Squire, P. W.; Caines, C. M. Pharm. J. 1905, 74, 784.
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]
(2) Water; H₂O; [7732-18-5]
Squire, P. W.; Caines, C. M.

VARIABLES:

T/I K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>V₁/V₂</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.25 × 10⁻³</td>
<td>0.361</td>
<td>2.582</td>
</tr>
</tbody>
</table>

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: Not specified.

REFERENCES:


COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]
(2) Water; H₂O; [7732-18-5]

VARIABLES:

T/I K = 288 - 303

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>1000 g₁/g₂</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>3.01</td>
<td>0.301</td>
<td>2.15</td>
</tr>
<tr>
<td>30</td>
<td>3.19</td>
<td>0.319</td>
<td>2.28</td>
</tr>
</tbody>
</table>

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co., further purified by fractional freezing before use.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: ± 1.5 %
Temperature: ± 0.02 K.

REFERENCES:

(2) Saylor, J. H. *Ph. D. Thesis*, Duke University, Durham, **1930**.
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]

(2) Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

van Arkel, A. E.; Vles, S. E.


### VARIABLES:

\( T/K = 303 \)

### EXPERIMENTAL VALUES:

<table>
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<th>( t/°C )</th>
<th>( 100 n_1/g_2 )</th>
<th>( 100 w_i ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.0</td>
<td>( 1.26 \times 10^{-3} )</td>
<td>0.318</td>
<td>0.227</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) Tribromomethane (bromoform); CHBr₃; [75-25-2]

(2) Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Booth, H. S.; Everson, H. E.


### VARIABLES:

\( T/K = 298 \)

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( V_1/V_2 )</th>
<th>( 100 w_i ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>&lt; 0.02</td>
<td>&lt; 0.058</td>
<td>&lt; 4.1</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

#### METHOD/APPARATUS/PROCEDURE:

The equilibrium was ensured by repeated shaking and centrifuging of a tribromomethane and water mixture in a stoppered Goetz tube and returning it to a constant temperature water bath. The difference between the total amount of tribromomethane which was added and the amount remaining in excess was taken as the amount of tribromomethane dissolved in the known volume of water.

The determination of the excess amount of tribromomethane added is described by Hamslick (ref. 1).

#### SOURCE AND PURITY OF MATERIALS:

(1) Source not given. Commercial reagent, C. P. grade, used as received.

(2) Distilled.

#### ESTIMATED ERRORS:

Solubility: < 100 %.

Temperature: ± 1 K (compiler).

#### REFERENCES:

COMPONENTS:
(1) Tribromomethane (bromoform);
CHBr\textsubscript{3}; [75-25-2]
(2) Water; H\textsubscript{2}O; [7732-18-5]

ORIGINAL MEASUREMENTS:
O'Connell, W. L.

VARIABLES:
\( T/K = 293 \)

EXPERIMENTAL VALUES:
\[
\begin{array}{cccc}
 t/°C & 100 g/g & 100 \text{ w}_f \text{ (compiler)} & 10^4 \text{ x}_f \text{ (compiler)} \\
 20 & 0.311 & 0.310 & 2.22 \\
\end{array}
\]

SOURCE AND PURITY OF MATERIALS:
(1) Dow Chemicals Co., used as received.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).

REFERENCES:

AUXILIARY INFORMATION

COMPONENTS:
(1) Tribromomethane (bromoform);
CHBr\textsubscript{3}; [75-25-2]
(2) Water; H\textsubscript{2}O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Symons, J. M. *et al.*

VARIABLES:
\( T/K = 298 \)

EXPERIMENTAL VALUES:
\[
\begin{array}{cccc}
 t/°C & \text{Henry's law constant} H/\text{dimensionless} & 100 \text{ w}_f \text{ (compiler)} & 10^4 \text{ x}_f \text{ (compiler)} \\
 25 & 2.4 \times 10^2 & 0.3107 & 2.221 \\
\end{array}
\]

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Cincinnati tap water.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K.

REFERENCES:
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Tribromomethane (bromoform); CHBr₃; [75-25-2]  
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Mackay, D. et al.  

### VARIABLES:

\[ T/K = 298 \]

PREPARED BY:  
A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c/mol m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10⁴ x₁ (compiler)</th>
<th>10⁵ w₂ (compiler)</th>
<th>10³ x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>12.0</td>
<td>0.3032</td>
<td>2.168</td>
<td>7.14 × 10⁻¹</td>
<td>1.0</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

An aqueous solution with an excess of tribromomethane was stirred for 1 day before being introduced into a 1 liter 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 tribromomethane in water was determined by gas chromatography. The GC was equipped with both flame ionization detector and an electron capture detector.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: Not specified.  
Temperature: ± 1.0 K.

### REFERENCES:

1. McNally, M. E.; Grob, R. L.  
*J. Chromatogr.* 1984, 284, 105-16.
## COMPONENTS:

1. Tribromomethane (bromoform); CHBr₃; [75-25-2]
2. Water; H₂O; [7732-18-5]

## ORIGINAL MEASUREMENTS:

Nicholson, B. C.; Maguire, B. P.; Bursill, D. B. 

## VARIABLES:

\( T/k = 293 \)

## EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3\ atm\ mol^{-1} )</th>
<th>( 100 w_j ) (compiler)</th>
<th>( 10^4 x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 4.3 \times 10^4 )</td>
<td>0.3093</td>
<td>2.211</td>
</tr>
</tbody>
</table>

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The apparatus consisted of a stripping vessel similar to that described by Mackay _et al._ (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**

1. Source and purity not given.
2. Distilled and deionized.

**ESTIMATED ERRORS:**

Solubility: ± 3.9 \%.
Temperature: ± 0.5 K.

**REFERENCES:**

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. 
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Tribromomethane (bromoform); CHBr₃; [75-25-2]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.


### VARIABLES:

\[ T_K = 298 \]

### PREPARED BY:

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry’s law constant, ( H/m^2\text{ atm mol}^{-1} )</th>
<th>( 100 w_f ) (compiler)</th>
<th>( 10^4 x_f ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>( 5.32 \times 10^{-4} )</td>
<td>0.3512</td>
<td>2.511</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The original method and apparatus for the determination of Henry’s law constants, described by Mackay et al. (ref. 1), were used. The general procedure was to add an excess quantity of tribromomethane to distilled deionized water and mix the system overnight. A portion of the solution was returned to the stripping vessel. Tribromomethane 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. Source not given. Purest quality available and was used without further purification, stated purity of > 99%.
2. Distilled and deionized.

**ESTIMATED ERRORS:**

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

### REFERENCES:


---

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Tribromomethane (bromoform); CHBr₃; [75-25-2]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Wright, D. A.; Sandler, S. I.; DeVoll, D.


### VARIABLES:

\[ T_K = 293 - 323 \]

### PREPARED BY:

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( \gamma^* )</th>
<th>( 100 w_f ) (compiler)</th>
<th>( 10^4 x_f ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>3530 ± 260</td>
<td>0.396</td>
<td>2.83</td>
</tr>
<tr>
<td>35</td>
<td>3080 ± 425</td>
<td>0.454</td>
<td>3.25</td>
</tr>
<tr>
<td>50</td>
<td>4050 ± 220</td>
<td>0.345</td>
<td>2.47</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 tribromomethane (\( \gamma^* \)) in water. Cells containing degassed water were submerged in a thermostated water bath. Tribromomethane was injected into the mixture cells, a magnetic stirrer was turned on, and 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: See above.
Temperature: ± 0.05 K.
COMPONENTS:
(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]
(2) Milang water

NICHOLSON, B. C.; MAGUIRE, B. P.; BURSILL, D. B.

VARIABLES:

T/K = 293

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry’s law constant, ( \frac{H}{m^3 \text{ atm mol}^{-1}} )</th>
<th>( 100 \ \omega_i ) (compiler)</th>
<th>( 10^4 \ \chi_i ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>( 4.6 \times 10^{-4} )</td>
<td>0.289</td>
<td>2.068</td>
</tr>
</tbody>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate was maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) \( pH = 8.4 \), 700 mg salt/dm³, 140 mg CaCO₃/dm³, 13 mg organic carbon/dm³, 110 mg suspended solid/dm³.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

COMPONENTS:
(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]
(2) Myponga water

NICHOLSON, B. C.; MAGUIRE, B. P.; BURSILL, D. B.

VARIABLES:

T/K = 293

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry’s law constant, ( \frac{H}{m^3 \text{ atm mol}^{-1}} )</th>
<th>( 100 \ \omega_i ) (compiler)</th>
<th>( 10^4 \ \chi_i ) (compiler)</th>
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<tbody>
<tr>
<td>20</td>
<td>( 4.1 \times 10^{-4} )</td>
<td>0.324</td>
<td>2.32</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate was maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) \( pH = 7.6 \), 370 mg salt/dm³, 60 mg CaCO₃/dm³, 10 mg organic carbon/dm³.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Tribromomethane (bromoform); CHBr₃; [75-25-2]</td>
<td>Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.</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>
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<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>Henry's law constant, $H$/m$^3$ atm mol$^{-1}$</td>
</tr>
<tr>
<td>-------</td>
<td>-----------------------------------------------</td>
</tr>
<tr>
<td>20</td>
<td>$4.3 \times 10^{-4}$</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow rate maintained. Samples of the solution being stripped were taken for analysis. After samples were extracted, they were analyzed by gas chromatograph equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**

1. Source and purity not given.
2. pH = 7.9, 20 mg humic acid/dm$^3$, 370 mg salt/dm$^3$, 68 mg CaCO$_3$/dm$^3$, 77 mg organic carbon/dm$^3$.

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 0.1 K.

**REFERENCES:**

COMPONENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

CRITICAL EVALUATION:

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

Part 1. The solubility of trichloromethane (1) in water (2) has been studied by 54 workers with reasonable agreement of reported values from a majority of the investigators.

The experimental data of most investigators in the 273 to 333 K temperature interval are sufficiently reliable to use in the smoothing equation, see Figure 1. (The solid curve in the figure was obtained from the regression of all values shown in the figure.) The experimental work of several workers was not used for the smoothing equation for a variety of reasons. The solubility data of Herz (ref. 1), Salkowski (ref. 2), Ababi et al. (ref. 3), Svetlanov et al. (ref. 4), Sato and Nakijima (ref. 5), Veith et al. (ref. 6), McNally and Grob (ref. 7), and Howe et al. (ref. 8) are markedly lower than other results and are therefore rejected. The data of McCollum (ref. 9), Booth and Everson (ref. 10), Aref’eva et al. (ref. 11), Coca et al. (ref. 12), and Warner et al. (ref. 13) are several per cent higher than the smoothed solubility values and are also rejected. Although, the measured solubility data of Okuda (ref. 14) above 310 K are in reasonable agreement, the low temperature data, that is, below 303 K are very uncertain. Consequently, the low temperature data were not included in the regression analysis. Similar inconsistency was found in the data of Hunter-Smith et al. (ref. 15) and were excluded from further considerations. Lincoff and Gossett (ref. 16) presented two methods for the determination of the solubility. The data determined by the Batch Air Stripping method shows more compatible results and are in good agreement, whereas it appears the EPICS method gave values too low. Therefore, only the solubility data measured by the Batch Air Stripping method were used for fitting the regression equation.

The combined data of 40 laboratories were correlated to obtain the following mass per cent (1) equation:

Solubility [100 w₁] = 12.5333 - 7.40557 x 10⁻² (T/K) + 1.16374 x 10⁴ (T/K)²

which shows a standard deviation of 5.6 x 10⁻². This equation, which shows a maximum deviation of 18 % (but much less for most of the data), may be considered as representing the combined solubility values in the 273 to 333 K temperature range.

The solubility minimum (see Figure 1) calculated from the regression equation is, in mass per cent (1), 0.752 at 318.18 K. The presence of a minimum in the solubility versus temperature behavior for the halogenated hydrocarbon-water systems is discussed in the Preface.

The recommended solubility values in mass per cent at 5 K intervals for trichloromethane (1) in water (2) are presented in Table 1.

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w₁</th>
<th>10² x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.988</td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.938</td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.895</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.857</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.825</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.798</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.778</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.763</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.755</td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.752</td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.755</td>
</tr>
<tr>
<td>55</td>
<td>328.15</td>
<td>0.763</td>
</tr>
<tr>
<td>60</td>
<td>333.15</td>
<td>0.778</td>
</tr>
</tbody>
</table>

(continued next page)
COMPONENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

March 1993.

CRITICAL EVALUATION: (continued)

Figure 1. Solubility of Trichloromethane (1) in Water (2).

Part 2. The solubility of water (2) in trichloromethane (1) has been studied by 25 workers as recorded in the Compilation Sheets immediately following this Critical Evaluation. The reported solubilities in the 263 to 323 K temperature interval are quite acceptable for using the smoothing equation as seen in Figure 2.

All the available data for the solubility of water (2) in trichloromethane (1) have been included for the fitting of the correlating equation with the following exceptions. The measured data of Herz (ref. 1), Evans (ref. 17), De Minjer (ref. 18), Reinders and De Minjer (ref. 19), and Kudryavtseva and Krutikova (ref. 20) are rejected because they are significantly higher than later studies. The data of Donahue and Bartell (ref. 21), Tettamanti et al. (ref. 22), Christyakov and Shapurova (ref. 23), and Antropov et al. (ref. 24) are markedly lower than other determinations and are therefore rejected.

The remaining data of 16 laboratories are in good agreement and the correlated values above 253 K are recommended although the low temperature data (below 273 K) are probably dubious. Further studies are required to establish reliable values in the lower temperature range below 273 K.

The equation for the mass per cent solubility of water (2) in trichloromethane (1) between 263 and 323 K is as follows:

\[
\text{Solubility (100 w_r)} = 6.1195 \times 10^{-2} - 2.0623 \times 10^{-3} (T/K) + 7.20879 \times 10^{-6} (T/K)^2
\]

This equation represents the combined data with a standard deviation of 2.2 x 10⁻² and a correlation coefficient of 0.916.

The recommended mass per cent solubility values at 5 K intervals for water (2) in trichloromethane (1) are presented in the Table 2.

(continued next page)
COMPONENTS:

(1) Trichloromethane (chloroform); CHCl₃ [67-66-3]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

March 1993.

CRITICAL EVALUATION: (continued)

The curve obtained from the smoothing equation is shown in Figure 2. It may be noted that all the studies show a general increase in the solubility with temperature, which is consistent with the discussion of water solubility versus temperature in the Preface. Often the temperature dependence of the solubility is plotted on a Cox chart, that is, log₁₀ x₂ versus 1/T, where a straight line represents the solubility behavior. This procedure is very useful for the illustration of data covering a limited temperature range. However, for the water (2) trichloromethane (1) system, this method of correlation was found to be less satisfactory than the regression with the normal polynomial equation.

Table 2. Recommended Solubility of Water (2) in Trichloromethane (1)

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w₂</th>
<th>10¹ x₂</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10</td>
<td>263.15</td>
<td>0.0177</td>
</tr>
<tr>
<td>-5</td>
<td>268.15</td>
<td>0.0265</td>
</tr>
<tr>
<td>0</td>
<td>273.15</td>
<td>0.0357</td>
</tr>
<tr>
<td>5</td>
<td>278.15</td>
<td>0.0453</td>
</tr>
<tr>
<td>10</td>
<td>283.15</td>
<td>0.0552</td>
</tr>
<tr>
<td>15</td>
<td>288.15</td>
<td>0.0655</td>
</tr>
<tr>
<td>20</td>
<td>293.15</td>
<td>0.0761</td>
</tr>
<tr>
<td>25</td>
<td>298.15</td>
<td>0.0871</td>
</tr>
<tr>
<td>30</td>
<td>303.15</td>
<td>0.0985</td>
</tr>
<tr>
<td>35</td>
<td>308.15</td>
<td>0.1102</td>
</tr>
<tr>
<td>40</td>
<td>313.15</td>
<td>0.1223</td>
</tr>
<tr>
<td>45</td>
<td>318.15</td>
<td>0.1347</td>
</tr>
<tr>
<td>50</td>
<td>323.15</td>
<td>0.1475</td>
</tr>
</tbody>
</table>

Figure 2. Solubility of Water (2) in Trichloromethane (1).
COMPONENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

(2) Water; H₂O; [7732-18-5]

CRITICAL EVALUATION: (continued)

Figure 3 shows the log₁₀ x₂ versus the reciprocal of absolute temperature behavior for comparison with the behavior shown in Figure 2.

Figure 3. Solubility of Water (2) in Trichloromethane (1); log₁₀ x₂ versus 1000/T.

REFERENCES:


## COMPONENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

## EVALUATOR:

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

## CRITICAL EVALUATION: (continued)

### REFERENCES:


COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Chancel, G.; Parmentier, F.
*Compt. Rend. 1885, 100A, 773-6.*

VARIABLES:

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>g₁V₁/kg m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>9.87</td>
<td>0.987</td>
<td>1.502</td>
</tr>
<tr>
<td>3.2</td>
<td>8.90</td>
<td>0.890</td>
<td>1.353</td>
</tr>
<tr>
<td>17.4</td>
<td>7.12</td>
<td>0.713</td>
<td>1.082</td>
</tr>
<tr>
<td>29.4</td>
<td>7.05</td>
<td>0.708</td>
<td>1.075</td>
</tr>
<tr>
<td>41.6</td>
<td>7.12</td>
<td>0.717</td>
<td>1.089</td>
</tr>
<tr>
<td>54.9</td>
<td>7.75</td>
<td>0.784</td>
<td>1.191</td>
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</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Details are not available.

SOURCE AND PURITY OF MATERIALS:
(1) Prepared from chloral and purified by distillation.
(2) Distilled (compiler).

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

COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Herz, W.

VARIABLES:

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 V₁/V₂</th>
<th>100 w₁ (compiler)</th>
<th>100 V₂/V₁</th>
<th>100 w₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>22</td>
<td>0.420</td>
<td>0.620</td>
<td>0.152</td>
<td>0.102</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The mutual solubility between trichloromethane and water was determined by a volumetric method at constant temperature. The change in the volume upon mixing was measured in a calibrated cylinder. The specific weight of the pure components and the solutions were also determined.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given, d₁ = 1.4760 g/cm³ at 22°C.
(2) Distilled (compiler), d₂ = 0.9980 g/cm³ at 22°C.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Moore, B.; Roaf, H. E.

VARIABLES:
T/K = 286

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁</th>
<th>10¹ x₁</th>
<th>100 wₘ/M₁/mol g⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>0.95</td>
<td>1.445</td>
<td>7.96 x 10⁻³</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Pure trichloromethane was dropped from a fine capillary pipette into a tared graduated flask containing distilled water. Samples in a series of flasks of various sizes were prepared and placed on a rotary shaking machine. After several days shaking, an equilibrium was established. The solubility was determined from the decreased amount of trichloromethane.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: ± 5%.
Temperature: ± 1 K (compiler).

COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Rex, A.

VARIABLES:
T/K = 273 - 303

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g₁/g₄</th>
<th>100 w₀</th>
<th>10¹ x₀</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.062</td>
<td>1.05</td>
<td>1.60</td>
</tr>
<tr>
<td>10</td>
<td>0.895</td>
<td>0.887</td>
<td>1.35</td>
</tr>
<tr>
<td>20</td>
<td>0.822</td>
<td>0.815</td>
<td>1.24</td>
</tr>
<tr>
<td>30</td>
<td>0.776</td>
<td>0.770</td>
<td>1.17</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The solubility of trichloromethane in water was determined in specially designed flasks with calibrated cylinders. After equilibration in a thermostatic bath, the volume and the weight of the samples were measured and the solubility calculated.

SOURCE AND PURITY OF MATERIALS:
(1) Commercial, dried, redistilled and washed before use. B. P. = 61.7°C.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

Antonov, G. N.

VARIABLES:
\[ T/K = 293 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 100 w_1 )</th>
<th>( 10^3 x_i ) (compiler)</th>
<th>( 100 w_i M_i^{-1}/mol g^{-1} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.79</td>
<td>1.20</td>
<td>( 6.62 \times 10^{-3} )</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: \( ± 1 \text{ K} \) (compiler).

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

Salkowski, E.
*Biochem. Z.* 1920, 107, 191-201.

VARIABLES:
\[ T/K = 293 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( g_1 V_1/l/kg \text{ m}^{-1} )</th>
<th>( 100 w_1 ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>7.5</td>
<td>0.746</td>
<td>1.13</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A volumetric method similar to that introduced by Alexejew was used. Trichloromethane was gradually added to water from a pipet under constant agitation. The appearance of clouding was the indication of saturation.

SOURCE AND PURITY OF MATERIALS:
(1) Kahlbaum reagent, used as received.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( ± 2 \text{ K} \) (compiler).
**COMPONENTS:**

(1) Water; H$_2$O; [7732-18-5]

(2) Trichloromethane (chloroform); CHCl$_3$; [67-66-3]

**ORIGINAL MEASUREMENTS:**

Clifford, C. W.


**VARIABLES:**

$T/K = 298 - 301$

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>$100 \ w_1$</th>
<th>$10^3 \ x_1$</th>
<th>$100 \ w_1 M_1^{-1}$/mol g$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.5</td>
<td>0.084</td>
<td>0.554</td>
<td>$4.66 \times 10^{-3}$</td>
</tr>
<tr>
<td>26.6</td>
<td>0.107</td>
<td>0.705</td>
<td>$5.94 \times 10^{-3}$</td>
</tr>
<tr>
<td>27.8</td>
<td>0.116</td>
<td>0.764</td>
<td>$6.44 \times 10^{-3}$</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The calcium chloride method was used for the determination of water in trichloromethane. The water was measured as the moisture abstracted from the samples by air and absorbed in two calcium chloride tubes. The tubes were weighed before and after absorption. For further details, see the paper by Clifford (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled (compiler).

(2) U. S. P. grade, used after dehydration with CaCl$_2$.

**ESTIMATED ERRORS:**

Solubility: About 1 mg.

Temperature: ± 0.5 K (compiler).

**REFERENCES:**


---

**COMPONENTS:**

(1) Trichloromethane (chloroform); CHCl$_3$; [67-66-3]

(2) Water; H$_2$O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Nicloux, M.; Scotti-Foglieni, L.


**VARIABLES:**

$T/K = 286 - 313$

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
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<tr>
<th>$t/°C$</th>
<th>Ostwald coefficient, $L$/dimensionless</th>
<th>$100 \ w_1$ (compiler)</th>
<th>$10^3 \ x_1$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>12.9</td>
<td>0.974</td>
<td>1.48</td>
</tr>
<tr>
<td>20</td>
<td>7.7</td>
<td>0.787</td>
<td>1.20</td>
</tr>
<tr>
<td>25</td>
<td>7.0</td>
<td>0.877</td>
<td>1.33</td>
</tr>
<tr>
<td>30</td>
<td>6.2</td>
<td>0.944</td>
<td>1.44</td>
</tr>
<tr>
<td>37</td>
<td>3.8</td>
<td>0.753</td>
<td>1.14</td>
</tr>
<tr>
<td>40</td>
<td>3.5</td>
<td>0.772</td>
<td>1.17</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 the measurements. Water was saturated with trichloromethane gas at a pressure of 750 mmHg. The absorbed gas volume was calculated from the initial dry gas and final water vapor saturated gas volume. The amount of water was determined by measuring the mass of mercury displacement.

**SOURCE AND PURITY OF MATERIALS:**

(1) Laboratory reagent, source and purity not given.

(2) Distilled (compiler).

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 0.5 K (compiler).
COMPONENTS: 
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3] 
(2) Water; H₂O; [7732-18-5] 

ORIGINAL MEASUREMENTS: 
McCollum, J. L. 

VARIABLES: 
\( T / K = 310 \) 

PREPARED BY: 
A. L. Horvath 

EXPERIMENTAL VALUES: 

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 ( g V_i^2/g ) cm³</th>
<th>100 ( w_j ) (compiler)</th>
<th>( 10^5 x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>37.5</td>
<td>1.0</td>
<td>0.997</td>
<td>1.517</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION 

METHOD/APPARATUS/PROCEDURE: 
A colorimetric method was used. A 2.5 g trichloromethane sample was pipetted into a centrifuge tube containing 20 cm³ water. The tube was then vigorously shaken in a thermostat bath for 2 days. After shaking, the tube was centrifuged at high speed to give a clear upper water layer. From this layer the concentration of trichloromethane was determined by using a colorimetric method.

SOURCE AND PURITY OF MATERIALS: 
(1) Source and purity not given. 
(2) Distilled (compiler).

ESTIMATED ERRORS: 
Solubility: ± 1 %. 
Temperature: ± 1 K (compiler). 

COMPONENTS: 
(1) Water; H₂O; [7732-18-5] 
(2) Trichloromethane (chloroform); CHCl₃; [67-66-3] 

ORIGINAL MEASUREMENTS: 
Gibby, C. W.; Hall, J. 

VARIABLES: 
\( T / K = 248 - 327 \) 

PREPARED BY: 
A. L. Horvath 

EXPERIMENTAL VALUES: 

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 ( w_j )</th>
<th>( 10^6 x_i ) (compiler)</th>
<th>( 100 w_j M_i^2/z/mol g^{-1} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-25</td>
<td>0.6 ( \times 10^{-2} )</td>
<td>4.0</td>
<td>3.33 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>-15</td>
<td>0.9 ( \times 10^{-2} )</td>
<td>6.0</td>
<td>5.00 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>-1</td>
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<td>9.3</td>
<td>7.77 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>3</td>
<td>1.9 ( \times 10^{-2} )</td>
<td>12.6</td>
<td>1.05 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>17</td>
<td>6.1 ( \times 10^{-2} )</td>
<td>40.3</td>
<td>2.39 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>22</td>
<td>6.5 ( \times 10^{-2} )</td>
<td>42.9</td>
<td>3.39 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>23</td>
<td>7.2 ( \times 10^{-2} )</td>
<td>47.5</td>
<td>3.61 ( \times 10^{-4} )</td>
</tr>
<tr>
<td>31</td>
<td>1.00 ( \times 10^{-1} )</td>
<td>65.9</td>
<td>4.00 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>45</td>
<td>1.18 ( \times 10^{-1} )</td>
<td>77.7</td>
<td>5.55 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>48</td>
<td>1.44 ( \times 10^{-1} )</td>
<td>94.7</td>
<td>6.55 ( \times 10^{-3} )</td>
</tr>
<tr>
<td>54</td>
<td>1.65 ( \times 10^{-1} )</td>
<td>108.3</td>
<td>8.00 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION 

METHOD/APPARATUS/PROCEDURE: 
Known weight mixtures of trichloromethane and water were prepared in glass tubes. The tubes were heated until all the water had dissolved. Upon cooling, the temperature at which the first detected appearance of turbidity was noted. Stirring was ensured by gentle rocking of the tubes.

SOURCE AND PURITY OF MATERIALS: 
(1) Distilled (compiler). 
(2) Source not given. Pure B. P., treated with H₂SO₄, NaOH, and H₂O. Dried with Na₂CO₃ and refluxing with Mg₃N₂ before use.

ESTIMATED ERRORS: 
Solubility: Not specified.
Temperature: ± 1 K.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]</td>
<td>Gross, P. M; Saylor, J. H.</td>
</tr>
<tr>
<td>VARIABLES:</td>
<td>PREPARED BY:</td>
</tr>
<tr>
<td>T/K = 288 - 303</td>
<td>A. L. Horvath</td>
</tr>
<tr>
<td>EXPERIMENTAL VALUES:</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>100 w₁</td>
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<tr>
<td>15</td>
<td>0.852</td>
</tr>
<tr>
<td>30</td>
<td>0.771</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

An excess of trichloromethane in 500 g water was shaken for 12 hours in a thermostat bath. Samples were then withdrawn and read against water in the interferometer made by Zeiss (ref. 1). A detailed description of the complete procedure is given in a Ph. D. thesis (ref. 2).

**SOURCE AND PURITY OF MATERIALS:**

(1) Eastman Kodak Co., shaken with H₂SO₄, Hg, and distilled water and fractionated before use.
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: ± 1.0 %.
Temperature: ± 0.02 K.

**REFERENCES:**


---

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
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<td>Evans, T. W.</td>
</tr>
<tr>
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<td>PREPARED BY:</td>
</tr>
<tr>
<td>T/K = 293</td>
<td>A. L. Horvath</td>
</tr>
<tr>
<td>EXPERIMENTAL VALUES:</td>
<td></td>
</tr>
<tr>
<td>t/°C</td>
<td>100 w₁</td>
</tr>
<tr>
<td>20</td>
<td>0.8</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

An oil centrifuge bottle (so-called) which permitted an accurate reading of both the total volume and the small volume of upper or lower layer was used for the measurements. The necks of the solubility bottles were adapted to 0.05 cm³ over a 5 cm³ volume range. These bottles held approximately 50 cm³. Following the Hill method, weighted amounts of the two liquids were introduced into the bottles and shaken until equilibrium was reached.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: ± 0.2.
Temperature: ± 0.5 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 303 \]

### EXPERIMENTAL VALUES:

<table>
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<th>100 ( w_w )</th>
<th>10² ( x_w ) (compiler)</th>
<th>100 ( w_wM)²/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.0</td>
<td>0.764</td>
<td>0.116</td>
<td>6.46 \times 10⁻³</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: ORIGINAL MEASUREMENTS:

1. Water; H₂O; [7732-18-5]
2. Trichloromethane (chloroform); CHCl₃; [67-66-3]

### VARIABLES:

\[ T/K = 288 \]

### EXPERIMENTAL VALUES:

<table>
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<th>10² ( x_w ) (compiler)</th>
<th>100 ( w_wM)²/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>0.20</td>
<td>1.31</td>
<td>1.11 \times 10⁻²</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Weighted mixtures of water and trichloromethane were shaken in sealed tubes in a water bath until the equilibrium had been established. After separation in two layers, a sample of the organic phase was taken and the water content of the mixture was determined by titration with a solution of cobalt chloride in anhydrous acetone. For further details, see (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

1. Distilled.
2. Commercial grade, washed with H₂SO₄ and K₂CO₃ solutions, followed by distillation before use.

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 0.05 K (compiler).

**REFERENCES:**

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Water; H₂O; [7732-18-5]
(2) Trichloromethane (chloroform); CHCl₃; [67-66-3]
Staverman, A. J.

VARIABLES:
T/K = 273 - 303

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁</th>
<th>10² x₁ (compiler)</th>
<th>100 w₁Mₑ⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>5.29 × 10⁻²</td>
<td>3.52</td>
<td>2.94 × 10⁻²</td>
</tr>
<tr>
<td>25</td>
<td>9.32 × 10⁻³</td>
<td>6.23</td>
<td>5.17 × 10⁻³</td>
</tr>
<tr>
<td>30</td>
<td>1.13 × 10⁻¹</td>
<td>7.50</td>
<td>6.27 × 10⁻³</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Trichloromethane was shaken with water for about 12 hours in a paraffin thermostat bath. The water content of the organic phase was determined by the Karl Fischer titration method. All measurements were carried out in duplicates. The result is the average of two determinations. A full description of the method used is given in a thesis (ref. 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: ORIGINAL MEASUREMENTS:
(1) Water; H₂O; [7732-18-5]
(2) Trichloromethane (chloroform); CHCl₃; [67-66-3]
Hutchison, C. A.; Lyon, A. M.

VARIABLES:
T/K = 298

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t/°C</th>
<th>100 w₁Mₑ⁻¹/mol g⁻¹</th>
<th>10³ x₁ (compiler)</th>
<th>100 w₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>4.88 × 10⁻³</td>
<td>5.80</td>
<td>8.79 × 10⁻³</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A 1 to 15 volume ratio mixture of water and trichloromethane was introduced into an equilibration flask and then lowered into a water thermostat bath. The assembly was shaken mechanically for about 90 minutes at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration. The measurement was done in triplicate.
The description was taken from a secondary source (ref. 1), because the original report is no longer available.

SOURCE AND PURITY OF MATERIALS:
(1) Distilled.
(2) Source not given. Purified and dried before use.

ESTIMATED ERRORS:
Solubility: ± 0.1 × 10⁻⁴ avg. dev.
Temperature: ± 0.05 K.

REFERENCES:
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
McGovern, E. W.

VARIABLES:
\( T/K = 273 - 323 \)

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( w₁ )</th>
<th>10³ ( x_1 ) (compiler)</th>
<th>100 ( w₂ )</th>
<th>10³ ( x₂ ) (compiler)</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>1.02</td>
<td>1.55</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>10</td>
<td>0.91</td>
<td>1.38</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>20</td>
<td>0.82</td>
<td>1.25</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>25</td>
<td>0.79</td>
<td>1.20</td>
<td>0.097</td>
<td>6.39</td>
</tr>
<tr>
<td>30</td>
<td>0.77</td>
<td>1.17</td>
<td>0.100</td>
<td>6.59</td>
</tr>
<tr>
<td>40</td>
<td>0.74</td>
<td>1.12</td>
<td>0.135</td>
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</tr>
<tr>
<td>50</td>
<td>0.76</td>
<td>1.15</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Solubility as function of temperature was presented in graphical form only, except at 25°C.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Details are not available.

SOURCE AND PURITY OF MATERIALS:
(1) Source not given. Commercial reagent, used as received.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( ± 1.0 \) K (compiler).
COMPONENTS:  
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]  
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:  
Reinders, W.; De Minjer, C. H.  

VARIABLES:  
*T/𝐾* = 273 - 333

PREPARED BY:  
A. L. Horvath

EXPERIMENTAL VALUES:  
<table>
<thead>
<tr>
<th><em>t</em>/°C</th>
<th>100 *w₁</th>
<th>10³ <em>x₁</em> (compiler)</th>
<th>100 *w₂</th>
<th>10³ <em>x₂</em> (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.98</td>
<td>1.49</td>
<td>0.1</td>
<td>6.59</td>
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<tr>
<td>25</td>
<td>0.90</td>
<td>1.37</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>42</td>
<td>0.71</td>
<td>1.08</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>60</td>
<td>0.75</td>
<td>1.14</td>
<td>0.17</td>
<td>11.2</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:  
The saturation between trichloromethane and water took place in a water bath. The composition of both the organic and water phases were determined from their density and refractive index. The constant density and refractive index calibration curves were established by using several synthetic mixtures.

SOURCE AND PURITY OF MATERIALS:  
(1) Commercial grade washed with H₂SO₄ and K₂CO₃ solutions, followed by distillation before use.  
(2) Distilled.

ESTIMATED ERRORS:  
Solubility: Not specified.  
Temperature: ± 0.05 K (compiler).

COMPONENTS:  
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]  
(2) Water; H₂O; [7732-18-5]

PREPARED BY:  
A. L. Horvath

EXPERIMENTAL VALUES:  
<table>
<thead>
<tr>
<th><em>t</em>/°C</th>
<th>100 *V₁/V₂</th>
<th>10³ <em>x₁</em> (compiler)</th>
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<tr>
<td>25.0</td>
<td>0.90</td>
<td>2.01</td>
<td>1.32</td>
<td></td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:  
Equilibrium was ensured through repeated shaking and centrifuging of the trichloromethane and water mixture in a stoppered Goetz tube and returned to a constant temperature water bath. The difference between the total amount of trichloromethane which was added and the amount remaining in excess was taken as the amount of trichloromethane dissolved in the known volume of water. The determination of the excess amount of trichloromethane added is described by Hanslick (ref. 1).

SOURCE AND PURITY OF MATERIALS:  
(1) Commercial reagent, C. P. grade, used as received.  
(2) Distilled.

ESTIMATED ERRORS:  
Solubility: Not specified.  
Temperature: ± 1 K (compiler).

REFERENCES:  
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 298 \]

### EXPERIMENTAL VALUES:

<table>
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<tr>
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<th>( 10^3 x_1 )</th>
<th>( 100 w_j ) (compiler)</th>
<th>( 10^3 x_2 )</th>
<th>( 100 w_z ) (compiler)</th>
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<tbody>
<tr>
<td>25</td>
<td>1.2</td>
<td>0.790</td>
<td>5.0</td>
<td>7.58 \times 10^{-2}</td>
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</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A mixture of trichloromethane and water was placed in a glass stoppered flask and was shaken intermittently for at least three days in a water bath held at constant temperature. The organic phase was analyzed for water content by the Karl Fischer titration method, whereas the aqueous phase was analyzed interferometrically.

**SOURCE AND PURITY OF MATERIALS:**

1. Source not given. Reagent grade, purified by fractional distillation.
2. Purified by distillation.

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 0.1 K.

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 293 \]

### EXPERIMENTAL VALUES:

<table>
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<th>( 10^3 x_j )</th>
<th>( 100 w_z ) (compiler)</th>
<th>( 10^2 x_z ) (compiler)</th>
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<tr>
<td>20</td>
<td>0.84</td>
<td>1.28</td>
<td>0.99</td>
<td>6.21</td>
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</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The mutual solubility between trichloromethane and water was determined by titration from a microburet until turbidity appeared. The end point of the titration, when turbidity first appeared, was determined with an accuracy of 0.3 - 0.5 %. The titration of the solution took place in a thermostat bath at 20°C. The caprolactam-water-trichloromethane ternary system was also studied.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: 0.3 - 0.5.
Temperature: ± 0.5 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

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<thead>
<tr>
<th>Component</th>
<th>Chemical Formula</th>
<th>CAS Number</th>
</tr>
</thead>
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<tr>
<td>(1) Water</td>
<td>H₂O</td>
<td>[7732-18-5]</td>
</tr>
<tr>
<td>(2) Trichloromethane (chloroform)</td>
<td>CHCl₃</td>
<td>[67-66-3]</td>
</tr>
</tbody>
</table>

**ORIGINAL MEASUREMENTS:**


### VARIABLES:

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<th>T/K</th>
<th>Value</th>
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</table>

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 ( w_i )</th>
<th>( 10^3 x_j ) (compiler)</th>
<th>( 100 w_i M_j ^{-1}/mol g^{-1} ) (compiler)</th>
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<tr>
<td>20</td>
<td>0.084 ± 0.003</td>
<td>5.54</td>
<td>4.66 ( \times 10^{-3} )</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A 50 g trichloromethane sample was shaken with pure water in a 100 cm³ Erlenmeyer flask. When equilibrium had been 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 (compiler).

### REFERENCES:

**COMPONENTS:**

(1) Water; H$_2$O; [7732-18-5]
(2) Trichloromethane (chloroform); CHCl$_3$; [67-66-3]

**ORIGINAL MEASUREMENTS:**

Desnoyer, M.  

**VARIABLES:**

$T/K = 299$

**PREPARED BY:**

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
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<th>$10^3 \ x_1$ (compiler)</th>
<th>$100 \ w_2$</th>
<th>$10^3 \ x_2$ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>26</td>
<td>8.6 x 10$^{-2}$</td>
<td>5.67</td>
<td>4.77 x 10$^{-3}$</td>
<td></td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The saturation of trichloromethane with water took place at room temperature under vigorous stirring. The concentration of water in the organic rich phase was determined by infrared spectrometry.

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled.  
(2) Source not given. Commercial reagent, washed and dried before use.

**ESTIMATED ERRORS:**

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

---

**COMPONENTS:**

(1) Trichloromethane (chloroform); CHCl$_3$; [67-66-3]  
(2) Water; H$_2$O; [7732-18-5]

**PREPARED BY:**

Z. Maczynska

**EXPERIMENTAL VALUES:**

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<th>$100 \ w_2$</th>
<th>$10^3 \ x_2$ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>0.82</td>
<td>1.25</td>
<td>7.0 x 10$^{-2}$</td>
<td>4.62</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

Turbidimetric titrations were used for both the aqueous and the organic phases. First, trichloromethane was titrated with water from a microburet until the appearance of turbidity. Then, water was titrated with trichloromethane. The amount of trichloromethane or water in the flask was weighted to an accuracy of 0.01 g. The temperature was maintained constant by using ultrathermostat bath. The trichloromethane-water-caprolactam ternary system was also studied.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: ± 1.0 %.  
Temperature: ± 0.1 K.
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. **Trichloromethane (chloroform);** CHCl₃; [67-66-3]
2. **Water;** H₂O; [7732-18-5]

### VARIABLES:

\( T/k = 298 - 329 \)

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/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>0.75</td>
<td>1.139</td>
<td>8.0 \times 10^{-2}</td>
<td>5.278</td>
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<td>56.1</td>
<td>0.80</td>
<td>1.216</td>
<td>1.7 \times 10^{-4}</td>
<td>11.16</td>
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</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A flask was charged with a trichloromethane and water mixture of approximately the desired composition. The system was allowed to equilibrate in a water bath at the desired temperature. Samples were withdrawn from the two layers and concentrations were determined. The analytical techniques are described elsewhere (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

1. U. S. P. grade. Washed with H₂SO₄ and K₂CO₃ solutions and then distilled. Only the center cut was used.
2. Deionized, distilled twice before use.

### REFERENCES:


---

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. **Trichloromethane (chloroform);** CHCl₃; [67-66-3]
2. **Water;** H₂O; [7732-18-5]

### VARIABLES:

\( T/k = 294 \)

### EXPERIMENTAL VALUES:

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</tr>
</thead>
<tbody>
<tr>
<td>20.5</td>
<td>0.7</td>
<td>1.4</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The isothermic titration method described by Ababi and Popa (refs. 1, 2) was used. A trichloromethane-water-allyl alcohol ternary system was also studied. Further details are not available in the article.

**SOURCE AND PURITY OF MATERIALS:**

1. Source and purity not given, \( n_B = 1.4454 \) at 20°C.
2. Distilled (compiler).

### REFERENCES:

<table>
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<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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<tr>
<td>(1) Water; H(_2)O; [7732-18-5]</td>
<td>Chistyakov, V. M.; Shapurova, V. V.</td>
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<th>PREPARED BY:</th>
</tr>
</thead>
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<tr>
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<td>A. L. Horvath</td>
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</tbody>
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<th>EXPERIMENTAL VALUES:</th>
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</tr>
</thead>
<tbody>
<tr>
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<td>(100 w_i) (compiler)</td>
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<tr>
<td>----------------------</td>
<td>------------------</td>
</tr>
<tr>
<td>20</td>
<td>(6.3 \times 10^{-2})</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
Details are not available.

**SOURCE AND PURITY OF MATERIALS:**
(1) Distilled (compiler).
(2) Source and purity not given.

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: ± 1 K (compiler).

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
</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>
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<th>EXPERIMENTAL VALUES:</th>
<th></th>
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<tbody>
<tr>
<td>(t/\degree C)</td>
<td>(c_i/\text{mol m}^{-3})</td>
</tr>
<tr>
<td>----------------------</td>
<td>------------------</td>
</tr>
<tr>
<td>25</td>
<td>73.8</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
Trichloromethane was equilibrated with water in an apparatus described elsewhere (ref. 1). The equilibration was allowed to take place for 2 days with the entire apparatus immersed in a water bath. The organic phase was analyzed for water by the Karl Fischer method (dead-stop end point). The microburet used for the titration was read to ± 0.01 cm\(^3\). All titrations were carried out in an atmosphere of dry nitrogen.

**SOURCE AND PURITY OF MATERIALS:**
(1) Distilled.
(2) Source not given. Reagent grade, washed with distilled water and the purity was checked with GC.

**ESTIMATED ERRORS:**
Solubility: ± 0.2 \times 10^{-3} avg. dev.
Temperature: ± 0.05 K.

**REFERENCES:**
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Lowe, H. J.

VARIABLES:

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

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<th>Ostwald coefficient, L/dimensionless</th>
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<th>10⁴ x_L (compiler)</th>
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</thead>
<tbody>
<tr>
<td>37</td>
<td>3.80</td>
<td>0.753</td>
<td>1.14</td>
</tr>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The direct injection technique was used for the investigation of the solubility of trichloromethane in water. Ostwald coefficients were determined by equilibration of trichloromethane with water in a capped syringe. After thoroughly mixing, a sample was withdrawn and analyzed in a gas chromatograph equipped with a hydrogen flame detector. The concentration was proportional to the recorded peak height.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Okuda, Y.

VARIABLES:

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

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<th>10⁴ x_L (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>7.15 ± 2.03</td>
<td>0.5915</td>
<td>8.971</td>
</tr>
<tr>
<td>20</td>
<td>5.95 ± 1.35</td>
<td>0.6092</td>
<td>9.241</td>
</tr>
<tr>
<td>25</td>
<td>5.08 ± 0.83</td>
<td>0.6378</td>
<td>9.677</td>
</tr>
<tr>
<td>30</td>
<td>4.40 ± 0.53</td>
<td>0.6717</td>
<td>10.195</td>
</tr>
<tr>
<td>35</td>
<td>3.85 ± 0.40</td>
<td>0.7091</td>
<td>10.766</td>
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<tr>
<td>37</td>
<td>3.70 ± 0.39</td>
<td>0.7501</td>
<td>11.392</td>
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<tr>
<td>40</td>
<td>3.40 ± 0.34</td>
<td>0.7499</td>
<td>11.389</td>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: See above.
Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

VARIABLES:

EXPERIMENTAL VALUES:

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: ± 0.06.
Temperature: ± 0.5 K (compiler).

COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

VARIABLES:

EXPERIMENTAL VALUES:

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined in a manometric apparatus consisting of a chamber and a transducer. The bottom plate of the chamber contained two wells; one was filled with mercury and the other was filled with introduced water and trichloromethane. The mixing and equilibrium between trichloromethane and water took place in the chamber under vigorous stirring. With the pressures before and after the equilibrium measured, the Ostwald coefficient was calculated from the chamber volume and the injected liquid volume.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: ± 0.5 K (compiler).
COMPONENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.


VARIABLES:

T/K = 288 - 333

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

\[ t/°C \quad 1000 \ g_l/g_s \quad 100 w_l \quad 10^4 x_l \]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>1000 g_l/g_s</th>
<th>100 w_l (compiler)</th>
<th>10^4 x_l (compiler)</th>
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<tr>
<td>15</td>
<td>4.82</td>
<td>0.480</td>
<td>7.27</td>
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<tr>
<td>30</td>
<td>3.20</td>
<td>0.319</td>
<td>4.83</td>
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<tr>
<td>45</td>
<td>2.05</td>
<td>0.205</td>
<td>3.10</td>
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<tr>
<td>60</td>
<td>1.30</td>
<td>0.130</td>
<td>1.96</td>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic method was used for the determination of the solubility. It consisted of the saturation of nitrogen with trichloromethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of water. After 2 - 3 hours the solution became saturated and samples were taken periodically (ref. 1). The concentration of trichloromethane in water was determined by GLC. On average, 3 - 5 measurements were taken at each temperature.

ESTIMATED ERRORS:

Solubility: ± 15 %
Temperature: ± 0.05 K

REFERENCES:


COMPONENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Karger, B. L; Chatterjee, A. K.; King, J. W.


VARIABLES:

T/K = 286

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

\[ t/°C \quad \text{Partition coefficient,}^1 \quad 100 w_l \quad 10^4 x_l \]

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Partition coefficient, ( K_d )</th>
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<th>10^4 x_l (compiler)</th>
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<tbody>
<tr>
<td>12.5</td>
<td>13.8</td>
<td>1.02</td>
<td>1.55</td>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Gas-liquid chromatography was used for the determination of the partition of trichloromethane with thin layers of water coated on Porasil D. Helium carrier gas was presaturated with water at the column temperature. The eluents were detected with an F & M flame ionization detector. The partition coefficient \( (K_d) \) was calculated from the slope of the straight line plot of \( V_L/A_L \) versus \( V_L/A_L \).

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.05 K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Antropov, L. I.; Populyai, V. E.; Simonov, V. D.; Shamsudinov, T. M.
(VINITI No. 3739-71).

VARIABLES:
T/K = 288 - 299

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t/°C</th>
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<th>( 10^3 \ x_1 ) (compiler)</th>
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<th>( 10^3 \ x_2 ) (compiler)</th>
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<tr>
<td>15</td>
<td>1.0</td>
<td>1.52</td>
<td>-</td>
<td>-</td>
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<tr>
<td>18</td>
<td>-</td>
<td>-</td>
<td>6.2 \times 10^{-2}</td>
<td>4.09</td>
</tr>
<tr>
<td>22</td>
<td>-</td>
<td>-</td>
<td>6.5 \times 10^{-2}</td>
<td>4.29</td>
</tr>
<tr>
<td>26</td>
<td>-</td>
<td>-</td>
<td>7.9 \times 10^{-2}</td>
<td>5.21</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The Alexejev’s synthetic method of solubility determination was used (ref. 1). A fixed weight of trichloromethane and water was sealed in a tube and 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, while the tube was constantly agitated, the temperature of the first appearance of opalescence was recorded. 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; H₂O; [7732-18-5]
(2) Trichloromethane (chloroform); CHCl₃; [67-66-3]

ORIGINAL MEASUREMENTS:
Ödberg, L.; Löfvenberg, A.; Högfeldt, E.; Fredlund, F.

VARIABLES:
T/K = 298

EXPERIMENTAL VALUES:

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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The equilibrium between water and trichloromethane was reached after the samples were left at least 40 hours in an equilibration vessel. The Karl Fischer titration method was used for the water analysis once equilibrium had been established. At least two samples were studied.

SOURCE AND PURITY OF MATERIALS:
(1) Distilled.
(2) Source not given. Purity is > 99.9 %.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.3 K.
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
McConnell, G.; Ferguson, D. M.; Pearson, C. R.

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:
<table>
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<tr>
<th>t/°C</th>
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<th>10¹ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>8200</td>
<td>0.813</td>
<td>1.24</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The solubility of trichloromethane in water was determined by using a gas-liquid chromatograph (GLC) equipped with 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) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Pearson, C. R.; McConnell, G.

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:
<table>
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<th>10¹ x₁ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>8200</td>
<td>0.813</td>
<td>1.24</td>
</tr>
</tbody>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Saturated solutions were prepared in a constant temperature thermostat. Water samples were extracted with n-pentane and an aliquot of the extract taken for GLC 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 K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.

VARIABLES:
T/K = 293

EXPERIMENTAL VALUES:
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<tr>
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<td>67.5</td>
<td>0.807</td>
<td>8.02</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Trichloromethane was added from a micro-
buret to an aqueous solution of octanoic acid
containing KCl under vigorous stirring. The pH of
the solution at first remained constant right up to the
appearance of a second phase, i.e., up to the satura-
tion of the aqueous phase with trichloromethane, after
which it began to rise. The solubility was calculated
from the volume of the aqueous phase and the volume
of trichloromethane used for the saturation.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: ± 10 %.
Temperature: ± 0.5 K (compiler).

COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Sato, A.; Nakijima, T.
Arch. Envir. Health 1979, 34, 69-75.

VARIABLES:
T/K = 310

EXPERIMENTAL VALUES:
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<th>10¹ x₁ (compiler)</th>
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<tbody>
<tr>
<td>37</td>
<td>3.5</td>
<td>0.677</td>
<td>1.027</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Trichloromethane vapor was equilibrated in an
airtight vial between water and the overlying air.
When equilibrium was reached, a portion of the e-
quilibrated air in the vessel was withdrawn using an
airtight syringe and was injected into a gas chro-
matograph and analyzed. The height of the chromat-
ogram peak was used to calculate the partition coef-
ficient.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: ± 0.3 std. dev.
Temperature: ± 0.5 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Freed, V. H.; Chiou, C. T.; Schmedding, D.; Kohnert, R.

*Environ. Health Perspect* 1979, 30, 75-80.

### VARIABLES: PREPARED BY:

\( T/K = 298 \)

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
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<th>( 10^4 w_j )</th>
<th>( 10^4 x_j )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>7950</td>
<td>0.795</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A known volume of water was mixed with trichloromethane in an Erlenmeyer flask. The flask was immersed in a water bath and magnetically stirred. All samples were analyzed using a gas-liquid chromatograph 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 standard grade, greater than 95% purity.
2. Distilled and run through a resin column before use.

**ESTIMATED ERRORS:**

- Solubility: ± 5% variation of 5 samples.
- Temperature: ± 0.5 K.

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Arefeva, R. P.; Korenman, I. M.; Gorokhov, A. A.


### VARIABLES: PREPARED BY:

\( T/K = 293 \)

A. L. Horvath

### EXPERIMENTAL VALUES:

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<tr>
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<th>( g/V_j^2/\text{kg m}^3 )</th>
<th>( 10^4 w_j )</th>
<th>( 10^4 x_j )</th>
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<tbody>
<tr>
<td>20</td>
<td>12.7 ± .2</td>
<td>1.274</td>
<td>1.944</td>
</tr>
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</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Equal quantities of diphenylthiocarbazone were added to aqueous solutions with different amounts of trichloromethane in several flasks. The contents of the flasks were shaken for 5 minutes and left to stand for 1 hour. The mixtures were filtered through filter paper before their analysis by spectrophotometry. The turning point on the graph of optical density versus trichloromethane concentration provided the saturation value.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

- Solubility: See above.
- Temperature: ± 1 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichloromethane (chloroform); \( \text{CHCl}_3; [67-66-3] \)

(2) Water; \( \text{H}_2\text{O}; [7732-18-5] \)

### VARIABLES:

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

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/\circ\text{C} )</th>
<th>( 100 w_1 )</th>
<th>( 10^4 x_1 ) (compiler)</th>
<th>( 100 w_2 )</th>
<th>( 10^4 x_2 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.19</td>
<td>1.814</td>
<td>8.0 \times 10^{-2}</td>
<td>5.278</td>
</tr>
</tbody>
</table>

---

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The mutual solubility data were determined by the method as described by Othmer et al. (ref. 1). Ten cm³ trichloromethane 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 from 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: \( \pm 0.5 \text{ K} \) (compiler).

**REFERENCES:**


---

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichloromethane (chloroform); \( \text{CHCl}_3; [67-66-3] \)

(2) Water; \( \text{H}_2\text{O}; [7732-18-5] \)

### VARIABLES:

\( T/\mathcal{K} = 293 - 298 \)

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/\circ\text{C} )</th>
<th>Henry's law constant ( H/\text{dimensionless} )</th>
<th>( 100 w_1 ) (compiler)</th>
<th>( 10^3 x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.112 ( \pm 0.038 )</td>
<td>0.847</td>
<td>1.393</td>
</tr>
<tr>
<td>25</td>
<td>0.166 ( \pm 0.100 )</td>
<td>0.699</td>
<td>1.149</td>
</tr>
</tbody>
</table>

---

**METHOD/APPARATUS/PROCEDURE:**

The method involved repeated equilibrations of nitrogen with a water sample containing trichloromethane. The sample was shaken vigorously at the required temperature in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph. The experiments were performed at least three times at 20 and 25°C; each experiment involved about six equilibrations.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source and purity not given.

(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: See above.

Temperature: \( \pm 0.5 \text{ K} \) (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]

(2) Water; H₂O; [7732-18-5]

Hutchinson, T. C.; Hellebust, J. A.; Tam, D.; *et al.*


### VARIABLES:

\[ T/K = 298 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
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<th>( t/°C )</th>
<th>( \rho/\text{kg m}^{-3} )</th>
<th>( 10^6 \rho \text{ (compiler)} )</th>
<th>( 10^3 x_I \text{ (compiler)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>7.95</td>
<td>0.7973</td>
<td>1.21</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

An excess quantity of trichloromethane was added to water and stirred vigorously for 24 hours. After settling at 25°C for 48 hours, the solution was extracted with cyclohexane. The samples were analyzed using an Aminco-Bowman spectrophotofluorometer. A detailed description of the method has been reported elsewhere (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

(1) Aldrich Chemicals, highest grade, used as received.

(2) Double distilled.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 0.2 K (compiler).

**REFERENCES:**


---

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]

(2) Water; H₂O; [7732-18-5]

Veith, G. D.; Macek, K. J.; Petrucelli, S. R.; Carroll, J.


### VARIABLES:

\[ T/K = 293 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
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<th>( n/V_{mol} \text{ mol m}^{-3} )</th>
<th>( 100 \omega_I \text{ (compiler)} )</th>
<th>( 10^3 x_I \text{ (compiler)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>61.7</td>
<td>0.732</td>
<td>1.11</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

An excess of trichloromethane was added to 10 cm³ distilled water in a 50 cm³ flask. The mixture was magnetically stirred in a constant temperature water bath. Samples taken from the solution were analyzed using radioactive techniques. The \(^{14}\text{C}\) activity of the water samples was measured in a liquid scintillation spectrometer by recording the number of counts per minute.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source and purity not given.

(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 1 K.
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C.

VARIABLES:
T/K = 298

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>n jPanel Vₐ/mol m⁻³</th>
<th>100 wᵢ (compiler)</th>
<th>10⁻¹ xᵢ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>60.5</td>
<td>0.719</td>
<td>1.09</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An excess of trichloromethane was added to a stainless steel tube containing water and the tube was sealed. It was allowed to equilibrate during shaking for a week at 25°C. After centrifugation, the sample was analyzed for radioactivity using a liquid scintillation counter. The solubility determination was carried out at least twice for each sample and the analysis was done in duplicate.

ESTIMATED ERRORS:
Solubility: ± 4.3% std. dev.
Temperature: ± 0.3 K.

REFERENCES:
COMPONENTS:
(1) Water; H₂O; [7732-18-5]
(2) Trichloromethane (chloroform); CHCl₃; [67-66-3]

ORIGINAL MEASUREMENTS:
Wu, X.

VARIABLES:
\( T/K = 278 - 328 \)

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^4 w_i )</th>
<th>( 100 w_i ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
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<tr>
<td>5</td>
<td>417</td>
<td>0.0417</td>
<td>2.76</td>
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<td>10</td>
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<td>0.0568</td>
<td>3.75</td>
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<td>15</td>
<td>606</td>
<td>0.0606</td>
<td>4.00</td>
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<td>20</td>
<td>758</td>
<td>0.0758</td>
<td>5.00</td>
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<tr>
<td>25</td>
<td>872</td>
<td>0.0872</td>
<td>5.75</td>
</tr>
<tr>
<td>30</td>
<td>909</td>
<td>0.0909</td>
<td>5.99</td>
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<td>35</td>
<td>1061</td>
<td>0.1061</td>
<td>6.99</td>
</tr>
<tr>
<td>40</td>
<td>1099</td>
<td>0.1099</td>
<td>7.24</td>
</tr>
<tr>
<td>45</td>
<td>1251</td>
<td>0.1251</td>
<td>8.23</td>
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<tr>
<td>50</td>
<td>1289</td>
<td>0.1289</td>
<td>8.48</td>
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<tr>
<td>55</td>
<td>1402</td>
<td>0.1402</td>
<td>9.22</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A known volume of water was added to dried trichloromethane to prepare a series of standard samples for establishing calibration curves and obtaining the saturated solutions at each temperature. The determination of the water content of trichloromethane was made with a RM-250 NMR spectrometer (radiation frequency = 250 MHz). The water peak amplitudes were the mean of four readings taken at a particular temperature.

SOURCE AND PURITY OF MATERIALS:
(1) Distilled.
(2) Source not given. Grade 2 purity was washed with KOH solution, H₂SO₄, and distilled water. Dried on molecular sieve before use.

ESTIMATED ERRORS:
Solubility: ± 72 std. dev.
Temperature: \( \pm 1 \) - 2 K.
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]
Leighton, D. T.; Calo, J. M.

VARIABLES:
T/K = 275 - 298

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Distribution coefficient¹, Dₓ/dimensionless</th>
<th>10⁵ wₓ (compiler)</th>
<th>10⁷ xₓ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>1.9</td>
<td>68.9</td>
<td>0.8251</td>
<td>1.254</td>
</tr>
<tr>
<td>13.5</td>
<td>128.7</td>
<td>0.7846</td>
<td>1.192</td>
</tr>
<tr>
<td>15.7</td>
<td>146.7</td>
<td>0.7565</td>
<td>1.149</td>
</tr>
<tr>
<td>17.1</td>
<td>155.0</td>
<td>0.7676</td>
<td>1.166</td>
</tr>
<tr>
<td>22.0</td>
<td>194.5</td>
<td>0.7669</td>
<td>1.165</td>
</tr>
<tr>
<td>24.9</td>
<td>204.8</td>
<td>0.8297</td>
<td>1.261</td>
</tr>
</tbody>
</table>

¹ Gas-liquid system analysis parameter, from calibration measurements.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A 5 µL trichloromethane sample was injected into a 2.3 liter equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 minutes, 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 trichloromethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: ± 10.0 %
Temperature: ± 0.5 K.

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]
Mackay, D.; et al.

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>ρ/kg m⁻³</th>
<th>10⁵ wₓ (compiler)</th>
<th>10⁷ xₓ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>7.95</td>
<td>0.7950</td>
<td>1.203</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
An aqueous solution with an excess amount of trichloromethane was stirred for 1 day before being introduced into a 1 liter 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 trichloromethane in water was determined using gas chromatography. The GC was equipped with both dual flame ionization detector and an electron capture detector.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Double distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1.0 K.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
</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 VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>( g_1v_1/\text{kg m}^3 )</td>
</tr>
<tr>
<td>25</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

Water was added gradually to 50 cm³ tri-chloromethane in a flask which was then lowered into a thermostat bath. The flask was shaken vigorously until the first cloud (turbidity) appeared. The sample water content was determined using the Karl Fischer titration method.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

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

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]</td>
<td>Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S.</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T/K = 293 - 298 )</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>( t/°C )</td>
<td>Henry's law constant, ( H/\text{dimensionless} )</td>
</tr>
<tr>
<td>20</td>
<td>0.1044</td>
</tr>
<tr>
<td>25</td>
<td>0.1686</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The multiple equilibration technique was used to measure the Henry's law constant as described elsewhere (ref. 1). A known volume of water in a syringe was shaken with a known volume of pure trichloromethane. After equilibration, the headspace was separated and analyzed for trichloromethane. 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) Trichloromethane (chloroform); CHCl₃; [67-66-3]  
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:  
Orlandini, M.; Fermeglia, M.; Kikic, I.; Alessi, P.  

VARIABLES:  
$T/K = 293$

EXPERIMENTAL VALUES:

<table>
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<th>$10^3 x_2$</th>
<th>$100 w_1$ (compiler)</th>
<th>$100 w_2$ (compiler)</th>
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<tbody>
<tr>
<td>20</td>
<td>1.23</td>
<td>5.17</td>
<td>0.809</td>
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EXPERIMENTAL VALUES:

EPICS Method

<table>
<thead>
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<th>$t/°C$</th>
<th>Henry's law constant, ( H/m^3\text{atm}\text{mol}^{-1} )</th>
<th>$100 w_1$ (compiler)</th>
<th>$10^3 x_2$ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>3.33 \times 10^3</td>
<td>0.7442</td>
<td>1.130</td>
</tr>
</tbody>
</table>

\[ \log_e H = - \frac{4180}{T(K)} + 8.553 \]

(continued)

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 bottles and the equilibrated headspaces contained concentrations proportional to original concentrations in the aqueous samples. Full equilibrium was achieved in a few hours.

SOURCE AND PURITY OF MATERIALS:  
(1) Source and purity not given.  
(2) Distilled.

ESTIMATED ERRORS:

Solubility: \( \pm 5 - 10 \% \).  
Temperature: \( \pm 0.1 K \).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCI₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
T/K = 293

EXPERIMENTAL VALUES: (continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>H/m³ atm mol⁻¹</th>
<th>100 wᵢ (compiler)</th>
<th>10¹ xᵢ (compiler)</th>
</tr>
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<tbody>
<tr>
<td>20</td>
<td>3.04 × 10⁻³</td>
<td>0.8152</td>
<td>1.239</td>
</tr>
</tbody>
</table>

\[ \log_{\varepsilon} H = - \frac{4322}{T(K)} + 8.956 \]

COMPONENTS:
(1) Trichloromethane (chloroform); CHCI₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
T/K = 303

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>gVᵢ/kg m³</th>
<th>100 wᵢ (compiler)</th>
<th>10¹ xᵢ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>2.524</td>
<td>0.2529</td>
<td>3.825</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Standard increasing concentration solutions of trichloromethane were prepared in volumetric flasks as described elsewhere (ref. 1). The aqueous-organic phase was 25 cm³ and the vapor phase above 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., U. S. A., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

ESTIMATED ERRORS:

Solubility: ± 1.85 % std. dev.
Temperature: ± 0.5 K (compiler).

REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.


VARIABLES:

\[ T/K = 293 \]

PREPARED BY:

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 100 w_p ) (compiler)</th>
<th>( 10^3 x_p ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>20</td>
<td>3.0 \times 10^{-3}</td>
<td>0.8257</td>
<td>1.255</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow was maintained. Samples of the solution being stripped were taken for analysis. After extraction of the samples, the extracts were analyzed by gas chromatography equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: \( \pm 0.1 \times 10^{-3} \) std. dev.
Temperature: \( \pm 0.1 \) K.

**REFERENCES:**


COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

Munz, C. D.


VARIABLES:

\[ T/K = 283 - 303 \]

PREPARED BY:

A. L. Horvath

**EXPERIMENTAL VALUES:**

<table>
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<th>( t/°C )</th>
<th>Henry's Law Constant, ( H/\text{dimensionless} )</th>
<th>( \rho/\text{kg m}^{-3} )</th>
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<th>( 10^3 x_p ) (compiler)</th>
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<tr>
<td>10</td>
<td>7.69 \times 10^{-2}</td>
<td>8.750</td>
<td>0.8750</td>
<td>1.330</td>
</tr>
<tr>
<td>20</td>
<td>1.24 \times 10^{-1}</td>
<td>8.320</td>
<td>0.8320</td>
<td>1.264</td>
</tr>
<tr>
<td>30</td>
<td>1.94 \times 10^{-1}</td>
<td>7.880</td>
<td>0.7880</td>
<td>1.197</td>
</tr>
</tbody>
</table>

**METHOD/APPARATUS/PROCEDURE:**

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

**SOURCE AND PURITY OF MATERIALS:**

(1) J. T. Baker Chemicals Co., N.J. > 99.9 % pure.
(2) Distilled and deionized.

**ESTIMATED ERRORS:**

Solubility: \( \pm 2.22 \times 10^{-3} \) std. dev.
Temperature: \( \pm 0.5 \) K.
<table>
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<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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<td>(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]</td>
<td>Takano, J.; Ishihara, Y.; Yasuoka, T.; Mitsuzawa, S.</td>
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<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>

<p>| EXPERIMENTAL VALUES: |  |</p>
<table>
<thead>
<tr>
<th>t/°C</th>
<th>ρᵣ/kg m⁻³</th>
<th>10₀ wᵣ (compiler)</th>
<th>10⁹ xᵣ (compiler)</th>
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<tbody>
<tr>
<td>20</td>
<td>7.77</td>
<td>0.7770</td>
<td>1.180</td>
</tr>
<tr>
<td>9.33</td>
<td>0.9330</td>
<td>1.419</td>
<td></td>
</tr>
<tr>
<td>6.33</td>
<td>0.6330</td>
<td>0.9604</td>
<td></td>
</tr>
<tr>
<td>8.55</td>
<td>0.8550</td>
<td>1.300</td>
<td></td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

A mixture of 1 cm³ trichloromethane and 30 cm³ water was introduced into a centrifuge tube which was then shaken for 60 minutes in a shaker at room temperature. After an additional shaking of 48 hours, samples were filtered through four types of filter paper in order to free the solution 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) Tokyo Chemical Co., analytical grade reagent, redistilled before use.  
(2) Double distilled.

**ESTIMATED ERRORS:**

Solubility: 0 - 2.5 % coeff. of var. Temperature: ± 1.0 K.

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]</td>
<td>Lo, J. M.; Tseng, C. L.; Yang, J. Y.</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>

<p>| EXPERIMENTAL VALUES: |  |</p>
<table>
<thead>
<tr>
<th>t/°C</th>
<th>10₀ wᵣ</th>
<th>10⁹ xᵣ (compiler)</th>
<th>10₀ wᵣMᵣ⁻¹/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>0.82</td>
<td>1.25</td>
<td>6.87 × 10⁻³</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

A 5 cm³ trichloromethane sample containing labeled complex cobalt(III) pyrrolidinecarbodithioate was placed together with 1000 cm³ of water into a separation funnel. After vigorous shaking for 5 minutes, the mixture was left for 30 minutes before the separation of the two phases. Samples were withdrawn for activity measurement using a Nal (Tl) scintillation detector. Several factors were adjusted to obtain accurate measurements.

**SOURCE AND PURITY OF MATERIALS:**

(1) E. Merck reagent, used as received.  
(2) Demineralized and subboiled.

**ESTIMATED ERRORS:**

Solubility: ± 0.02 std. dev. Temperature: ± 1.0 K (compiler).
COMPONENTS:  
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]  
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:  
Barr, R. S.; Newsham, D. M. T.  
*Fluid Phase Equilibr.* 1987, 35, 189-205.

VARIABLES:  
7TK = 293 - 323

PREPARED BY:  
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t/°C</th>
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<th>100 w₁ (compiler)</th>
<th>10³ x₂</th>
<th>100 w₂ (compiler)</th>
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<td>5.06</td>
<td>0.0767</td>
</tr>
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<td>35</td>
<td>1.121</td>
<td>0.7382</td>
<td>8.29</td>
<td>0.126</td>
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<tr>
<td>50</td>
<td>1.099</td>
<td>0.7238</td>
<td>11.6</td>
<td>0.177</td>
</tr>
</tbody>
</table>

Mole fraction of trichloromethane (x₁) was calculated from the activity coefficient at infinite dilution (γ*) using the relation \( x₁ = \frac{γ*}{Y} \).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water-rich mixture was studied using gas-liquid chromatography in which a mixture of methane and trichloromethane vapor passed through the sampling loop. The eluted trichloromethane was determined with a flame ionization detector.

The Organic-rich mixture was studied using an isopiestic method in which a CaCl₂ 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) Mullinckrodt reagent, ACS, preserved with 0.75 % ethanol.  
(2) Distilled.

ESTIMATED ERRORS:

Solubility: Not specified.  
Temperature: ± 0.05 K.

COMPONENTS:  
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]  
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:  
Gossett, J. M.  

VARIABLES:  
7TK = 283 - 308

PREPARED BY:  
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's Law Constant, ( H/m^3 \text{atm/mol}^1 )</th>
<th>CV'</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.6</td>
<td>1.50 × 10⁻³</td>
<td>6.16</td>
<td>1.0330</td>
<td>1.571</td>
</tr>
<tr>
<td>17.5</td>
<td>2.46 × 10⁻³</td>
<td>1.96</td>
<td>0.8980</td>
<td>1.365</td>
</tr>
<tr>
<td>24.8</td>
<td>3.67 × 10⁻³</td>
<td>3.75</td>
<td>0.8424</td>
<td>1.280</td>
</tr>
<tr>
<td>34.6</td>
<td>5.63 × 10⁻³</td>
<td>3.76</td>
<td>0.8332</td>
<td>1.2662</td>
</tr>
</tbody>
</table>

\(^1 \text{CV} = \text{coefficient of variation} (\approx 100 \text{ S.D./mean}).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A modification of the EPICS method was used to measure Henry's law constants. Precise quantities of trichloromethane were injected into serum bottles which contained distilled water. The bottles were incubated for 18 - 24 hours at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured by a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was approximately 4.3 %.

SOURCE AND PURITY OF MATERIALS:

(1) Mullinckrodt reagent, ACS, preserved with 0.75 % ethanol.  
(2) Distilled.

ESTIMATED ERRORS:

Solubility: See above.  
Temperature: ± 0.1 K.
### Components:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.


### Variables:

\[ T/K = 298 \]

### Experimental Values:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3\ atm\ mol^{-1} )</th>
<th>100 ( w_j ) (compiler)</th>
<th>10(^3) ( x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>3.39 \times 10^{-3}</td>
<td>0.9169</td>
<td>1.397</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

The original method and apparatus for the determination of Henry's law constants have been described elsewhere (ref. 1). The general procedure was to add an excess of trichloromethane to distilled, deionized water and, following, to mix the system overnight. A portion of the solution was returned to the stripping vessel. Trichloromethane was stripped isothermally from the solution at a known gas flow rate. The Henry's law constant was calculated from the log of the concentration versus time plot. The experimental data values are averages of two or more replicates.

**Source and Purity of Materials:**

1. Purest quality available and was used without further purification, that is > 99 %.
2. Distilled and deionized.

**Estimated Errors:**

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

### References:


### Components:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Water; H₂O; [7732-18-5]

### Original Measurements:

Howe, G. B.; Mullins, M. E.; Rogers, T. N.


### Variables:

\[ T/K = 283 - 303 \]

### Experimental Values:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>10(^4) ( w_j )</th>
<th>100 ( w_j ) (compiler)</th>
<th>10(^4) ( x_j ) (compiler)</th>
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<tbody>
<tr>
<td>10</td>
<td>3471</td>
<td>0.3471</td>
<td>5.2535</td>
</tr>
<tr>
<td>20</td>
<td>2963</td>
<td>0.2963</td>
<td>4.4827</td>
</tr>
<tr>
<td>30</td>
<td>3596</td>
<td>0.3596</td>
<td>5.4432</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

250 cm³ bottles were filled with distilled deionized water and sealed. A measured volume of trichloromethane was injected into the bottles through each bottle septum using a microliter syringe. Trichloromethane was in excess of the anticipated solubility limit. The bottles were shaken for 1 hour 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 the calibration plot.

**Source and Purity of Materials:**

1. Probable a commercial reagent at least 99 % purity. Used as received.
2. Distilled and deionized.

**Estimated Errors:**

Solubility: Not specified.
Temperature: ± 0.5 K (compiled).
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
T/°K = 293

EXPERIMENTAL VALUES:

\[
\begin{array}{ccc}
\text{t°C} & 100 \, w_i & 10^3 \, x_i \\
20.0 & 0.82 & 1.25 \\
& & 6.87 \times 10^{-3}
\end{array}
\]

AUXILIARY INFORMATION
METHOD/APPARATUS/PROCEDURE:
The solubility determination was done in small test tubes (e.g., 100 x 12 mm) to permit vigorous shaking of the trichloromethane and water mixture. During the experiment, 0.20 cm³ trichloromethane was added to 3.0 cm³ of water and shaken. The amount of trichloromethane in the water was analyzed by passing the sample through a chromatographic column.

SOURCE AND PURITY OF MATERIALS:
(1) Commercial grade, dried over anhydrous CaCl₂ before use.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1 K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Milang water

ORIGINAL MEASUREMENTS:
Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.

VARIABLES:
\( T/K = 293 \)

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:
\[
\begin{array}{ccc}
t/^{\circ}C & \text{Henry's law constant, } H/m^3 \text{ atm mol}^{-1} & 100 w_j \text{ (compiler)} & 10^3 x_j \text{ (compiler)} \\
20 & 3.3 \times 10^{-3} & 0.7506 & 1.1407 \\
\end{array}
\]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1).
The air entered through the top of the vessel and the diffuser was close to the bottom. The solution was added to the stripping vessel and the desired flow was maintained. A sample of the solution being stripped was taken for analysis. After extraction of the sample, the extracts were analyzed by gas chromatograph equipped with a capillary column.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) \( pH = 8.4, 700 \text{ mg salt}/\text{dm}^3, 140 \text{ mg CaCO}_3/\text{dm}^3, 15 \text{ mg organic carbon}/\text{dm}^3, 110 \text{ mg suspended solid}/\text{dm}^3. \)

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: \( \pm 0.1 \text{ K}. \)

REFERENCES:
(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P.

COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) MQ-Water

ORIGINAL MEASUREMENTS:
Munz, C. D.

VARIABLES:
\( T/K = 293 \)

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:
\[
\begin{array}{ccc}
t/^{\circ}C & \text{Henry's law constant, } H/\text{dimensionless} & 100 w_j \text{ (compiler)} & 10^3 x_j \text{ (compiler)} \\
20 & 0.244 & 0.4207 & 6.371 \\
\end{array}
\]

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 trichloromethane and MQ-water was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected direct into a gas chromatograph, the liquid samples were preconcentrated by liquid-liquid extraction before analysis. The experiments were carried out in duplicates.

SOURCE AND PURITY OF MATERIALS:
(1) J. T. Baker Chemicals Co., NJ., \( > 99.5 \% \) purity.
(2) \( 0.25 \text{ mg total organic carbon per dm}^3, 0.75 \text{ mg COD/dm}^3. \)

ESTIMATED ERRORS:
Solubility: \( \pm 0.016 \text{ std. dev.} \)
Temperature: \( \pm 0.5 \text{ K}. \)
### COMPONENTS: ORIGINAL MEASUREMENTS:
1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Municipal tap water (PASE)

### VARIABLES:
\[ T/K = 293 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/\text{dimensionless} )</th>
<th>( 100 \ w_j ) (compiler)</th>
<th>( 10^4 \ x_j ) (compiler)</th>
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<tr>
<td>20</td>
<td>0.324</td>
<td>0.3174</td>
<td>4.803</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 trichloromethane and municipal tap water was introduced into a syringe and allowed to equilibrate. The ratio of gas to liquid volume was maintained constant. While vapor samples were injected direct into a gas chromatograph, the liquid samples were preconcentrated by liquid-liquid extraction before analysis. The experiments were carried out in duplicate.

**SOURCE AND PURITY OF MATERIALS:**
2. 10 mg total organic carbon per dm³, 40 mg COD/dm³.

**ESTIMATED ERRORS:**
Solubility: ± 0.020 std. dev.
Temperature: ± 0.5 K.

### COMPONENTS: ORIGINAL MEASUREMENTS:
1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Myponga water

### VARIABLES:
\[ T/K = 293 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 100 \ w_j ) (compiler)</th>
<th>( 10^4 \ x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>2.9×10⁻³</td>
<td>0.8542</td>
<td>1.299</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**
The apparatus consisted of a stripping vessel similar to that described by Mackay et al. (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The mixture was added to the stripping vessel and the desired flow was maintained. A sample of the solution being stripped was taken for analysis. After extraction of the sample, the extracts were analyzed by gas chromatograph equipped with a capillary column.

**SOURCE AND PURITY OF MATERIALS:**
1. Source and purity not given.
2. \( pH = 7.6, 370 \text{ mg salt/dm}³, 60 \text{ mg CaCO}_3/\text{dm}³, 10 \text{ mg organic carbon/dm}³. \)

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: ± 0.1 K.

**REFERENCES:**
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Myponga water + humic acid
Nicholson, B. C.; Maguire, B. P.; Bursill, D. B.

VARIABLES: PREPARED BY:
$T/K = 293$
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>Henry's law constant, $H/\text{cm}^2\text{ atmos} \text{ mol}^{-1}$</th>
<th>100 $w_f$</th>
<th>$10^4 x_f$</th>
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<tr>
<td>20</td>
<td>$3.1 \times 10^3$</td>
<td>0.7991</td>
<td>1.2145</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The apparatus consisted of a stripping vessel similar to that described by Mackay *et al.* (ref. 1). The air entered through the top of the vessel and the diffuser was close to the bottom. The mixture was added to the stripping vessel and the desired flow was maintained. A sample of the solution being stripped was taken for analysis. After extraction of the sample, the extracts were analyzed by gas chromatography equipped with a capillary column.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) $pH = 7.9$, 20 mg humic acid/cm³, 370 mg salt/dm³, 68 mg CaCO₃/dm³, 17 mg organic carbon/dm³.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: $\pm 0.1$ K.

REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Seawater
Balls, P. W.

VARIABLES: PREPARED BY:
$T/K = 283 - 298$
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>$t/°C$</th>
<th>Henry's law constant, $H/dimensionless$</th>
<th>100 $w_f$</th>
<th>$10^4 x_f$</th>
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<tbody>
<tr>
<td>10</td>
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<td>0.569</td>
<td>9.33</td>
</tr>
<tr>
<td>15</td>
<td>$0.125 \pm 0.039$</td>
<td>0.614</td>
<td>10.07</td>
</tr>
<tr>
<td>20</td>
<td>$0.161 \pm 0.027$</td>
<td>0.605</td>
<td>9.92</td>
</tr>
<tr>
<td>25</td>
<td>$0.197 \pm 0.057$</td>
<td>0.603</td>
<td>9.89</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The method involved repeated equilibrations of nitrogen with seawater sample containing trichloromethane. The sample was shaken vigorously at the required temperatures in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph. The experiments were performed at least three times at 10, 15, 20, and 25°C, each experiment involving about six equilibrations.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Salinity = 20%.

ESTIMATED ERRORS:
Solubility: See above.
Temperature: $\pm 0.5$ K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Seawater

VARIABLES:
T/K = 283 - 298

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, ( H/\text{dimensionless} )</th>
<th>100 ( w_t ) (compiler)</th>
<th>10(^4 ) ( x_t ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.6500</td>
<td>9.864</td>
</tr>
<tr>
<td>15</td>
<td>0.1399</td>
<td>0.6470</td>
<td>9.818</td>
</tr>
<tr>
<td>20</td>
<td>0.1624</td>
<td>0.6428</td>
<td>9.753</td>
</tr>
<tr>
<td>25</td>
<td>0.2001</td>
<td>0.6377</td>
<td>9.675</td>
</tr>
</tbody>
</table>

The Henry's law constants (dimensionless) were derived from the best-fit lines of van't Hoff plots:

\[ \log_e H = - \frac{3649}{T(K)} + 10.63 \]

ORIGINAL MEASUREMENTS:
Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S.

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Henry's law constant, ( H/\text{dimensionless} )</th>
<th>100 ( w_t ) (compiler)</th>
<th>10(^4 ) ( x_t ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.1046</td>
<td>0.6500</td>
<td>9.864</td>
</tr>
<tr>
<td>15</td>
<td>0.1399</td>
<td>0.6470</td>
<td>9.818</td>
</tr>
<tr>
<td>20</td>
<td>0.1624</td>
<td>0.6428</td>
<td>9.753</td>
</tr>
<tr>
<td>25</td>
<td>0.2001</td>
<td>0.6377</td>
<td>9.675</td>
</tr>
</tbody>
</table>

The Henry's law constants (dimensionless) were derived from the best-fit lines of van't Hoff plots:

\[ \log_e H = - \frac{3649}{T(K)} + 10.63 \]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The multiple equilibrium technique was used to measure the Henry's law constant as described elsewhere (ref. 1). A known volume of seawater in a syringe was shaken with a known volume of trichloromethane. After equilibration, the headspace was separated and analyzed for trichloromethane. 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) Samples from 45° N to 65° S in the Atlantic in late 1981.

ESTIMATED ERRORS:
Solubility: ± 5.5 % std. dev.
Temperature: ± 0.2 K.

REFERENCES:
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Cesium chloride; CsCl; [7647-17-8]
(3) Water; H₂O; [7732-18-5]

VARIABLES:
T/K = 293
Concentration

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c₂/mol dm⁻³</th>
<th>c₁/mol m⁻³</th>
<th>100 w₁/ (compiler)</th>
<th>10⁻³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.5</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>1.0</td>
<td>64.5</td>
<td>0.6828</td>
<td>1.221</td>
</tr>
<tr>
<td></td>
<td>1.5</td>
<td>58.5</td>
<td>0.5830</td>
<td>1.143</td>
</tr>
<tr>
<td></td>
<td>2.0</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>2.5</td>
<td>56.0</td>
<td>0.5081</td>
<td>-</td>
</tr>
<tr>
<td></td>
<td>3.0</td>
<td>52.5</td>
<td>0.4560</td>
<td>1.237</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Trichloromethane was introduced from a microburet into an aqueous solution of cesium chloride which contained octanoic acid as an indicator. The mixture was vigorously stirred. The pH of the solution at first remained constant right up to the appearance of a second phase, i.e., up to the saturation of the aqueous phase with trichloromethane, after which the pH began to rise. The solubility was calculated from the volume of the aqueous phase and the volume of trichloromethane used for the saturation.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: ± 10 %.
Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
(2) Hydrogen chloride; HCl; [7647-01-0]
(3) Water; H₂O; [7732-18-5]

VARIABLES:

T/K = 288 - 333

EXPERIMENTAL VALUES:

Solubility of CHCl₃ in 10 % HCl solution:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10³ wᵢ</th>
<th>100 wᵢ (compiler)</th>
<th>10⁴ xᵢ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>6.70</td>
<td>0.670</td>
<td>10.71</td>
</tr>
<tr>
<td>30</td>
<td>4.44</td>
<td>0.444</td>
<td>7.086</td>
</tr>
<tr>
<td>45</td>
<td>2.36</td>
<td>0.236</td>
<td>3.759</td>
</tr>
<tr>
<td>60</td>
<td>1.34</td>
<td>0.134</td>
<td>2.132</td>
</tr>
</tbody>
</table>

Solubility of CHCl₃ in 20 % HCl solution:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10³ wᵢ</th>
<th>100 wᵢ (compiler)</th>
<th>10⁴ xᵢ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>9.20</td>
<td>0.920</td>
<td>15.58</td>
</tr>
<tr>
<td>30</td>
<td>5.16</td>
<td>0.516</td>
<td>8.706</td>
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<tr>
<td>45</td>
<td>2.84</td>
<td>0.284</td>
<td>4.781</td>
</tr>
<tr>
<td>60</td>
<td>1.50</td>
<td>0.150</td>
<td>2.522</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic method which was used for the solubility determination consisted of the saturation of nitrogen with the solute vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of trichloromethane. After 2 - 3 hours, the solution became saturated and samples were taken periodically (ref. 1). The trichloromethane concentration in the aqueous solution was determined by GLC. On average, 3 - 5 measurements were taken at each temperature.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: ± 15 %.
Temperature: ± 0.05 K.

REFERENCES:

### COMPONENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Lithium chloride; LiCl; [7447-41-8]
3. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.


### VARIABLES:

\[ \text{T}/\text{K} = 293 \]

Concentration

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(c_x/\text{mol dm}^3)</th>
<th>(c_y/\text{mol m}^3)</th>
<th>100 (w_x) (compiler)</th>
<th>10⁵ (x_y) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.5</td>
<td>66.8</td>
<td>0.7880</td>
<td>1.212</td>
</tr>
<tr>
<td>1.0</td>
<td>64.5</td>
<td>0.7503</td>
<td>1.168</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>60.0</td>
<td>0.6921</td>
<td>1.091</td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>58.5</td>
<td>0.6675</td>
<td>1.065</td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>56.0</td>
<td>0.6320</td>
<td>1.022</td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>52.0</td>
<td>0.5805</td>
<td>1.003</td>
<td></td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Trichloromethane was introduced from a microburet into an aqueous solution of lithium chloride which contained octanoic acid as indicator. The mixture was vigorously stirred. The pH of the solution at first remained constant right up to the appearance of a second phase, i.e., up to the saturation of the aqueous phase with trichloromethane, after which the pH began to rise. The solubility was calculated from the volume of the aqueous phase and the volume of trichloromethane used for the saturation.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: ± 10 %.
Temperature: ± 0.5 K (compiler).

### COMPONENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Potassium chloride; KCl; [7447-40-7]
3. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.


### VARIABLES:

\[ \text{T}/\text{K} = 293 \]

Concentration

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>(t/°C)</th>
<th>(c_x/\text{mol dm}^3)</th>
<th>(c_y/\text{mol m}^3)</th>
<th>100 (w_x) (compiler)</th>
<th>10⁵ (x_y) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.5</td>
<td>56.0</td>
<td>0.6535</td>
<td>1.021</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Trichloromethane was introduced from a microburet into an aqueous solution of potassium chloride which contained octanoic acid as indicator. The mixture was vigorously stirred. The pH of the solution at first remained constant right up to the appearance of a second phase, i.e., up to the saturation of the aqueous phase with trichloromethane, after which the pH began to rise. The solubility was calculated from the volume of the aqueous phase and the volume of trichloromethane used for the saturation.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: ± 10 %.
Temperature: ± 0.5 K (compiler).
### COMPONENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Potassium chloride; KCl; [7447-40-7]
3. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.


### VARIABLES:

T/K = 293
Concentration

### EXPERIMENTAL VALUES: (continued)

<table>
<thead>
<tr>
<th>t/°C</th>
<th>c₁/mol dm⁻³</th>
<th>c₂/mol m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10¹ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.0</td>
<td>50.0</td>
<td>0.5692</td>
<td>0.9160</td>
</tr>
<tr>
<td>1.5</td>
<td>41.0</td>
<td></td>
<td>0.4591</td>
<td>0.7610</td>
</tr>
<tr>
<td>2.0</td>
<td>29.2</td>
<td></td>
<td>0.3131</td>
<td>0.5542</td>
</tr>
<tr>
<td>2.5</td>
<td>24.2</td>
<td></td>
<td>0.2546</td>
<td>0.4639</td>
</tr>
</tbody>
</table>

### COMPONENTS:

1. Trichloromethane (chloroform); CHCl₃; [67-66-3]
2. Rubidium chloride; RbCl; [7791-11-9]
3. Water; H₂O; [7732-18-5]

### ORIGIN OF MATERIALS:

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

### METHOD/APPARATUS/PROCEDURE:

Trichloromethane was introduced from a microburet into an aqueous solution of rubidium chloride which contained octanoic acid as indicator. The mixture was vigorously stirred. The pH of the solution at first remained constant right up to the appearance of a second phase, i. e., up to the saturation of the aqueous phase with trichloromethane, after which the pH began to rise. The solubility was calculated from the volume of the aqueous phase and the volume of trichloromethane used for the saturation.

### ESTIMATED ERRORS:

Solubility: ± 10 %.
Temperature: ± 0.5 K (compiler).
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); CHCl₃; [67-66-3]
Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H₂O; [7732-18-5]

VARIABLES:

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>cᵣ/mol dm⁻³</th>
<th>cᵣ/mol m⁻³</th>
<th>10⁷ wᵣ</th>
<th>10³ xᵣ</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.5</td>
<td>57.2</td>
<td>0.6707</td>
<td>1.0390</td>
</tr>
<tr>
<td>1.0</td>
<td>51.0</td>
<td>0.5837</td>
<td>0.9236</td>
<td></td>
</tr>
<tr>
<td>1.5</td>
<td>42.6</td>
<td>0.4791</td>
<td>0.7730</td>
<td></td>
</tr>
<tr>
<td>2.0</td>
<td>37.6</td>
<td>0.4156</td>
<td>0.6850</td>
<td></td>
</tr>
<tr>
<td>2.5</td>
<td>30.9</td>
<td>0.3361</td>
<td>0.5660</td>
<td></td>
</tr>
<tr>
<td>3.0</td>
<td>25.8</td>
<td>0.2754</td>
<td>0.4742</td>
<td></td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Trichloromethane was introduced from a microburet into an aqueous solution of sodium chloride which contained octanoic acid as indicator. The mixture was vigorously stirred. The pH of the solution at first remained constant right up to the appearance of a second phase, i.e., up to the saturation of the aqueous phase with trichloromethane, after which the pH began to rise. The solubility was calculated from the volume of the aqueous phase and the volume of trichloromethane used for the saturation.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: ± 10 %. Temperature: ± 0.5 K (compiler).

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Water-d₂; D₂O; [7789-20-0]
(2) Trichloromethane (chloroform); CHCl₃; [67-66-3]
Hutchison, C. A.; Lyon, A. M.

VARIABLES:

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 wᵣMᵣ⁺/mol g⁻¹</th>
<th>10⁷ wᵣ</th>
<th>10³ xᵣ</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>4.15 × 10⁻³</td>
<td>8.31 × 10⁻²</td>
<td>4.93</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 1 to 15 volume ratio mixture of heavy water and trichloromethane was introduced into an equilibration flask and then lowered into a water thermostat. The assembly was shaken mechanically for about 90 minutes 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.

The description was taken from a secondary source (ref. 1). The original 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: ± 0.6 × 10⁻⁴ avg. dev. Temperature: ± 0.05 K.

REFERENCES:
### COMPONENTS:
1. Triiodomethane (iodoform); CHI₃; [75-47-8]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:
Dehn, W. M.

### VARIABLES:

| T/K | 293 - 298 |

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g/˚˚</th>
<th>100 w/ (compiler)</th>
<th>10² x/ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 - 25</td>
<td>1.0 × 10⁴</td>
<td>1.0 × 10⁴</td>
<td>4.57</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**
Excess triiodomethane in 5 cm³ water samples were enclosed in small vials which, when stoppered, were shaken until equilibria were established. The solutions were filtered into weighed crucibles and reweighed. After drying in vacuum desiccators, the crucibles were again weighed and the loss of water calculated. No great accuracy was claimed for the experiments.

**SOURCE AND PURITY OF MATERIALS:**
1. From reliable firms; "not always pure."
2. Distilled (compiler).

**ESTIMATED ERRORS:**
Solubility: Not specified.
Temperature: ± 5 K.

### COMPONENTS:
1. Triiodomethane (iodoform); CHI₃; [75-47-8]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:
van Arkel, A. E.; Vles, S. E.

### VARIABLES:

| T/K | 303 |

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>m_k/mol kg⁻¹</th>
<th>100 w/ (compiler)</th>
<th>10² x/ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>3 × 10⁴</td>
<td>1.18 × 10²</td>
<td>5.41</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 (compiler).
**COMPONENTS:**

1. Triiodomethane (iodoform); CHI₃; [75-47-8]
2. Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Booth, H. S.; Everson, H. E.  

---

**VARIABLES:**

77K = 298

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>t°C</th>
<th>(g/V_i) kg m⁻³</th>
<th>(100 , w_i) (compiler)</th>
<th>(10^3 , x_i) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>&lt; 0.2</td>
<td>&lt; 0.02</td>
<td>&lt; 4.6</td>
</tr>
</tbody>
</table>

**PREPARED BY:**

A. L. Horvath

---

**METHOD/APPARATUS/PROCEDURE:**

Equilibrium was ensured through repeated shaking and centrifuging of a triiodomethane and water mixture in a stoppered Goetz tube and returning it to a constant temperature water bath. The difference between the total amount of triiodomethane which was added and the amount remaining in excess was taken as the amount of triiodomethane dissolved in the known volume of water. The determination of the excess amount of triiodomethane added is described by Hanslick (ref. 1).

---

**SOURCE AND PURITY OF MATERIALS:**

1. Commercial reagent, C. P. grade, used as received.
2. Distilled.

**ESTIMATED ERRORS:**

Solubility: < 100 %.
Temperature: ± 1 K (compiler).

**REFERENCES:**

COMPONENTS:
(1) Bromochloromethane; CH₂BrCl; [74-97-5]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

CRITICAL EVALUATION:

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

The solubility of bromochloromethane (1) in water (2) has been studied by three workers, whereas the solu­bility of water (2) in bromochloromethane (1) has been reported in one paper only.

Part 1. The solubility of bromochloromethane (1) in water (2) has been studied by three workers. The ex­perimental data of Tewari et al. (ref. 1) and Miller et al. (ref. 2) are in excellent agreement and the mass per cent (1) value of 1.646 at 298.15 K is recommended. In both cases the modified generator column method was used, but the analytical method was more advanced in the latter case. (For a comparison, see the two compilation sheets.) The single mass per cent (1) data point of 1.5 g(1)/100 g soln. at 293.15 K, reported by O’Connell (ref. 3) is considered as tentative. Whether the solubilities at 293.15 and 298.15 K are consistent with the general trend of temperature dependence remains to be investigated.

Part 2. The solubility of water (2) in bromochloromethane (1) has been reported in only one paper, that of O’Connell (ref. 3) and there are no other measurements for comparison. Therefore, it is not possible to perform a critical evaluation. The readers are referred to the compilation sheet for further details.

REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Bromochloromethane; CH₂BrCl; [74-97-5]
(2) Water; H₂O; [7732-18-5]

O'Connell, W. L.

VARIABLES:

\[ T/K = 293 \]

PREPARED BY:

A. L. Horvath

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( g_1/g_2 )</th>
<th>( 10^3 x_2 ) (compiler)</th>
<th>100 ( g_2/g_1 )</th>
<th>( 10^3 x_2 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.5</td>
<td>2.08</td>
<td>9.0 \times 10^{-2}</td>
<td>6.43</td>
</tr>
</tbody>
</table>

EXPERIMENTAL VALUES:

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Details are not available.

SOURCE AND PURITY OF MATERIALS:
(1) Dow Chemicals Co., used as received.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

(1) Bromochloromethane; CH₂BrCl; [74-97-5]
(2) Water; H₂O; [7732-18-5]

Tewari, Y. B.; Miller, M. M.; Wasik, S. P.; Martire, D. E.


VARIABLES:

\[ T/K = 298 \]

PREPARED BY:

A. L. Horvath

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( c_1/mol \cdot m^3 )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>( 10^3 x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>125</td>
<td>1.646</td>
<td>2.325</td>
</tr>
</tbody>
</table>

EXPERIMENTAL VALUES:

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The modified generator column method was used. A chromatographic column was coated with bromochloromethane. An aqueous phase was generated by pumping water through the coated generator column. The aqueous solution was analyzed by gas chromatography. The gas chromatograph was equipped with a flame ionization detector. On average, at least three measurements were taken.

SOURCE AND PURITY OF MATERIALS:
(1) Source not known, at least 99 % pure by GC analysis.
(2) Baker-analyzed HPLC grade.

ESTIMATED ERRORS:
Solubility: ± 1.0 %.
Temperature: ± 0.1 K.
### COMPONENTS:
1. Bromochloromethane; CH₂BrCl; [74-97-5]
2. Water; H₂O; [7732-18-5]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>nV₂⁻¹/mol m⁻³</th>
<th>100 w₁ (compiler)</th>
<th>10¹ x₁ (compiler)</th>
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</thead>
<tbody>
<tr>
<td>25</td>
<td>129.0</td>
<td>1.646</td>
<td>2.325</td>
</tr>
</tbody>
</table>

### ORIGINAL MEASUREMENTS:
Miller, M. M.; Wasik, S. P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

### VARIABLES:
T/K = 298

### PREPARED BY:
A. L. Horvath

### METHOD/APPARATUS/PROCEDURE:
A saturated aqueous solution was prepared by passing water through a column which was packed with glass beads coated with bromochloromethane. The saturated solution was then pumped through an extractor column and bromochloromethane was extracted into an analytical column. The samples were analyzed with a liquid chromatograph equipped with both an UV absorbance and a fluorescent detector with excitation filters. The peak area was established using a Hewlett-Packard integrator.

### SOURCE AND PURITY OF MATERIALS:
1. Eastman Kodak Co., Commercial quality, used as received.
2. Double distilled.

### ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1 K (compiler).
COMPONENTS:
(1) Dibromomethane; CH₂Br₂; [74-95-3]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

CRITICAL EVALUATION:

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

Part 1. The solubility of dibromomethane (1) in water (2) has been studied by 6 workers. The Compilation Sheets immediately follow this Critical Evaluation.

The experimental data of all investigators in the 273 to 323 K temperature range are sufficiently reliable for use in the smoothing equation (see Figure 1) with the exception of the experimental work of Booth and Everson (ref. 1) which is markedly higher than other results and is therefore rejected. The combined data of 5 laboratories were correlated to give the following equation for mass per cent (1) solubility:

\[ \text{Solubility} \left[ \text{100 w}_1 \right] = 10.1890 - 0.06336789 \left( \frac{T}{K} \right) + 1.10906 \times 10^4 \left( \frac{T}{K} \right)^2 \]

which produced a standard deviation of 4.4 x 10⁻². This equation represents the combined solubility data with a maximum deviation of 6.0 % (usually less) and may be considered recommended to represent the data in the 273 to 323 K temperature interval.

The recommended mass per cent solubility values at 5 K intervals for dibromomethane (1) in water (2) are recorded in Table 1.

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w₁</th>
<th>10² x₁</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 273.15</td>
<td>1.155</td>
<td>1.209</td>
</tr>
<tr>
<td>5 278.15</td>
<td>1.144</td>
<td>1.198</td>
</tr>
<tr>
<td>10 283.15</td>
<td>1.138</td>
<td>1.191</td>
</tr>
<tr>
<td>15 288.15</td>
<td>1.138</td>
<td>1.191</td>
</tr>
<tr>
<td>20 293.15</td>
<td>1.144</td>
<td>1.198</td>
</tr>
<tr>
<td>25 298.15</td>
<td>1.155</td>
<td>1.209</td>
</tr>
<tr>
<td>30 303.15</td>
<td>1.171</td>
<td>1.226</td>
</tr>
<tr>
<td>35 308.15</td>
<td>1.194</td>
<td>1.251</td>
</tr>
<tr>
<td>40 313.15</td>
<td>1.221</td>
<td>1.279</td>
</tr>
<tr>
<td>45 318.15</td>
<td>1.254</td>
<td>1.313</td>
</tr>
<tr>
<td>50 323.15</td>
<td>1.293</td>
<td>1.356</td>
</tr>
</tbody>
</table>

Part 2. The solubility of water (2) in dibromomethane (1) has been reported in one work (ref. 2) and, therefore, no Critical Evaluation has not been performed. The readers are referred to the relevant Compilation Sheet.
COMPONENTS:
(1) Dibromomethane; CH₂Br₂; [74-95-3]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

CRITICAL EVALUATION: (continued)

![Graph of solubility of Dibromomethane (1) in Water (2).]

Figure 1. Solubility of Dibromomethane (1) in Water (2).

REFERENCES:


## COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dibromomethane; CH₂Br₂; [74-95-3]

(2) Water; H₂O; [7732-18-5]

VARIABLES: PREPARED BY:

T/K = 273 - 303

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g₁/g₂</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.173</td>
<td>1.15</td>
<td>1.20</td>
</tr>
<tr>
<td>10</td>
<td>1.146</td>
<td>1.13</td>
<td>1.18</td>
</tr>
<tr>
<td>20</td>
<td>1.148</td>
<td>1.13</td>
<td>1.18</td>
</tr>
<tr>
<td>30</td>
<td>1.176</td>
<td>1.16</td>
<td>1.21</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The solubility of dibromomethane in water was determined in specially designed flasks with calibrated capillary cylinders. After the samples reached equilibrium in a thermostatic bath, their volumes and weights were used to determine the solubility values.

**SOURCE AND PURITY OF MATERIALS:**

(1) Merck reagent, redistilled and washed before use, b. p. = 97.8°C.

(2) Distilled.

**ESTIMATED ERRORS:**

- Solubility: ± 0.5%.
- Temperature: ± 0.02 K.

**REFERENCES:**


COMPONENTS:
(1) Dibromomethane; CH₂Br₂; [74-95-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
van Arkel, A. E.; Vles, S. E.

VARIABLES:
TIK = 303

EXPERIMENTAL VALUES:
<table>
<thead>
<tr>
<th>t/°C</th>
<th>m/mol kg⁻¹</th>
<th>10² x₁</th>
<th>100 w₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30.0</td>
<td>6.86 × 10⁻²</td>
<td>0.123</td>
<td>1.174</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) Dibromomethane; CH₂Br₂; [74-95-3]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Both, H. S.; Everson, H. E.

VARIABLES:
TIK = 298

EXPERIMENTAL VALUES:
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<tr>
<th>t/°C</th>
<th>100 V₁/V₂</th>
<th>100 w₁ (compiler)</th>
<th>10¹ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.0</td>
<td>0.70</td>
<td>1.71</td>
<td>1.80</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The equilibrium was ensured through repeated shaking and centrifuging of a dibromomethane and water mixture in a stoppered Goetz tube and returning the sample to a constant temperature water bath. The difference between the total amount of dibromomethane which was added and the amount remaining in excess was taken as the amount of dibromomethane dissolved in the known volume of water. The determination of the excess amount of dibromomethane added is described by Hanslick (ref. 1).

SOURCE AND PURITY OF MATERIALS:
(1) Commercial reagent, C. P. grade, used as received.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 1 K (compiler).

REFERENCES:
## COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dibromomethane; CH₂Br₂; [74-95-3]

(2) Water; H₂O; [7732-18-5]

---

## EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 w₁</th>
<th>10¹ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10¹ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td></td>
<td></td>
<td>0.07</td>
<td>6.71</td>
</tr>
<tr>
<td>25</td>
<td>1.1</td>
<td>1.14</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient for dibromomethane (γ⁺) in water. Degasged water cells were submerged in a thermostated water bath. Dibromomethane was injected into a mixture cell, a magnetic stirrer was turned on, and 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) Dow Chemicals Co., used as received.

---

**PREPARED BY:**
A. L. Horvath
The dichloromethane (1) and water (2) binary system is discussed in two parts; part 1 is dichloromethane (1) in water (2) and part 2 is water (2) in dichloromethane (1).

Part 1. The solubility of dichloromethane (1) in water (2) has been studied by at least 32 groups of workers. Most of the data reported have been considered for inclusion in the smoothing equation with the following exclusions. The experimental data of Salkowski (ref. 1) are markedly lower than the other results and are therefore rejected. The solubility data of Booth and Everson (ref. 2), Alexandrova et al. (ref. 3), and Sadovnikova et al. (refs. 4 and 5) are several per cent higher than the smoothed solubility values and are also rejected. The data of Sabinin et al. (ref. 6) between 293.15 and 303.15 K show a temperature dependence of solubility much too large and are therefore rejected. The data of Svetlanov et al. (ref. 7) also show a change in solubility far too large between 288.15 and 333.15 K and are rejected; however, the value at 303.15 K is retained. The solubilities calculated from the distribution coefficients of Prosyanov et al. (ref. 8) are in very poor agreement, providing no confidence in their values which are regarded as dubious. The solubility data of Howe et al. (ref. 9) between 283.15 and 303.15 K show a maximum which is inconsistent with the trend of temperature dependence of solubility and are rejected; however, the value at 293.15 K is retained.

The remaining data of 25 laboratories by Rex (ref. 10), van Arkel and Vles (ref. 11), Bakowski and Treszczanowicz (ref. 12), Niini (ref. 13), McGovern (ref. 14), Donahue and Bartell (ref. 15), Kudryavtseva and Krutikova (ref. 16), Maretic and Sirocic (ref. 17), du Pont (ref. 18), Svetlanov et al. (ref. 7), Karger et al. (ref. 19), Antropov et al. (ref. 20), McConnell et al. (ref. 21), Pearson and McConnell (ref. 22), Archor and Stevens (ref. 23), Sato and Nakijima (ref. 24), Coca et al. (ref. 25), Hutchinson et al. (ref. 26), Leighton and Calo (ref. 27), Lincoff and Gossett (ref. 28), Gossett (ref. 29), Warner et al. (ref. 30), Howe et al. (ref. 9), Vogel (ref. 31), and Wright et al. (ref. 32), were used to obtain the following smoothing equation for solubility in mass per cent (1):

\[
\text{Solubility} \left[100 \, w_1\right] = 58.838 - 0.38224 \left(T/K\right) + 6.3928 \times 10^{-4} \left(T/K\right)^2
\]

This equation represents the combined data with a 0.37 standard deviation in the 273 to 310 K temperature range.

The curve obtained from the smoothing equation shows a distinct minimum at 299 K as seen in Figure 1. The appearance of the minimum for the solubility versus temperature behavior is discussed in the Preface.

The recommended mass per cent solubility values at 5 K intervals for dichloromethane (1) in water (2) are presented in the Table 1.

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility [100 , w_1]</th>
<th>\text{10}^3 \times x_t</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.126</td>
<td>4.587</td>
</tr>
<tr>
<td>5</td>
<td>1.977</td>
<td>4.260</td>
</tr>
<tr>
<td>10</td>
<td>1.860</td>
<td>4.004</td>
</tr>
<tr>
<td>15</td>
<td>1.766</td>
<td>3.799</td>
</tr>
<tr>
<td>20</td>
<td>1.722</td>
<td>3.703</td>
</tr>
<tr>
<td>25</td>
<td>1.701</td>
<td>3.657</td>
</tr>
<tr>
<td>30</td>
<td>1.712</td>
<td>3.681</td>
</tr>
<tr>
<td>35</td>
<td>1.754</td>
<td>3.773</td>
</tr>
</tbody>
</table>

(continued next page)
COMPONENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

March 1993.

CRITICAL EVALUATION: (continued)

Part 2. The solubility of water (2) in dichloromethane (1) has been reported from 19 laboratories. The solubility measurements cover the 253 to 313 K temperature range as represented in Figure 2.

The data reported have been considered for inclusion in the smoothing equation with the following exclusions. The data of Bakowski and Tersczanowicz (ref. 12), Niini (ref. 13), Donahue and Bartell (ref. 15), and Kudryavtseva and Krutikova (ref. 16) are markedly higher than other results and are therefore rejected. The measured solubility of Alexandrova et al. (ref. 3), and Sadovnikova et al. (refs. 4 and 5) are several per cent lower than the smoothed solubility and are also rejected. The solubilities calculated from the distribution coefficients of Prosyanov et al. (ref. 33), are in very poor agreement, providing no confidence in their values which are regarded as dubious.

The remaining data of 11 laboratories by Staverman (Ref. 34), McGovern (ref. 14), Davies et al. (ref. 35), Maretic and Sirocic (ref. 17), Sabinin et al. (ref. 6), Lees and Sarram (ref. 36), Antropov et al. (ref. 20), Archer and Stevens (ref. 23), Coca et al. (ref. 25), Wu (ref. 37), and Ohtsuka and Kazama (ref. 38) were compiled or used for the smoothing equation. The fitting equation used was:

\[ \log_{10} x_2 = 1.8214 - 1164.63/(T/K) \]

The equation represents the combined data with a standard deviation of \( 5.8 \times 10^{-2} \) in the 253 to 313 K temperature range.

The recommended mass per cent solubility values at 5 K intervals for water (2) in dichloromethane (1) are presented in the Table 2.

The linear relation between the solubility expressed as \( \log_{10} x_2 \) versus the reciprocal of absolute temperature behavior is illustrated in Figure 2. The straight line behavior of such plots is characteristic of the solubility of water in halogenated hydrocarbons, as discussed in the Preface.

(continued next page)
CRITICAL EVALUATION: (continued)

Table 2. Recommended Solubility of Water (2) in Dichloromethane (1)

<table>
<thead>
<tr>
<th>Temperature °C</th>
<th>Solubility 100 w_2</th>
<th>10^3 x_2</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20</td>
<td>0.0353</td>
<td>1.663</td>
</tr>
<tr>
<td>-15</td>
<td>0.0434</td>
<td>2.042</td>
</tr>
<tr>
<td>-10</td>
<td>0.0522</td>
<td>2.487</td>
</tr>
<tr>
<td>-5</td>
<td>0.0640</td>
<td>3.008</td>
</tr>
<tr>
<td>0</td>
<td>0.0768</td>
<td>3.612</td>
</tr>
<tr>
<td>5</td>
<td>0.0917</td>
<td>4.308</td>
</tr>
<tr>
<td>10</td>
<td>0.109</td>
<td>5.109</td>
</tr>
<tr>
<td>15</td>
<td>0.128</td>
<td>6.021</td>
</tr>
<tr>
<td>20</td>
<td>0.151</td>
<td>7.057</td>
</tr>
<tr>
<td>25</td>
<td>0.176</td>
<td>8.226</td>
</tr>
<tr>
<td>30</td>
<td>0.204</td>
<td>9.541</td>
</tr>
<tr>
<td>35</td>
<td>0.236</td>
<td>11.015</td>
</tr>
<tr>
<td>40</td>
<td>0.271</td>
<td>12.656</td>
</tr>
</tbody>
</table>

Figure 2. Solubility of Water (2) in Dichloromethane (1).
COMPONENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

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

March 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:


17. Maretic, M.; Sirocic, V. Nafra (Zagreb) 1962, 13, 126.


(continued next page)
COMPONENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:

COMPONENTS:  
(1) Dichloromethane; CH₂Cl₂; [75-09-2]  
(2) Water; H₂O; [7732-18-5]  

ORIGINAL MEASUREMENTS:  
Rex, A.  
*Z. Phys. Chem. 1906, 55, 355-70.*

VARIABLES:  
77K = 273 - 303  

PREPARED BY:  
A. L. Horvath

EXPERIMENTAL VALUES:  

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 g₁/g₂ (compiler)</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>2.363</td>
<td>2.30</td>
<td>4.97</td>
</tr>
<tr>
<td>10</td>
<td>2.122</td>
<td>2.08</td>
<td>4.48</td>
</tr>
<tr>
<td>20</td>
<td>2.000</td>
<td>1.96</td>
<td>4.22</td>
</tr>
<tr>
<td>30</td>
<td>1.969</td>
<td>1.93</td>
<td>4.16</td>
</tr>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:  
The dichloromethane in water solubility was determined in specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostatic bath, their volumes and weights were determined in order to calculate the solubilities.

SOURCE AND PURITY OF MATERIALS:  
(1) Kahlbaum, redistilled and washed before use, b.p. = 41°C.  
(2) Distilled.

ESTIMATED ERRORS:  
Solubility: Not specified.  
Temperature: ± 0.5 K (compiler).

COMPONENTS:  
(1) Dichloromethane; CH₂Cl₂; [75-09-2]  
(2) Water; H₂O; [7732-18-5]  

ORIGINAL MEASUREMENTS:  
Salkowski, E.  
*Biochem. Z. 1920, 107, 191-201.*

VARIABLES:  
77K = 293  

PREPARED BY:  
A. L. Horvath

EXPERIMENTAL VALUES:  

<table>
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<tr>
<th>t/°C</th>
<th>g₁V₁/kg m³ (compiler)</th>
<th>100 w₁ (compiler)</th>
<th>10³ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>12.24</td>
<td>1.211</td>
<td>2.59</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:  
A volumetric method similar to that introduced by Alexejev was used. Dichloromethane was gradually added to water from a pipet under constant agitation. The appearance of clouding was the indication of saturation.

SOURCE AND PURITY OF MATERIALS:  
(1) Kahlbaum, used as received.  
(2) Distilled (compiler).

ESTIMATED ERRORS:  
Solubility: Not specified.  
Temperature: ± 2 K (compiler).
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<th>ORIGINAL MEASUREMENTS:</th>
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</thead>
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<tr>
<td>(1) Dichloromethane; CH₂Cl₂; [75-09-2]</td>
<td>van Arkel, A. E.; Vles, S. E.</td>
</tr>
</tbody>
</table>

<table>
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<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
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<tbody>
<tr>
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<td>A. L. Horvath</td>
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<table>
<thead>
<tr>
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<tr>
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<td>METHOD/APPARATUS/PROCEDURE:</td>
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<tr>
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</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Source and purity not given.</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>

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dichloromethane; CH₂Cl₂; [75-09-2]</td>
<td>Bakowski, S.; Treszczanowicz, E.</td>
</tr>
<tr>
<td>(2) Water; H₂O; [7732-18-5]</td>
<td><em>Przemysł Chemiczny 1937, 21, 204-6.</em></td>
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<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
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</thead>
<tbody>
<tr>
<td>T/K = 293</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</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>
<tbody>
<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
</tr>
<tr>
<td>The water content of a liquid mixture was determined in a specially constructed apparatus which consisted of a 250 cm³ flask, a Vigreux type column, two water condensers, a U-shaped measuring tube, an electric heater, and a thermometer. The volume of water was determined in a calibrated tube with an accuracy of 0.01 cm³.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Merck reagent, dried by means of CaCl₂ before use.</td>
</tr>
<tr>
<td>(2) Distilled (compiler).</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>ESTIMATED ERRORS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solubility: ± 0.01 cm³.</td>
</tr>
<tr>
<td>Temperature: ± 0.5 K (compiler).</td>
</tr>
</tbody>
</table>
### COMPONENTS: ORIGINAL MEASUREMENTS:

<table>
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<tr>
<th>Component</th>
<th>Original Measurements</th>
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<tbody>
<tr>
<td>(2) Dichloromethane; CH₂Cl₂; [75-09-2]</td>
<td></td>
</tr>
</tbody>
</table>

### VARIABLES:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K</td>
<td>293</td>
</tr>
</tbody>
</table>

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 wᵦ</th>
<th>10⁵ xᵦ (compiler)</th>
<th>100 wₓ</th>
<th>10⁵ xₓ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.629</td>
<td>3.50</td>
<td>0.239</td>
<td>1.12</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The changes resulting from the addition of dichloromethane to water were determined by the measurement of both the density and refractive index of the saturated solutions. A conventional refractometer and a dilatometer were used for the measurements.

**SOURCE AND PURITY OF MATERIALS:**

(1) Kahlbaum, dried over P₂O₅ and redistilled before use.
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: ± 12 %.
Temperature: ± 0.5 K (compiler).

---

### COMPONENTS: ORIGINAL MEASUREMENTS:

<table>
<thead>
<tr>
<th>Component</th>
<th>Original Measurements</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Dichloromethane; CH₂Cl₂; [75-09-2]</td>
<td></td>
</tr>
</tbody>
</table>

### VARIABLES:

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K</td>
<td>273 - 303</td>
</tr>
</tbody>
</table>

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t°C</th>
<th>100 wᵦ</th>
<th>10⁵ xᵦ (compiler)</th>
<th>100 wₓMᵦₓ/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>8.49 × 10⁻²</td>
<td>400</td>
<td>4.71 × 10⁻²</td>
</tr>
<tr>
<td>25</td>
<td>1.67 × 10⁻¹</td>
<td>788</td>
<td>9.27 × 10⁻¹</td>
</tr>
<tr>
<td>30</td>
<td>1.96 × 10⁻¹</td>
<td>925</td>
<td>10.90 × 10⁻¹</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Dichloromethane was shaken with water for about 12 hours in a paraffin thermostat bath. The water content of the organic phase was determined using the Karl Fischer titration method. All measurements were carried out in duplicate and the average of the two measurements was reported. A full description of the method is given in a thesis (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

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

**REFERENCES:**

COMPONENTS: 
(1) Dichloromethane; CH₂Cl₂; [75-09-2] 
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS: 
McGovern, E. W. 

VARIABLES: 
T/K = 263 - 308

PREPARED BY: 
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁</th>
<th>10³ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10³ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-10</td>
<td>-</td>
<td>0.056</td>
<td>2.63</td>
<td></td>
</tr>
<tr>
<td>0</td>
<td>2.00</td>
<td>4.31</td>
<td>0.079</td>
<td>3.71</td>
</tr>
<tr>
<td>10</td>
<td>1.62</td>
<td>3.48</td>
<td>0.110</td>
<td>5.17</td>
</tr>
<tr>
<td>20</td>
<td>1.40</td>
<td>3.00</td>
<td>0.150</td>
<td>7.03</td>
</tr>
<tr>
<td>25</td>
<td>1.32</td>
<td>2.83</td>
<td>0.198</td>
<td>9.27</td>
</tr>
<tr>
<td>30</td>
<td>1.29</td>
<td>2.76</td>
<td>0.200</td>
<td>9.36</td>
</tr>
<tr>
<td>35</td>
<td>1.27</td>
<td>2.72</td>
<td>0.228</td>
<td>10.66</td>
</tr>
</tbody>
</table>

Solubility data as a function of temperature were presented in graphical form only, except the tabulated data point at 25°C.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: 
Equilibrium was ensured through repeated shaking and centrifuging of a dichloromethane and water mixture in a stoppered Goetz tube and returning the sample to a constant temperature water bath. The difference between the total amount of dichloromethane which was added and the amount remaining in excess was taken as the amount of dichloromethane dissolved in the known volume of water. The determination of the excess amount of dichloromethane added is described by Hanslick (ref. 1).

REFERENCE:
COMPONENTS:
(1) Water; H₂O; [7732-18-5]
(2) Dichloromethane; CH₂Cl₂; [75-09-2]

ORIGINAL MEASUREMENTS:
Davies, W.; Jagger, J. B.; Whalley, H. K.

VARIABLES:

| T/K | 253 - 313 |

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^3 x_i</th>
<th>10^3 x_j (compiler)</th>
<th>100 w_i/M_i/mol g⁻¹ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-20</td>
<td>0.3 x 10⁻¹</td>
<td>1.4</td>
<td>1.66 x 10⁻³</td>
</tr>
<tr>
<td>-10</td>
<td>0.4 x 10⁻¹</td>
<td>1.9</td>
<td>2.22 x 10⁻³</td>
</tr>
<tr>
<td>0</td>
<td>0.7 x 10⁻¹</td>
<td>3.3</td>
<td>3.88 x 10⁻³</td>
</tr>
<tr>
<td>10</td>
<td>1.0 x 10⁻¹</td>
<td>4.7</td>
<td>5.55 x 10⁻³</td>
</tr>
<tr>
<td>20</td>
<td>1.4 x 10⁻¹</td>
<td>6.6</td>
<td>7.77 x 10⁻³</td>
</tr>
<tr>
<td>30</td>
<td>1.9 x 10⁻¹</td>
<td>8.9</td>
<td>10.5 x 10⁻³</td>
</tr>
<tr>
<td>40</td>
<td>2.6 x 10⁻¹</td>
<td>12.1</td>
<td>14.4 x 10⁻³</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A mixture of water and dichloromethane was agitated in a flask until equilibrium was established. The apparatus was assembled in a water thermostat bath. The equilibrium was established after 30 minutes. The pipette used for withdrawing samples from the mixture was fitted with a cotton wool filter at the tip to prevent ice particles from being withdrawn at low temperatures. The organic layer was titrated with Karl Fischer reagent.

SOURCE AND PURITY OF MATERIALS:
(1) Distilled.
(2) Commercial quality, source and purity not given.

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

COMPONENTS:
(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Donahue, D. J.; Bartell, F. E.

VARIABLES:

| T/K | 298 |

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>10^3 x_i</th>
<th>100 w_j</th>
<th>10^2 x_j (compiler)</th>
<th>100 w_j (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>4.2</td>
<td>1.950</td>
<td>1.13</td>
<td>0.242</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A mixture of dichloromethane and water was placed in a glass stoppered flask and was shaken intermittently for at least three days in a water bath held at constant temperature. The organic phase was analyzed for water content using the Karl Fischer titration methods. The concentration of dichloromethane in the aqueous phase was analyzed interferometrically.

SOURCE AND PURITY OF MATERIALS:
(1) Reagent grade, purified by fractional distillation before use.
(2) Purified by distillation.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.1 K.
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]  
   Kudryavtseva, G. I.; Krutikova, A. D.  

(2) Water; H₂O; [7732-18-5]  

### VARIABLES:

\[ T/K = 293 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( w_{1} )</th>
<th>10³ ( x_{1} ) (compiler)</th>
<th>100 ( w_{2} )</th>
<th>10³ ( x_{2} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.89</td>
<td>4.07</td>
<td>1.92</td>
<td>8.45</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**  
The mutual solubility between dichloromethane and water was determined by titration from a micro-buret until a turbidity appeared. The end point of the titration, when turbidity first appeared, was determined with an accuracy of 0.3 - 0.5 %. The titration of the solutions was done in a thermostat bath at 20°C.

**SOURCE AND PURITY OF MATERIALS:**  
(1) Source and purity not given.  
(2) Distilled (compiler).

**ESTIMATED ERRORS:**  
Solubility: ± 0.2 % by mass.  
Temperature: ± 0.5 K (compiler).

---

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]  
   Maretic, M.; Sirocic, V.  
   *Nafta (Zagreb)* 1962, 13, 126-31.

(2) Water; H₂O; [7732-18-5]  

### VARIABLES:

\[ T/K = 298 - 346 \]  
\[ P/mmHg = 750 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( w_{1} )</th>
<th>10³ ( x_{1} ) (compiler)</th>
<th>100 ( w_{2} )</th>
<th>10³ ( x_{2} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.4</td>
<td>3.00</td>
<td>0.2</td>
<td>9.36</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( P/mmHg )</th>
<th>10³ ( x_{1} ) (compiler)</th>
<th>100 ( w_{1} ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>38.3</td>
<td>750</td>
<td>0.39</td>
<td>1.81</td>
</tr>
<tr>
<td>44.0</td>
<td>750</td>
<td>0.19</td>
<td>0.89</td>
</tr>
<tr>
<td>58.0</td>
<td>750</td>
<td>0.15</td>
<td>0.70</td>
</tr>
<tr>
<td>73.0</td>
<td>750</td>
<td>0.10</td>
<td>0.47</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**  
The solubility was determined in a 50 cm³ flask containing a weighed quantity of water. Dichloromethane was added dropwise to the water until the first excess drop created turbidity. A slight turbidity immediately indicated the saturation point.

**SOURCE AND PURITY OF MATERIALS:**  
(1) Laboratory sample dried with CaCl₂ and distilled. The middle fraction was used.  
(2) Distilled.

**ESTIMATED ERRORS:**  
Solubility: ± 0.2 % by mass.  
Temperature: ± 2.0 K.
### COMPONENTS: ORIGIANL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]

(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

du Pont de Nemours & Company,


### VARIABLES:

\( T/K = 298 \)

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>100 ( w_i )</th>
<th>( 10^3 x_i ) ( (\text{compiler}) )</th>
<th>100 ( w_i M_i )/mol g(^{-1}) ( (\text{compiler}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.32</td>
<td>2.83</td>
<td>1.55 ( \times 10^2 )</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The solubility data were taken from a secondary source (ref. 1). Details and the original report are not available.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source and purity not given.

(2) Distilled (compiler).

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: \( \pm 1 \) K (compiler).

**REFERENCES:**


### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]

(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Sabinin, V. E.; Kiya-Oglu, N. V.; Gorichnina, V. P.


### VARIABLES:

\( T/K = 293 - 303 \)

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
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<tr>
<th>( t/°C )</th>
<th>100 ( w_i )</th>
<th>( 10^3 x_i ) ( (\text{compiler}) )</th>
<th>100 ( w_i M_i )/mol g(^{-1}) ( (\text{compiler}) )</th>
<th>( 10^3 x_i ) ( (\text{compiler}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>0.6</td>
<td>1.28</td>
<td>0.15</td>
<td>7.03</td>
</tr>
<tr>
<td>30</td>
<td>2.6</td>
<td>6.63</td>
<td>0.19</td>
<td>8.89</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

The saturation of dichloromethane and water mixtures occurred in a flask fitted with a thermostat jacket and a powerful stirrer. After a stirring time of 10 - 20 minutes, samples were withdrawn from both the organic and aqueous layers and the compositions were determined from their refractivity indices.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source not given. Purified by repeated distillation; density = 1.3252 g/cm\(^3\) and refractive index = 1.4233 at 20 °C.

(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: \( \pm 0.1 \) K.
### Components: Original Measurements

1. Water; \( \text{H}_2\text{O}; [7732-18-5] \)
2. Dichloromethane; \( \text{CH}_2\text{Cl}_2; [75-09-2] \)

VARIABLES:

\( T/K = 298 \)

**Experimental Values:**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^3 x_l ) (compiler)</th>
<th>( 100 w_f/M_f' ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>6.10</td>
<td>7.2 ( \times ) 10^3</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

An apparatus containing the mixture of dichloromethane and water was placed in a thermostat bath. The stirring of the mixture was accomplished by using a glass rod rotated by a horseshoe magnet for about 48 hours. 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 before use.

**Estimated Errors:**

- Solubility: \( \pm 2\% \).
- Temperature: \( \pm 0.1 \) K.

### Components: Original Measurements

1. Dichloromethane; \( \text{CH}_2\text{Cl}_2; [75-09-2] \)
2. Water; \( \text{H}_2\text{O}; [7732-18-5] \)

VARIABLES:

\( T/K = 288 - 333 \)

**Experimental Values:**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 1000 g_f/g_s )</th>
<th>( 100 w_f ) (compiler)</th>
<th>( 10^3 x_l ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>15</td>
<td>25.00</td>
<td>2.44</td>
<td>5.28</td>
</tr>
<tr>
<td>30</td>
<td>15.60</td>
<td>1.54</td>
<td>3.31</td>
</tr>
<tr>
<td>45</td>
<td>8.80</td>
<td>0.872</td>
<td>1.86</td>
</tr>
<tr>
<td>60</td>
<td>5.30</td>
<td>0.527</td>
<td>1.12</td>
</tr>
</tbody>
</table>

### Auxiliary Information

**Method/Apparatus/Procedure:**

A dynamic method was used for the solubility determination. It consisted of the saturation of nitrogen with dichloromethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of water. After 2 - 3 hours, the solution became saturated and samples were taken periodically (ref. 1). The concentration of dichloromethane in water was determined by gas-liquid chromatography. On average, 3 - 5 measurements were taken at each temperature.

### Source and Purity of Materials:

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

**Estimated Errors:**

- Solubility: \( \pm 15\% \).
- Temperature: \( \pm 0.05 \) K.

### References:

1. Treger, Yu. A.; Flid, R. M.; Spektor, S. S.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dichloromethane; CH₂Cl₂; [75-09-2]</td>
<td>Karger, B. L.; Chatterjee, A. K.; King, J. W.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>7T/K = 286</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
</tr>
</thead>
<tbody>
<tr>
<td>t°C</td>
</tr>
<tr>
<td>12.5</td>
</tr>
</tbody>
</table>

¹ Gas-liquid chromatographic parameter, from instrument calibration.

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
</thead>
<tbody>
<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
</tr>
<tr>
<td>Gas-liquid chromatography was used for the determination of the partition of dichloromethane with thin layers of water coated on Porasil D. Helium carrier gas was presaturated with water at the column temperature. The eluents were detected with an F &amp; M flame ionization detector. The partition coefficient was obtained from the slope of the straight line plot of Vᵢ/Vᵢₐ versus Vᵢ/ₐ.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) J. T. Baker Chemical Co., reagent grade, 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>

<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dichloromethane; CH₂Cl₂; [75-09-2]</td>
<td>Alexandrova, M. V.; Sadovnikova, L. V.; Martinov, W. W.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>7T/K = 293</td>
<td>Z. Maczynska</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</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>
<tbody>
<tr>
<td>METHOD/APPARATUS/PROCEDURE:</td>
</tr>
<tr>
<td>The titration method was used. Solubility data were also reported for the ternary dichloromethane-water-acetic acid system.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>SOURCE AND PURITY OF MATERIALS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Source not given. C. P. grade, used as received; n₀ = 1.4242 at 20 °C.</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: ± 0.1 K.</td>
</tr>
</tbody>
</table>
## COMPONENTS:

1. Dichloromethane; CH₂Cl₂; [75-09-2]
2. Water; H₂O; [7732-18-5]

## ORIGINAL MEASUREMENTS:

- Antropov, L. I.; Populyai, V. E.; Simonov, V. D.; Shamsutdinov, T. M.
  
  (VINITI No: 3739-71).

## VARIABLES:

\[ T/K = 291 - 299 \]

## EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°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>18</td>
<td>-</td>
<td>0.14</td>
<td>6.57</td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>2.0</td>
<td>4.31</td>
<td>-</td>
<td></td>
</tr>
<tr>
<td>22</td>
<td>-</td>
<td>0.16</td>
<td>7.50</td>
<td></td>
</tr>
<tr>
<td>26</td>
<td>-</td>
<td>0.18</td>
<td>8.43</td>
<td></td>
</tr>
</tbody>
</table>

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Alexejev’s synthetic solubility determination method was used (ref. 1). A fixed weight of dichloromethane 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:**

- Source and purity not given.
- Distilled.

**ESTIMATED ERRORS:**

- Solubility: Not specified.
- Temperature: \( \pm 0.2 \) K (compiler).

## REFERENCES:


---

## COMPONENTS:

1. Dichloromethane; CH₂Cl₂; [75-09-2]
2. Water; H₂O; [7732-18-5]

## ORIGINAL MEASUREMENTS:

Sadovnikova, L. V.; Komarova, V. P.; Alexandrova, M. V.


## VARIABLES:

\[ T/K = 311 \]

## EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°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>38</td>
<td>5.26</td>
<td>11.6</td>
<td>1.0 \times 10^2</td>
<td>0.47</td>
</tr>
</tbody>
</table>

## AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The titration method was used. The solubility was determined at the normal boiling point temperature. An ebulliometer was used to check the boiling point. The solubility data for the ternary dichloromethane-water-acetic acid system were also reported.

**SOURCE AND PURITY OF MATERIALS:**

- Source and purity not given.
- Distilled (compiler).

**ESTIMATED ERRORS:**

- Solubility: Not specified.
- Temperature: \( \pm 0.2 \) K (compiler).
COMPONENTS:
(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Sadovnikova, L. V.; Komarova, V. P.;
Alexandrova, M. V.; Serafimov, L. A.
1972, 15, 1891-4.

VARIABLES:

T/K = 293

PREPARED BY:
Z. Maczynska

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁</th>
<th>10⁶ x₁ (compiler)</th>
<th>100 w₂</th>
<th>10⁴ x₂ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>19.85</td>
<td>2.76</td>
<td>5.98</td>
<td>0.1</td>
<td>5.0</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available. Solubility data for the ternary dichloromethane-water-isobutyric acid system were also reported.

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) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Prosyannov, N. N.; Shalygin, V. A.; Zel’venskii, Ya. D.

VARIABLES:

T/K = 298 - 373

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Distribution coefficient¹, Dₓ/dimensionless</th>
<th>100 w₁</th>
<th>10⁶ x₁ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25.1</td>
<td>3920</td>
<td>0.0693</td>
<td>1.471</td>
</tr>
<tr>
<td>50.0</td>
<td>2480</td>
<td>0.2696</td>
<td>5.731</td>
</tr>
<tr>
<td>70.0</td>
<td>1650</td>
<td>0.7419</td>
<td>15.833</td>
</tr>
<tr>
<td>90.0</td>
<td>1240</td>
<td>1.6652</td>
<td>35.793</td>
</tr>
<tr>
<td>96.0</td>
<td>1130</td>
<td>2.1071</td>
<td>45.453</td>
</tr>
<tr>
<td>100</td>
<td>1080</td>
<td>2.4173</td>
<td>52.273</td>
</tr>
</tbody>
</table>

¹ Gas-liquid system analysis parameter, from calibration measurements.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The distribution coefficient was determined by distillation. An inert gas was used to take samples from the vapor phase at equilibrium. The concentration of dichloromethane 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: ± 0.5 K (compiler).
COMPONENTS:
(1) Water; H₂O; [7732-18-5]
(2) Dichloromethane; CH₂Cl₂; [75-09-2]

VARIABLES:

\[ T/K = 280 - 310 \]

EXPERIMENTAL VALUES:

\[
\log_{10} \alpha = \frac{547.33}{T(K)} - 1.0416
\]

where \( \alpha \) = Distribution Coefficient

At the normal boiling point of CH₂Cl₂, 313.15 K, \( \alpha = 50.0 \), the activity coefficient, \( \gamma_i = 67.0 \), and the mole fraction of (1) at saturation, \( x_i = 3.953 \times 10^{-3} \) (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

After equilibration of a dichloromethane and water mixture, the water content of the organic phase was determined radiometrically using tritium-labeled water. The experimental method is described in greater detail elsewhere (ref. 1).

REFERENCES:
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Dichloromethane; CH₂Cl₂; [75-09-2]  
2. Water; H₂O; [7732-18-5]  

**VARIABLES:**  
\( T/K = 298 \)

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^6 w_i )</th>
<th>( 100 w_j ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>13200</td>
<td>1.320</td>
<td>2.84</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
Saturated solutions were prepared and placed in a constant temperature thermostat bath. Water samples were extracted with n-pentane and an aliquot of the extract taken for analysis using a gas-liquid chromatograph. 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 K (compiler).

---

### REFERENCES:


---

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Dichloromethane; CH₂Cl₂; [75-09-2]  
2. Water; H₂O; [7732-18-5]  

**VARIABLES:**  
\( T/K = 298 \)

**EXPERIMENTAL VALUES:**

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 100 w_i )</th>
<th>( 10^3 x_i ) (compiler)</th>
<th>( 100 w_j )</th>
<th>( 10^3 x_j ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.0</td>
<td>4.22</td>
<td>0.20</td>
<td>9.34</td>
</tr>
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</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**
Details are not available.  
Data were reported elsewhere (ref. 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: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Sato, A.; Nakijima, T.

### VARIABLES:

\[
T/K = 310
\]

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Partition coefficient(^1), (K_t/\text{dimensionless})</th>
<th>100 (w_t) ((\text{compiler}))</th>
<th>10(^3) (x_t) ((\text{compiler}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>37</td>
<td>7.2</td>
<td>2.2</td>
<td>4.75</td>
</tr>
</tbody>
</table>

\(^1\) Gas-liquid chromatographic parameter, from instrument calibration.

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

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

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

Solubility: ± 0.6 std. dev.
Temperature: ± 0.5 K \((\text{compiler})\).

---

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

**ORIGINAL MEASUREMENTS:**

Coca, J.; Diaz, R. M.; Pazos, C.

### VARIABLES:

\[
T/K = 298
\]

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 (w_t)</th>
<th>10(^3) (x_t) ((\text{compiler}))</th>
<th>100 (w_t)</th>
<th>10(^3) (x_t) ((\text{compiler}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>1.37</td>
<td>2.94</td>
<td>0.18</td>
<td>8.43</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The mutual solubility data were determined by the method described by Othmer *et al.* (ref. 1). A 10 cm\(^3\) dichloromethane sample was added to water from a buret and agitated until the solution became turbid. The appearance of the turbidity indicated the formation of a second phase. The solubilities were calculated by means of known densities and volumes.

**SOURCE AND PURITY OF MATERIALS:**

(1) Probus reagent, further purified by distillation in a heli-packing column.
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 0.5 K \((\text{compiler})\).

### REFERENCES:

(1) Othmer, D. F.; White, R. E.; Trueges, E.
<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAl MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Dichloromethane; CH₂Cl₂ [75-09-2]</td>
<td>Hutchinson, T. C.; Hellebust, J. A.; Tam, D.; et al.</td>
</tr>
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<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 VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>ρ/thesized m³</td>
</tr>
<tr>
<td>25</td>
<td>19.4</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

An excess of dichloromethane was added to water and stirred vigorously for 24 hours. After settling at 25°C for 48 hours, the solution was extracted with cyclohexane. The samples were analyzed using an Aminco-Bowman spectrophotofluorometer. A detailed description of the method is reported elsewhere (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

(1) Aldrich Chemicals, highest grade, used as received. |
| (2) Double distilled. |

**ESTIMATED ERRORS:**

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

**REFERENCES:**


<table>
<thead>
<tr>
<th>COMPONENTS:</th>
<th>ORIGINAl MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(2) Dichloromethane; CH₂Cl₂ [75-09-2]</td>
<td><em>Huaxue, Shiji</em> 1981, 221-4.</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>VARIABLES:</th>
<th>PREPARED BY:</th>
</tr>
</thead>
<tbody>
<tr>
<td>T/K = 278 - 308</td>
<td>A. L. Horvath</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>EXPERIMENTAL VALUES:</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>t/°C</td>
<td>10⁶ w₁</td>
</tr>
<tr>
<td>5</td>
<td>1313</td>
</tr>
<tr>
<td>10</td>
<td>1440</td>
</tr>
<tr>
<td>15</td>
<td>1525</td>
</tr>
<tr>
<td>20</td>
<td>1609</td>
</tr>
<tr>
<td>25</td>
<td>1779</td>
</tr>
<tr>
<td>30</td>
<td>1948</td>
</tr>
<tr>
<td>35</td>
<td>2075</td>
</tr>
</tbody>
</table>

**AUXILIARY INFORMATION**

**METHOD/APPARATUS/PROCEDURE:**

A known volume of water was added to dried dichloromethane to prepare a series of standard solutions for establishing calibration curves and obtaining the saturated solutions at each temperature. The determination of the water content of dichloromethane was made with an RM-250 NMR spectrometer (radiation frequency of 250 MHz). The reported water peak amplitude was the mean of four readings taken at a particular temperature.

**SOURCE AND PURITY OF MATERIALS:**

(1) Distilled. |
| (2) Source not given, chromatographically pure, used as received. |

**ESTIMATED ERRORS:**

Solubility: ± 24 std. dev. |
| Temperature: 1 - 2 K. |
### COMPONENTS: ORIGINAL MEASUREMENTS:

- (1) Dichloromethane; CH₂Cl₂; [75-09-2]
- (2) Water; H₂O; [7732-18-5]

### VARIABLES:

| T/K | 275 - 298 |

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>Partition coefficient¹, $K_t$/dimensionless</th>
<th>$100 w_f$ (compiler)</th>
<th>$10^3 x_f$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.9</td>
<td>61.4</td>
<td>1.5871</td>
<td>3.409</td>
</tr>
<tr>
<td>13.5</td>
<td>111.5</td>
<td>1.4886</td>
<td>3.195</td>
</tr>
<tr>
<td>15.7</td>
<td>121.5</td>
<td>1.4904</td>
<td>3.199</td>
</tr>
<tr>
<td>17.1</td>
<td>141.6</td>
<td>1.3651</td>
<td>2.927</td>
</tr>
<tr>
<td>22.0</td>
<td>157.1</td>
<td>1.5144</td>
<td>3.251</td>
</tr>
<tr>
<td>24.9</td>
<td>161.9</td>
<td>1.6569</td>
<td>3.561</td>
</tr>
</tbody>
</table>

¹ Gas-liquid chromatographic parameter, from instrument calibration.

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A 5 μL dichloromethane sample was injected into a 2.3 liter equilibration cell containing distilled water. After the cell was shaken vigorously for about 5 minutes, 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 dichloromethane content was extracted and analyzed using a dual flame ionization detector gas chromatograph.

**SOURCE AND PURITY OF MATERIALS:**

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

### ESTIMATED ERRORS:

- Solubility: ± 4.8 %.
- Temperature: ± 0.5 K.

### COMPONENTS: ORIGINAL MEASUREMENTS:

- (1) Water; H₂O; [7732-18-5]
- (2) Dichloromethane; CH₂Cl₂; [75-09-2]

### VARIABLES:

| T/K | 298 |

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>t/°C</th>
<th>$g_i V^{-1}/kg m^3$</th>
<th>$100 w_i$ (compiler)</th>
<th>$10^3 x_i$ (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>2.00</td>
<td>0.151</td>
<td>7.08</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

Water was added gradually to 50 cm³ dichloromethane in a flask and then lowered into a thermostat bath. The flask was then shaken vigorously until the first cloud (turbidity) appeared. The water content of the sample was determined by the Karl Fischer titration method.

**SOURCE AND PURITY OF MATERIALS:**

- (1) Distilled (compiler).
- (2) Commercial JFS extra pure reagent, further purified by conventional methods before use.

**ESTIMATED ERRORS:**

- Solubility: Not specified.
- Temperature: ± 0.5 K (compiler).
COMPONENTS:
(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Lincoff, A. H.; Gossett, J. M.

VARIABLES:
\[ T/K = 293 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

EPICS Method:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 100 \ w )</th>
<th>( 10^3 \ x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 2.25 \times 10^{-3} )</td>
<td>1.7786</td>
<td>3.826</td>
</tr>
</tbody>
</table>

\[
\log_e H = -\frac{4191}{T(K)} + 8.200
\]

Batch Air Stripping Method:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 100 \ w )</th>
<th>( 10^3 \ x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>( 1.97 \times 10^{-3} )</td>
<td>2.0314</td>
<td>4.379</td>
</tr>
</tbody>
</table>

\[
\log_e H = -\frac{4472}{T(K)} + 9.035
\]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Henry's law constants were determined by EPICS and Batch Air Stripping methods. The Equilibrium Partitioning in Closed Systems (EPICS) technique compared the GL peak heights upon direct injection of headspace samples.

For the Batch Air Stripping procedure, equal volume samples were placed in serum bottles and allowed to reach equilibrium. The equilibrated headspaces containing concentrations proportional to original concentrations in the aqueous samples were analyzed. Full equilibrium was achieved in a few hours.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: \( \pm 5 - 10 \% \).
Temperature: \( \pm 0.1 \text{ K} \).
### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 283 - 308 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's Law Constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( CV \text{%} )</th>
<th>( 10^3 w_j \text{ (compiler)} )</th>
<th>( 10^3 x_j \text{ (compiler)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>9.6</td>
<td>( 1.15 \times 10^3 )</td>
<td>19.2</td>
<td>2.2513</td>
<td>4.862</td>
</tr>
<tr>
<td>17.5</td>
<td>( 1.31 \times 10^3 )</td>
<td>19.9</td>
<td>2.7492</td>
<td>5.960</td>
</tr>
<tr>
<td>24.8</td>
<td>( 2.19 \times 10^3 )</td>
<td>17.4</td>
<td>2.1422</td>
<td>4.842</td>
</tr>
<tr>
<td>34.6</td>
<td>( 3.26 \times 10^3 )</td>
<td>2.37</td>
<td>2.2150</td>
<td>4.782</td>
</tr>
</tbody>
</table>

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

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

A modification of the EPICS (Equilibrium Partitioning in Closed Systems) procedure was used for measuring Henry's law constants. A precise quantity of dichloromethane was injected into serum bottles which contained distilled water. The bottles were incubated for 18 - 24 hours at four desired temperatures in a reciprocating shaker bath. The headspace concentrations of the EPICS bottles were measured using a gas chromatograph which was equipped with a flame ionization detector. The mean of the coefficient of variation values was approximately 4.3 \%.  

**SOURCE AND PURITY OF MATERIALS:**

(1) Burdick & Jackson reagent, pesticide grade. Distilled in a glass set-up before use.
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: See above.
Temperature: \( \pm 0.1 \text{ K.} \)

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

### VARIABLES:

\[ T/K = 298 \]

### EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>Henry's law constant, ( H/m^3 \text{ atm mol}^{-1} )</th>
<th>( 100 w_j \text{ (compiler)} )</th>
<th>( 10^3 x_j \text{ (compiler)} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>24.85</td>
<td>( 3.19 \times 10^3 )</td>
<td>1.599</td>
<td>3.436</td>
</tr>
</tbody>
</table>

### SOURCE AND PURITY OF MATERIALS:

(1) Source not given. Purest quality available, used as received. Stated purity > 99 %.  
(2) Distilled and deionized.

**REFERENCES:**

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

**Howe, G. B.; Mullins, M. E.; Rogers, T. N.**


### VARIABLES:

\[ \text{VARIABLES:} \]

\[ T \text{K} = 283 - 303 \]

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
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<tr>
<th>( t/°C )</th>
<th>( 10^6 w_i )</th>
<th>( 100 w_i ) (compiler)</th>
<th>( 10^3 x_i ) (compiler)</th>
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</thead>
<tbody>
<tr>
<td>10</td>
<td>11092</td>
<td>1.1092</td>
<td>2.3736</td>
</tr>
<tr>
<td>20</td>
<td>13508</td>
<td>1.3508</td>
<td>2.8961</td>
</tr>
<tr>
<td>30</td>
<td>11211</td>
<td>1.1211</td>
<td>2.3993</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

250 cm³ bottles were filled with distilled deionized water and sealed. Measured volumes of dichloromethane were injected into the bottles through each bottle septum using a microliter syringe. Dichloromethane was in excess of the anticipated solubility limit. The bottles were shaken for one hour with 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 GL response was compared with the calibration plot.

**SOURCE AND PURITY OF MATERIALS:**

(1) Probably a commercial reagent at least 99 % pure. Used as received.
(2) Distilled and deionized.

**ESTIMATED ERRORS:**

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

### COMPONENTS: ORIGINAL MEASUREMENTS:

(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

**Vogel, A. I., rev. by Furniss, B. S.; et al.**


### VARIABLES:

\[ T \text{K} = 298 \]

**PREPARED BY:**

A. L. Horvath

### EXPERIMENTAL VALUES:

<table>
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<th>( t/°C )</th>
<th>( 100 w_i )</th>
<th>( 10^3 x_i ) (compiler)</th>
<th>( 100 w_i M_i^{-1}/mol \ g^{-1} ) (compiler)</th>
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<tbody>
<tr>
<td>25.0</td>
<td>1.30</td>
<td>2.79</td>
<td>( 1.53 \times 10^{-2} )</td>
</tr>
</tbody>
</table>

### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The solubility determination was carried out in small test tubes (e. g., 100 × 12 mm) to permit vigorous shaking of dichloromethane and water mixtures. During the experiment 0.20 cm³ dichloromethane was added to 3.0 cm³ of water and shaken. The amount of dichloromethane dissolved in water was analyzed by passing the samples through a chromatographic column.

**SOURCE AND PURITY OF MATERIALS:**

(1) Commercial reagent, purified by washing with concentrated sulfuric acid before use.
(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: Not specified.
Temperature: ± 1 K (compiler).
COMPONENTS:
(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Wright, D. A.; Sandler, S. I.; DeVoll, D.

VARIABLES:
\( T/K = 283 - 303 \)

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

\[
\begin{array}{cccc}
 t/K & \gamma^* & 100 \omega_i & 10^4 x_i \\
 10 & 235 \pm 5 & 1.977 & 4.26 \\
 20 & 251 \pm 14 & 1.849 & 3.98 \\
 30 & 250 \pm 8 & 1.858 & 4.00 \\
\end{array}
\]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of dichloromethane (\( \gamma^* \)) in water. Cells containing degassed water were submerged in a thermostated water bath. Dichloromethane was injected into the mixture cells and a magnetic stirrer was turned on. 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: See above.
Temperature: \( \pm 0.05 \) K.
COMPONENTS:
(1) Dichloromethane; CH₂Cl₂; [75-09-2]
(2) Hydrogen chloride; HCl; [7647-01-0]
(3) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

VARIABLES:
\( T/K = 288 - 333 \)
HCl concentration

EXPERIMENTAL VALUES:

Solubility of CH₂Cl₂ in 10 % HCl solution:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^3 \ w_1 )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10³ ( x_1 ) (compiler)</th>
</tr>
</thead>
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<tr>
<td>15</td>
<td>29.40</td>
<td>2.940</td>
<td>6.733</td>
</tr>
<tr>
<td>30</td>
<td>18.50</td>
<td>1.850</td>
<td>4.198</td>
</tr>
<tr>
<td>45</td>
<td>12.50</td>
<td>1.250</td>
<td>2.822</td>
</tr>
<tr>
<td>60</td>
<td>6.00</td>
<td>0.600</td>
<td>1.347</td>
</tr>
</tbody>
</table>

Solubility of CH₂Cl₂ in 20 % HCl solution:

<table>
<thead>
<tr>
<th>( t/°C )</th>
<th>( 10^3 \ w_1 )</th>
<th>100 ( w_1 ) (compiler)</th>
<th>10³ ( x_1 ) (compiler)</th>
</tr>
</thead>
<tbody>
<tr>
<td>30</td>
<td>24.50</td>
<td>2.450</td>
<td>5.909</td>
</tr>
<tr>
<td>45</td>
<td>12.00</td>
<td>1.200</td>
<td>2.862</td>
</tr>
<tr>
<td>60</td>
<td>6.50</td>
<td>0.650</td>
<td>1.543</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The dynamic method was used for the determination of the solubility. It consisted of the saturation of nitrogen with dichloromethane vapor which was then bubbled through a thermostatically controlled flask filled with a definite volume of solution. After 2 - 3 hours the solution became saturated and samples were taken periodically (ref. 1). The concentration of dichloromethane in the solution was determined by GLC. On average, 3 - 5 measurements were taken at each temperature.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Source and purity not given.
(3) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: ± 15 %
Temperature: ± 0.05 K.

REFERENCES:
(1) Treger, Yu. A.; Flid, R. M.; Spektor, S. S.
COMPONENTS:

(1) Diiodomethane; CH₂I₂; [75-11-6]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

CRITICAL EVALUATION:

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

Part 1. The solubility of diiodomethane (1) in water (2) has been studied by four groups of workers. The experimental data of Gross and Saylor (ref. 1) and Andrews and Keefer (ref. 2) are supported by the descriptions of the methods used for determining the reported data. Details are not available for methods, apparatus, and procedures used by van Arkel and Vles (ref. 3) and O'Connell (ref. 4) for obtaining the solubility data.

The three solubility values, see (refs. 1, 3, and 4), between 293.15 and 303.15 K compare favorably with the selected value, whereas the datum of Andrews and Keefer (ref. 2) at 298.15 K is low and classified as doubtful. More accurate solubility determinations are required, meanwhile, the tentative mas per cent solubility of diiodomethane (1) in water (2) is 0.124 at 303.15 K.

Part 2. The only datum available for the solubility of water (2) in diiodomethane (1) is that of Hutchison and Lyon (ref. 5) and so no Critical Evaluation is possible. The interested reader is referred to the relevant Compilation Sheet for the experimental solubility.

REFERENCES:

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<th>COMPONENTS:</th>
<th>ORIGINAl MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Diodomethane; CH$_2$I$_2$; [75-11-6]</td>
<td>Gross, P. M.; Saylor, J. H.</td>
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<table>
<thead>
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<th>VARIABLES:</th>
<th>PREPARED BY:</th>
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<tbody>
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<td>A. L. Horvath</td>
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<table>
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</table>

<table>
<thead>
<tr>
<th>AUXILIARY INFORMATION</th>
</tr>
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</table>

**METHOD/APPARATUS/PROCEDURE:**

An excess of diiodomethane in 500 g water was shaken for 12 hours in a thermostat bath. Samples were then withdrawn and read against water in an interferometer made by Zeiss (ref. 1). A detailed description of the complete method and procedure is given in a Ph. D. thesis (ref. 2).

**SOURCE AND PURITY OF MATERIALS:**

(1) Eastman Kodak Co., shaken with Na$_2$S$_2$O$_3$ solution, washed with distilled water, dried, and fractionally frozen twice before use.

(2) Distilled.

**ESTIMATED ERRORS:**

Solubility: ± 2.0 %.

Temperature: ± 0.02 K.

**REFERENCES:**


---

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<tr>
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<th>ORIGINAL MEASUREMENTS:</th>
</tr>
</thead>
<tbody>
<tr>
<td>(1) Diodomethane; CH$_2$I$_2$; [75-11-6]</td>
<td>van Arkel, A. E.; Vles, S. E.</td>
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</tr>
<tr>
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**METHOD/APPARATUS/PROCEDURE:**

Details are not available.

**SOURCE AND PURITY OF MATERIALS:**

(1) Source and purity not given.

(2) Distilled (compiler).

**ESTIMATED ERRORS:**

Solubility: Not specified.

Temperature: ± 0.5 K (compiler).
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Water; H$_2$O; [7732-18-5]
(2) Diiodomethane; CH$_2$I$_2$; [75-11-6]

Hutchison, C. A.; Lyon, A. M.
_Columbia University Report A-745, July 1, 1943._

VARIABLES:
$T/K = 298$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>$t/°C$</th>
<th>$100 , \omega_{MI} / \text{mol g}^{-1}$</th>
<th>$100 , \omega_{I}$ (compiler)</th>
<th>$10^3 , x_I$ (compiler)</th>
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<tbody>
<tr>
<td>25</td>
<td>$1.207 \times 10^{-3}$</td>
<td>2.174 $\times 10^{-2}$</td>
<td>3.222</td>
</tr>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A 1 to 15 volume ratio mixture of water and diiodomethane was introduced into an equilibration flask and then the flask was lowered into a water thermostat bath. The assembly was shaken mechanically for about 90 minutes at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fischer titration method. The determination was done in triplicate.

The description was taken from a secondary source (ref. 1). The original report is no longer available.

SOURCE AND PURITY OF MATERIALS:
(1) Distilled.
(2) Source not given, purified and dried before use.

ESTIMATED ERRORS:
Solubility: $\pm 1.5 \times 10^{-3}$ avg. dev.
Temperature: $\pm 0.05$ K.

REFERENCES:

COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Diiodomethane; CH$_2$I$_2$; [75-11-6]
(2) Water; H$_2$O; [7732-18-5]

Andrews, L. J.; Keefer, R. M.

VARIABLES:
$T/K = 298$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>$t/°C$</th>
<th>$c_i / \text{mol m}^{-3}$</th>
<th>$100 , \omega_{I}$ (compiler)</th>
<th>$10^3 , x_I$ (compiler)</th>
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<tbody>
<tr>
<td>25.0</td>
<td>3.11</td>
<td>8.35 $\times 10^{-2}$</td>
<td>5.62</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Water was mixed with diiodomethane in a glass-stoppered Erlenmeyer flask which was then placed in a constant temperature bath and rotated for 30 hours. The organic halide content of the aqueous solution was extracted with n-hexane. The optical density of the extract was measured against a n-hexane blank using a Beckman spectrophotometer (ref. 1).

SOURCE AND PURITY OF MATERIALS:
(1) Prepared from iodoform at the University of California; b. p. = 71.0 - 71.5 °C at 18 mmHg.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: $\pm 0.5$ K (compiler).

REFERENCES:
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<tr>
<th>COMPONENTS:</th>
<th>ORIGINAL MEASUREMENTS:</th>
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</thead>
<tbody>
<tr>
<td>(1) Diiodomethane; CH₂I₂; [75-11-6]</td>
<td>O’Connell, W. L.</td>
</tr>
</tbody>
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<table>
<thead>
<tr>
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<th>PREPARED BY:</th>
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<td>A. L. Horvath</td>
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<table>
<thead>
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<tbody>
<tr>
<td>t/°C</td>
</tr>
<tr>
<td>20</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Details are not available.

SOURCE AND PURITY OF MATERIALS:
(1) Dow Chemicals Co., used as received.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).

COMPONENTS:
(1) Water-d₂; D₂O; [7789-20-0]
(2) Diiodomethane; CH₂I₂; [75-11-6]

VARIABLES:
T/K = 298

EXPERIMENTAL VALUES:
<table>
<thead>
<tr>
<th>t/°C</th>
<th>100 w₁ M₁⁻¹/mol g⁻¹</th>
<th>10⁴ x₁</th>
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</thead>
<tbody>
<tr>
<td>25</td>
<td>1.017 x 10⁻³</td>
<td>2.04 x 10⁻²</td>
</tr>
</tbody>
</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
A 1 to 15 volume ratio mixture of heavy water and diiodomethane was introduced into an equilibration flask and then lowered into a water thermostat bath. The assembly was shaken mechanically for about 90 minutes 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.

The description was taken from a secondary source (ref. 1). The original 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: ± 0.3 x 10⁻⁴ avg. dev.
Temperature: ± 0.05 K.

REFERENCES:
CRITICAL EVALUATION:

The solubility of iodomethane (1) in water (2) has been studied by 8 groups of workers; whereas, the solubility of water (2) in iodomethane (1) has not been investigated yet.

The experimental data of Glew (ref. 1) covering the 273 to 323 K temperature range are significantly higher than the likely solubility. Furthermore, the continuous decrease in solubility with temperature between 273 and 323 is not consistent with the formation of a minimum shown by most similar binary systems. Therefore, these data are classed as doubtful and are rejected. The presence of a minimum in the solubility versus temperature behavior for the halogenated hydrocarbon-water systems is discussed in the Preface.

The solubility data of Balls (ref. 2) between 283 and 298 K show a continuous rise with temperature which is contrary to the trends shown by all other investigators and are therefore rejected. The single data point of Liss and Slater (ref. 3) at 293 K is lower than other results and is likewise rejected.

The remaining data of Rex (ref. 4), Fühner (ref. 5), van Arkel and Vles (ref. 6), Swain and Thornton (ref. 7), and Hunter-Smith et al. (ref. 8) are in reasonable agreement, although further studies are required before any values can be recommended. The tentative mass per cent solubilities of iodomethane (1) in water (2) over the 273 to 313 K temperature range were used to obtain the following equation:

$$\text{Solubility \[100 \text{ w}_1\] = 19.0036 - 0.11723 \frac{(T/K)}{T/K} + 1.95356 \times 10^{-4} \left(\frac{T}{K}\right)^2}$$

This regression equation was established using the combined data from (refs. 4 - 8), which yielded a standard deviation of $4.3 \times 10^{-2}$.

The tentative mass per cent solubility values at 5 K intervals for iodomethane (1) in water (2) are presented in Table 1. The curve obtained from the smoothing equation is shown in Figure 1. It shows a distinct minimum at 300.0 K, as discussed in the Preface.

Table 1. Tentative Solubility of Iodomethane (1) in Water (2)

<table>
<thead>
<tr>
<th>Temperature, °C</th>
<th>Solubility, 100 w_1</th>
<th>10^3 x_1</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1.557</td>
<td>2.003</td>
</tr>
<tr>
<td>5</td>
<td>1.510</td>
<td>1.942</td>
</tr>
<tr>
<td>10</td>
<td>1.472</td>
<td>1.893</td>
</tr>
<tr>
<td>15</td>
<td>1.444</td>
<td>1.856</td>
</tr>
<tr>
<td>20</td>
<td>1.425</td>
<td>1.831</td>
</tr>
<tr>
<td>25</td>
<td>1.417</td>
<td>1.821</td>
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<tr>
<td>30</td>
<td>1.418</td>
<td>1.822</td>
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<tr>
<td>35</td>
<td>1.430</td>
<td>1.838</td>
</tr>
<tr>
<td>40</td>
<td>1.450</td>
<td>1.864</td>
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</table>

(continued next page)
COMPONENTS:
(1) Iodomethane; CH₃I; [74-88-4]
(2) Water; H₂O; [7732-18-5]

EVALUATOR:
A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
March 1993.

CRITICAL EVALUATION: (continued)

Figure 1. Solubility of Iodomethane (1) in Water (2).

REFERENCES:
5. Fühner, H. Ber. 1924, 57, 510.
COMPONENTS:
(1) Iodomethane; CH$_3$I; [74-88-4]
(2) Water; H$_2$O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Rex, A.

VARIABLES:
$T/\mathbf{K} = 273 - 303$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

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<th>100 $g_{s}/g_{t}$</th>
<th>100 $w_r$ (compiler)</th>
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<tr>
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<td>1.419</td>
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<td>1.793</td>
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<tr>
<td>30</td>
<td>1.429</td>
<td>1.409</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The solubility of iodomethane in water was determined using specially designed flasks with calibrated capillary cylinders. After samples were equilibrated in a thermostatic bath, their volumes and weights were determined and their solubilities were calculated.

SOURCE AND PURITY OF MATERIALS:
(1) Kahlbaum reagent, redistilled and washed and equilibrated before use, b.p. = 42.8 °C.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).

COMPONENTS:
(1) Iodomethane; CH$_3$I; [74-88-4]
(2) Water; H$_2$O; [7732-18-5]

ORIGINAL MEASUREMENTS:
Fühner, H.
Ber. 1924, 57, 510-5.

VARIABLES:
$T/\mathbf{K} = 295$

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

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<td>1.75</td>
<td>$9.59 \times 10^3$</td>
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</table>

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Iodomethane was added gradually to 100 cm$^3$ water from a pipette under continuous stirring and shaking in an oil bath. The appearance of the first cloud (turbidity) indicated the saturation of the solution. The solubility was calculated from the volume of iodomethane added to a known quantity of water.

SOURCE AND PURITY OF MATERIALS:
(1) E. Merck, Darmstadt, further purified before use.
(2) Distilled (compiler).

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 0.5 K (compiler).
### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Iodomethane; CH₃I; [74-88-4]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

van Arkel, A. E.; Vles, S. E.


### VARIABLES:

\( \frac{T}{K} = 303 \)

### PREPARED BY:

A. L. Horvath

### EXPERIMENTAL VALUES:

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<th>( m_i/mol \cdot kg^{-1} )</th>
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<th>10³ ( x_i ) (compiler)</th>
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### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**
Details are not available.

**SOURCE AND PURITY OF MATERIALS:**

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

**ESTIMATED ERRORS:**

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

---

### COMPONENTS: ORIGINAL MEASUREMENTS:

1. Iodomethane; CH₃I; [74-88-4]
2. Water; H₂O; [7732-18-5]

### ORIGINAL MEASUREMENTS:

Glew, D. N.


### VARIABLES:

\( \frac{T}{K} = 273 - 323 \)

### PREPARED BY:

A. L. Horvath

### EXPERIMENTAL VALUES:

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<th>( ldm³ \cdot mmHg \cdot mol⁻¹ )</th>
<th>( P_i/c_i )</th>
<th>Henry's law constant, ( H/m³ \cdot atm \cdot mol⁻¹ ) (compiler)</th>
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<th>10³ ( x_i ) (compiler)</th>
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### AUXILIARY INFORMATION

**METHOD/APPARATUS/PROCEDURE:**

The experiment was performed in an Ostwald type solubility apparatus consisting of a gas burette and a solubility pipette. The gas burette containing iodomethane and the solubility pipette filled with water were connected and allowed to equilibrate in a thermostat bath. The volume, pressure, and temperature were monitored and Henry's law constants were calculated. A summary of the experiment is given elsewhere (ref. 1).

**SOURCE AND PURITY OF MATERIALS:**

1. British Drug House, washed with KOH solution, dried, redistilled and dried again with Ca metal filings.
2. Gas free, deionizes by ion exchange resin.

**ESTIMATED ERRORS:**

Solubility: ± 0.5 %. Temperature: ± 0.2 K.

**REFERENCES:**

COMPONENTS:
(1) Iodomethane; CH₃I; [74-88-4]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
$\frac{T}{k} = 303 - 313$
Pressure

EXPERIMENTAL VALUES:

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<th>$P_x/c_1$</th>
<th>Henry's law constant, $H/m^3 \text{atm} \text{mol}^{-1}$</th>
<th>$100 w_x$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
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<td>40.35</td>
<td>6920</td>
<td>$9.105 \times 10^3$</td>
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<td>1.881</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The measuring apparatus was described by Brown et al. (ref. 1). Iodomethane gas was admitted to the measurement apparatus from a storage bulb by distillation. The gas volume absorbed by water was estimated using a gas buret. The temperature was controlled by a water bath and the equilibrium was aided by a magnetic stirrer in the equilibration bulb. The concentration in the solution was calculated from the pressure and volume measured.

SOURCE AND PURITY OF MATERIALS:
(1) Eastman Kodak Co., redistilled before use.
(2) Double distilled.

ESTIMATED ERRORS:
Solubility: $\pm 3\%$.
Temperature: $\pm 0.01$ K.
Pressure: $\pm 0.05$ mmHg.

REFERENCES:

COMPONENTS:
(1) Iodomethane; CH₃I; [74-88-4]
(2) Water; H₂O; [7732-18-5]

VARIABLES:
$\frac{T}{k} = 283 - 298$

EXPERIMENTAL VALUES:

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<th>$t/°C$</th>
<th>Henry's law constant, $H$/dimensionless</th>
<th>$100 w_x$ (compiler)</th>
<th>$10^3 x_1$ (compiler)</th>
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<tr>
<td>10</td>
<td>0.12 ± 0.04</td>
<td>1.464</td>
<td>1.882</td>
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<td>15</td>
<td>0.15 ± 0.05</td>
<td>1.829</td>
<td>1.829</td>
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<tr>
<td>20</td>
<td>0.17 ± 0.03</td>
<td>1.514</td>
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<tr>
<td>25</td>
<td>0.20 ± 0.04</td>
<td>1.539</td>
<td>1.979</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The measurements involved repeated equilibration of nitrogen with a water sample containing iodomethane. The sample was shaken vigorously at the required temperature in a constant temperature bath for 30 minutes. The equilibrated gas phase was then injected into a gas chromatograph. The experiments were performed at least three times at 10, 15, 20, and 25 °C. Each experiments involved about six equilibrations.

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Distilled.

ESTIMATED ERRORS:
Solubility: See above.
Temperature: $\pm 0.5$ K (compiler).
COMPONENTS: ORIGINAL MEASUREMENTS:
(1) Iodomethane; CH₃I; [74-88-4]
(2) Water; H₂O; [7732-18-5]
Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S.

VARIABLES:
T/K = 283 - 298

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>℃</th>
<th>Henry’s law constant, H/dimensionless</th>
<th>100 wₓ (compiler)</th>
<th>10³ xₓ (compiler)</th>
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<tr>
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<td>0.1425</td>
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<td>25</td>
<td>0.2151</td>
<td>1.4308</td>
<td>1.839</td>
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The Henry’s law constant (H) was derived from the best-fit lines of van’t Hoff plots:

\[
\log_e H = -\frac{3541}{T(K)} + 10.34
\]

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The multiple equilibration technique as described elsewhere (ref. 1) was used to measure the Henry’s law constants. A known volume of water in a syringe was shaken with a known volume of pure iodomethane. 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: ORIGINAL MEASUREMENTS:
(1) Iodomethane; CH₃I; [74-88-4]
(2) Seawater
Liss, P. S.; Slater, P. G.

VARIABLES:
T/K = 293

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
<thead>
<tr>
<th>℃</th>
<th>Henry’s law constant, H/dimensionless</th>
<th>100 wₓ (compiler)</th>
<th>100 wₓMₓ/m mol g⁻¹ (compiler)</th>
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<tbody>
<tr>
<td>20</td>
<td>0.24</td>
<td>1.093</td>
<td>7.7 x 10⁻³</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
Details are not available except that the data originate from Lovelock (ref. 1).

SOURCE AND PURITY OF MATERIALS:
(1) Source and purity not given.
(2) Samples from Atlantic ocean.

ESTIMATED ERRORS:
Solubility: Not specified.
Temperature: ± 2 K (compiler).

REFERENCES:
(1) Lovelock, J. E. Personal communication.
COMPONENTS:
(1) Iodomethane; CH$_3$I; [74-88-4]
(2) Water-d$_2$; D$_2$O; [7789-20-0]

ORIGINAL MEASUREMENTS:
Swain, C. G.; Thornton, E. R.

VARIABLES:
\[ T/K = 303 - 313 \]

PREPARED BY:
A. L. Horvath

EXPERIMENTAL VALUES:

<table>
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<tr>
<th>t/°C</th>
<th>( \frac{P_i}{c_i} )</th>
<th>( H )</th>
<th>( 100 \omega_i )</th>
<th>( 10^3 x_i )</th>
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<td>7450</td>
<td>9.803 \times 10^4</td>
<td>1.226</td>
<td>1.748</td>
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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
The measuring apparatus was described by Brown *et al.* (ref. 1). Iodomethane gas was admitted to the measurement apparatus from a storage bulb by distillation. The gas volume absorbed by heavy water was determined in the gas buret. The temperature was controlled by a water bath and the equilibrium was aided by a magnetic stirrer in the equilibration bulb. The concentration of the solution was calculated from the pressures and volumes measured.

SOURCE AND PURITY OF MATERIALS:
(1) Eastman Kodak Co., redistilled before use.
(2) Liquid Carbonic Co., 99.5 % pure, used as received.

ESTIMATED ERRORS:
Solubility: ± 3 %
Temperature: ± 0.01 K.
Pressure: ± 0.05 mmHg.

REFERENCES:
(1) Brown, H. C.; Taylor, M. D.; Gerstein, M.
Bromoform
  see methane, tribromo-
Carbon tetrabromide
  see methane, tetrabromo-
Carbon tetrachloride
  see methane, tetrachloro-
Chloroform
  see methane, trichloro-
Iodoform
  see methane, triiodo-
Magnesium sulfate
  see sulfuric acid, magnesium salt

Methane, bromochloro-
  + water
  + water, Milang
  + water, Myponga
  + humic acid
    E143, 144-145
  + water, Myponga

Methane, bromodichloro-
  + water
  + water, Milang
  + water, Myponga
    E71, 72-74
  + water, Myponga

Methane, dibromo-
  + water
    E146-E147, 148-150
  + water, Milang
  + water, Myponga

Methane, dibromochloro-
  + water
  + water, Milang
  + water, Myponga
    E76, 77-79
  + water, Myponga

Methane, dichloro-
  + water
  + water, Milang
  + water, Myponga
  + water, Myponga
  + water-d2
  + water, sea-
    E151-E155, 156-175
  + water, sea-
  + water, sea-
  + water, sea-
  + water-

Methane, diiodo-
  + water
    E177, 178-180
  + water-d2
  + water-

Methane, iodo-
  + water
    E181-E182, 183-186
  + water-
  + water-

Methane, tetrabromo-
  + water
  + water, MQ-
  + water, Municipal tap, (PASE)
  + water, sea-
  + calcium chloride (aqueous)
  + water-d2
  + water-
  + water-
  + water-
  + water-

Methane, tetrachloro-
  + water
  + water, MQ-
  + water, Municipal tap, (PASE)
  + water, sea-
  + calcium chloride (aqueous)
  + water
  + water-
  + water-
  + water-
  + water-
  + water-
  + water-
  + water-
  + water-
  + water-
  + water-

E17-E21, 22-26, 28-30, 32, 34, 36, 39-44, 46-49, 51-57

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+ water 64
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+ water, Milang 90
+ water, Myponga 90
+ water, Myponga
+ humic acid 91
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+ water 1
Methane, trichloro-
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+ water, Milang 132
+ water, MQ- 132
+ water, Municipal tap, (PASE) 133
+ water, Myponga 133
+ water, Myponga
+ humic acid 134
+ water, sea 134-135
+ cesium chloride (aqueous)
+ water 136
+ hydrogen chloride (aqueous)
+ water 137
+ lithium chloride (aqueous)
+ water 138
+ potassium chloride (aqueous)
+ water 138-139
+ rubidium chloride (aqueous)
+ water 139
+ sodium chloride (aqueous)
+ water 140
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+ water E3-E5, 6-13
+ water, sea 13-16
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Sodium sulfate
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+ methane, trichloro-
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+ methane, diiodo- 180
+ methane, tetrachloro-
+ methane, trichloro- 69-70
+ methane, trichloro- 140
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Page numbers preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

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