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SOLUBILITY DATA SERIES

Volume 60

HALOGENATED METHANES WITH WATER

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES

Volume 60

HALOGENATED METHANES WITH WATER

Volume Editors

Ari L. Horváth
Imperial Chemical Industries PLC
Runcorn, UK

Forrest W. Getzen
North Carolina State University
Raleigh, NC, USA

Contributors

Z. Maczynska
Institute of Physical Chemistry
Warsaw, Poland

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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:

C_5H_8	cyclopentane
	2-methyl-1,3-butadiene
	1,4-pentadiene
	1-pentyne
C_5H_{10}	cyclopentane
	3-methyl-1-butene
	2-methyl-2-butene
	1-pentene
	2-pentene
C_5H_{12}	2,2-dimethylpropane
	2-methylbutane
	pentane
$C_5H_{12}O$	2,2-dimethyl-1-propanol
	2-methyl-1-butanol
	2-methyl-2-butanol
	3-methyl-1-butanol
	3-methyl-2-butanol
	1-pentanol
	2-pentanol
	3-pentanol
$C_6H_{12}O$	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 cpmponent 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 $x(1)$:

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

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

2. *Ionic mole fractions* of salt i, x_{i+}, x_{i-}:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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:

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

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

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

$$\rho_1 = g_1/V \qquad [11]$$

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

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

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*, ρ:

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

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

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

Thermodynamics of Solubility

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 ybe described in the Preface to that volume.

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

F.W. Getzen
Raleigh, NC, USA

G.T. Hefter
Perth, WA, Australia

D.G. Shaw
Fairbanks, AK, USA

January, 1994

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

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

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

PREFACE

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:

1. Wisniak, J.; Tamir, A. *Liquid-Liquid Equilibrium and Extraction. A Literature Source Book*, Elsevier, Amsterdam, 1980, 1252 pp.

2. Wisniak, J.; Herskowitz, M. *Solubility of Gases and Solids. A Literature Source Book*, Parts A and B, Elsevier, Amsterdam, 1984, 2070 pp.

B. Secondary Sources:

1. Ware, G. W. *Review of Environmental Contamination and Toxicology*, Vol. 116, Springer-Verlag, New York, 1990, 200 pp.

2. Freier, R. K. *Aqueous Solutions*, Vol. 1, Walter de Gruyter, Berlin, 1976, 477 pp.

3. Landolt-Börnstein Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik, *Gleichgewichte der Absorption von Gasen in Flüssigkeiten*, Vol. 4a/c1, Springer-Verlag, Berlin, 1976, 479 pp.

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Table 1. Sources of Solubility Data (continued)

8. *Beilsteins Handbuch der Organischen Chemie*, Beilstein Institut für Literatur der Organischen Chemie, Springer-Verlag, Berlin, Vol. 1, 1918-
9. *Kirk-Othmer Encyclopedia of Chemical Technology*, 1st, 2nd, 3rd, and 4th eds., Wiley, New York.
10. Seidell, A. *Solubility of Organic Compounds*, 3rd ed., Van Nostrand, New York, 1963, 926 pp.
11. Linke, W. F. *Solubilities of Inorganic and Metal-Organic Compounds*, 4th Ed., van Nostrand, Princeton, N. J., Vol. 1, 1958, Vol. 2, 1965.
12. Stephen, H.; Stephen, T. *Solubilities of Inorganic and Organic Compounds*, Vols. 1 and 2, Pergamon Press, Oxford, 1963.
13. Riddich, J. A.; Bunger, W. B. *Organic Solvents*, 3rd ed., Vol. 2, Wiley-Interscience, New York, 1970, 603 pp.
14. DECHEMA Data Serires, Gmeling, J.; Onken, U. *Vapor-Liquid Equilibrium Data Collection. Aqueous-Organic Systems, Vol. 1*, 1977.
15. Dreisbach, R. R. *Physical Properties of Chemical Compomds*, Am. Chem. Soc. Adv. in Chem. Ser. 15 (1955, 536 pp.), 22 (1959, 491 pp.), and 29(1961, 489 pp.), Washington, D. C.

C. Databases:

1. *AQUASOL database of Aqueous Solubility*, 5th., S. H. Yalkowsky, Ed., University of Arizona, Tucson, Arizona, 1991.

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 tem-perature. 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.

a. Henry's Law Constant (*H*):

$$\text{Mass }\% = \frac{\left[\dfrac{P_{vap}\,(\text{atm})\ M_{solute}}{H\,(\text{dimensionless})}\right]}{82.06\ T(\text{K})\, d_{solvent}\ \ (\text{g cm}^{-3})} \times 100$$

$$\text{Mass }\% = \frac{\left[\dfrac{P_{vap}\,(\text{atm})\ M_{solute}}{H\,(\text{m}^3\,\text{atm mol}^{-1})}\right]}{d_{solvent}\ \ (\text{g cm}^{-3})} \times 10^{-4}$$

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

b. Air/Water Partition Coefficient (K_{AW}):

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

c. Distribution Ratio (*p/c*):

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

d. Partition Coefficient (*K*):

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

e. Distribution Coefficient (K_l):

$$K_l = \text{Ostwald coefficient} = L = \frac{y_l}{x_l}$$

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

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

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

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 (CH_2Cl_2) is 2.363 g/100 g water at 0°C. The mass per cent solubility, 100 w_l, at the same temperature is required.

If 100 g water dissolves 2.363 g CH_2Cl_2, then the total mass of the solution becomes 102.363 g. This means that 100 g aqueous solution will dissolve less CH_2Cl_2 than 100 g pure water, that is,

$$100\ w_1 = \frac{2.363\ \text{g}\ CH_2Cl_2}{102.363\ \text{g soln.}}\ 100 = 2.3084\ .$$

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

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

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 relationhip suggests some inconsistency and introduces doubt concerning the reliablility of the data.

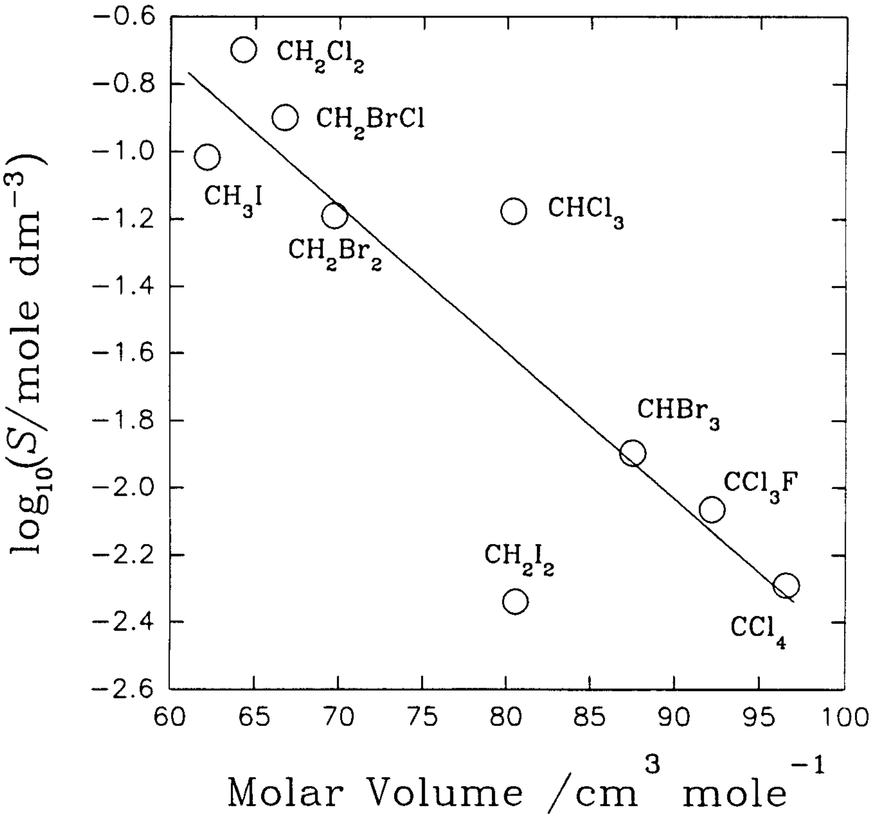

Figure 1. Logarithm of Saturated Molarity versus Solute Molar Volume at 25 °C for Halogenated Methanes in Water.

Correlation equation:

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

REFERENCES:

1. DIPPR, *Design Institute for Physical Property Data*, Am. Inst. Chem. Eng., New York, Software package for IBM PC, 1985.

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

3. Reid, R. C.; Prausnitz, J. M.; Poling, B. E. *The Properties of Gases and Liquids*, 4th ed., McGraw-Hill, New York, 1987, 742 pp.

4. Horvath, A. L. *Halogenated Hydrocarbons: Solubility-Miscibility with Water*, Marcel Dekker, New York, 1982, 889 pp.

5. Shinoda, K. *J. Phys. Chem.* 1977, *81*, 1300.

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8. Horvath, A. L.; Getzen, F. W. *Halogenated Benzenes, Toluenes and Phenols with Water*, IUPAC Solubility Data Series, *Vol. 20*, Pergamon Press, Oxford, 1985, 266 pp.

9. Horiba, S. *Memoires of the College of Science and Engineering*, Kyoto Imperial University, 1917, *Vol. 2*, p. 1-43.

COMPONENTS:

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

(2) Bromotrichloromethane; $CBrCl_3$; [75-62-7]

ORIGINAL MEASUREMENTS:

O'Connell, W. L.

Trans. Am. Inst. Mech. Eng. 1963, *226*, 126-32.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	6.0×10^{-3}	6.0×10^{-3}	6.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tribromofluoromethane; CBr_3F; [353-54-8]

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

ORIGINAL MEASUREMENTS:

O'Connell, W. L.

Trans. Am. Inst. Mech. Eng. 1963, *226*, 126-32.

VARIABLES:

T/K = 293 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	$10^5\ x_1$ (compiler)	100 g_2/g_1	$10^3\ x_2$ (compiler)
20	-	-	2.0×10^{-2}	3.0
25	4.0×10^{-2}	2.66	-	-

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) Tetrabromomethane (Carbon tetrabromide); CBr_4; [558-13-4]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.; Saylor, J. H.

J. Am. Soc. Soc. 1931, *53*, 1744-51.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	1000 g_1/g_2	100 w_1 (compiler)	10^5 x_1 (compiler)
30	0.24	2.4×10^{-2}	1.30

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:

(1) Gross, P. M. *J. Am. Chem. Soc.* 1929, *51*, 2362.
(2) Saylor, J. H. *Ph. D. thesis*, Duke University, Durham, 1930.

COMPONENTS:

(1) Tetrabromomethane (Carbon tetrabromide); CBr_4; [558-13-4]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	m_1/mol kg^{-1}	100 w_1 (compiler)	10^5 x_1 (compiler)
30	7.0×10^{-4}	2.32×10^{-2}	1.26

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:	EVALUATOR:
(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11 (2) Water; H_2O; [7732-18-5]	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 Sukornick (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:

$$\text{Solubility } [100\, w_1] = 25.0094 - 0.16263\,(T/\text{K}) + 2.6547 \times 10^{-4}\,(T/\text{K})^2$$

with a standard error of 5.0×10^{-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 Sukornick (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 Sukornick (ref. 7) at 304.15 K is low and classified as doubtful. More accurate solubility measurements are required for more reliable values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11 (2) Water; H_2O; [7732-18-5]	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)

Temperature		Solubility	
°C	K	100 w_1	$10^4 x_1$
0	273.15	0.393	5.18
5	278.15	0.312	4.10
10	283.15	0.244	3.21
15	288.15	0.189	2.48
20	293.15	0.148	1.94
25	298.15	0.119	1.56
30	303.15	0.104	1.36
35	308.15	0.103	1.35
40	313.15	0.114	1.50

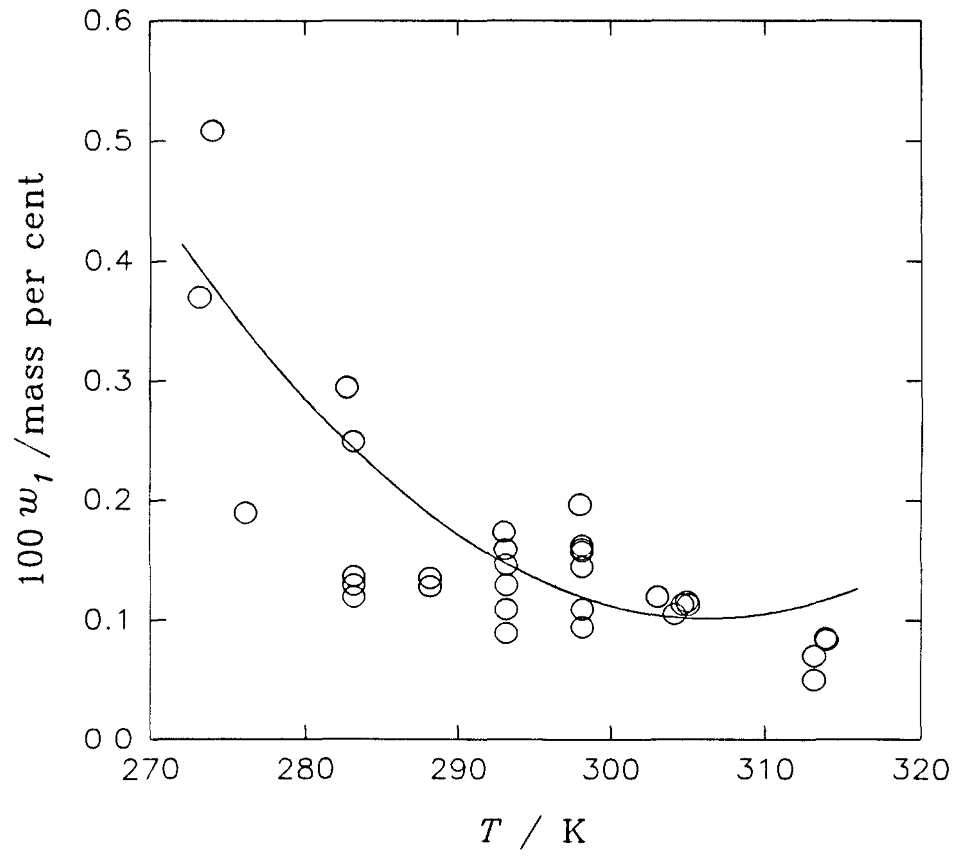

Figure 1. Solubility of Trichlorofluoromethane (1) in Water (2).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11 (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. January 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:

1. Howe, G. B.; Mullins, M. E.; Rogers, T. N. *AFESC Tyndall Air Force Base*, Report ESL-TR-86-66, Vol. 1, Florida, Sept. 1987, 86 pp. (AD-A188 517).

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

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

4. Rauws, A. G.; Olling, M.; Wibowo, A. E. *J. Pharm. Pharmac.* 1973, *25*, 718.

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8. Park, T.; Rettich, T. R.; Battino, R.; Peterson, D.; Wilhelm, E. *J. Chem. Eng. Data* 1982, *27*, 324.

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13. Privalov, P. L.; Gill, S. J. *Pure & Appl. Chem.* 1989, *61*, 1097.

14. Balls, P. W. *Ph. D. Thesis*, Univ. of East Anglia, Norwich, U. K., July 1980.

15. Zeininger, H. *Hoechst A. G.*, Internat Report, 1975.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

du Pont de Nemours & Company,

Solubility Relationship of the Freon Fluorocarbon Compounds, Tech. Bull. B-7, Wilmington, Del., 1966, 16 pp.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$100\,w_1$	$10^4\,x_1$ (compiler)	$100\,w_2$	$10^4\,x_2$ (compiler)
25	0.11	1.44	1.1×10^{-2}	8.38

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:

(1) Saunders, R. A. *Handbook of Aerosol Technology*, 2nd ed., Van Nostrand Reinhold Co., New York, 1979, p. 184.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

du Pont de Nemours & Company,

Solubility Relationships between Fluorocarbons and Water, Tech. Bull. B-43, Wilmington, Del., 1966, 17 pp.

VARIABLES:

T/K = 294 - 304

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$100\,w_1$	$10^4\,x_1$ (compiler)	$100\,w_2$	$10^4\,x_2$ (compiler)
21	-	-	9.0×10^{-3}	6.86
31	0.106	1.39	-	-

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:

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

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-5]; R-11

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

ORIGINAL MEASUREMENTS:

Rauws, A. G.; Olling, M.; Wibowo, A. E.

J. Pharm. Pharmac. 1973, *25*, 718-22.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.11	1.44	8.0 × 10^{-4}

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: ± 0.5 K (compiler).

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

McConnell, G.; Ferguson, D. M.; Pearson, C. R.

Endeavour, 1975, *34*, 13-8.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^6 g_1/g_2	100 w_1 (compiler)	10^4 x_1 (compiler)
20	1100	0.1099	1.443

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: ± 0.1 K (compiler).

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

Pearson, C. R.; McConnell, G.

Proc. Roy. Soc. B <u>1975</u>, *189*, 305-32.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6 w_1$	$100 w_1$ (compiler)	$10^4 x_1$ (compiler)
20	1100	0.110	1.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

Zeininger, H.

Hoechst A. G., Internat Report, <u>1975</u>.

VARIABLES:

$T/K = 273 - 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100 w_1$	$10^4 x_1$ (compiler)	$100 w_1 M_1^{-1}/mol\ g^{-1}$ (compiler)
0	0.37	4.87	2.69×10^{-3}
10	0.25	3.29	1.82×10^{-3}
20	0.16	2.10	1.17×10^{-3}
40	0.070	0.919	5.10×10^{-4}

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 PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

REFERENCES:

(1) Junge, C. *Z. Naturforsch.* <u>1976</u>, *31a*, 482.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, Univ. of East Anglia, Norwich, U. K., 1980, July 1980, 375 pp.

VARIABLES:

T/K = 283 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
10	2.60 ± 0.12	0.137	1.79
15	3.10 ± 0.18	0.136	1.79
20	3.40 ± 0.21	0.147	1.93
25	3.60 ± 0.22	0.163	2.14

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).

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1982, *27*, 324-6.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Bunsen coefficient, α/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
10	0.2491	0.1602	2.104

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:

(1) Douglas, E. *J. Phys. Chem.* 1964, *68*, 169.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 97-106.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Bunsen coefficient, α/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	0.246	0.158	2.08

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 CCl_3F was carried out using a Hewlett-Packard ^{63}Ni 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; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 1485-97.

VARIABLES:

$T/K = 274 - 313.95$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2\ c_1\ P_1^{-1}$ /mol dm^{-3} atm^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
0.85	3.7221	0.511	6.73
0.85	3.6555	0.502	6.61
0.85	3.6636	0.503	6.60
0.85	3.6818	0.506	6.66

(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 ^{63}Ni electron capture detector set in a constant cur-rent operating mode.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 1485-97.

VARIABLES:

T/K = 274 - 313.95

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

t/°C	$10^2\ c_1\ P_1^{-1}$ /mol dm^{-3} atm^{-1}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0.85	3.6561	0.502	6.62
0.85	3.6371	0.500	6.58
9.58	2.1092	0.290	3.81
9.59	2.1600	0.297	3.90
9.59	2.1532	0.296	3.89
9.59	2.1498	0.295	3.88
9.59	2.1760	0.299	3.93
9.59	2.1647	0.295	3.88
19.82	1.2561	0.174	2.28
19.87	1.2646	0.171	2.25
19.89	1.2756	0.176	2.30
19.89	1.2707	0.175	2.30
19.92	1.2785	0.176	2.31
19.93	1.2785	0.176	2.31
29.87	0.8697	0.120	1.58
29.87	0.8783	0.121	1.59
29.87	0.8715	0.120	1.58
29.89	0.8712	0.120	1.58
29.89	0.8645	0.120	1.58
31.50	0.8223	0.114	1.50
31.79	0.8366	0.116	1.52
31.79	0.8314	0.115	1.51
31.79	0.8543	0.118	1.55
31.89	0.8222	0.114	1.49
31.89	0.8129	0.113	1.48
31.89	0.8240	0.114	1.50
31.89	0.8263	0.114	1.50
40.73	0.6180	0.0856	1.12
40.73	0.6282	0.0870	1.14
40.73	0.5979	0.0828	1.09
40.73	0.6130	0.0849	1.11
40.76	0.6048	0.0837	1.10
40.80	0.6060	0.0839	1.10

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants, EPA Tech. Rept. PB87-212684, Cincinatti, OH., *July 1987.*

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
24.85	5.83×10^{-2}	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:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. D. *Environ. Sci. Techn.* 1979, *13*, 333.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

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

AFESC Tyndall Air Force Base, Rept. ESL-TR-86-66, Vol. 1, Florida, Sept. 1987, 86 pp. (AD-A188 571).

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
10	541	5.41×10^{-2}	7.098
20	341	3.41×10^{-2}	4.473
30	262	2.62×10^{-2}	3.437

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).

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

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

ORIGINAL MEASUREMENTS:

Sukornick, B.

Inter. J. Thermophys. 1989, *10*, 553-61.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_l$	$10^4\ x_l$ (compiler)	$100\ w_2$	$10^4\ x_2$ (compiler)
25	9.50×10^{-2}	1.25	7.0×10^{-3}	5.34

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

(1) Allied-Signal Inc., Buffalo, N. Y., purity not given.
(2) Distilled (compiler).

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

(2) Seawater

ORIGINAL MEASUREMENTS:

Zeininger, H.

Hoechst A. G., Internat Report, 1975.

VARIABLES:

$T/K = 276 - 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_l$	$10^4\ x_l$ (compiler)	$100\ w_l M_l^{-1}$/mol g^{-1} (compiler)
3	0.19	2.50	1.38×10^{-3}
10	0.12	1.58	8.74×10^{-4}
20	0.09	1.18	6.55×10^{-4}
40	0.05	0.656	3.64×10^{-4}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

The original report is not obtainable; therefore, the details were taken from Junge (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.
(2) North Atlantic suface water, salinity not given.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Junge, C. *Z. Naturforsch.* 1976, *31a*, 482.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

(2) Seawater

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, Univ. of East Anglia, Norwich, U. K., July 1980, 375 pp.

VARIABLES:

T/K = 283 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
10	2.82 ± 0.13	0.130	1.71
15	3.38 ± 0.17	0.129	1.70
20	3.95 ± 0.30	0.130	1.71
25	4.15 ± 0.06	0.145	1.90

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method involved repeated equilibrations of nitrogen with a water sample containing trichlorofluoromrthane. 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:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

(2) Seawater

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 97-106.

VARIABLES:

T/K = 273 - 305

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

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

(continued)

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 CCl_3F was carried out using a Hewlett-Packard ^{63}Ni 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) Collected from Puget Sound, Washington with salinity of 35.0×10^{-3}.

ESTIMATED ERRORS:

Solubility: ± 2.0 %.
Temperature: ± 0.5 K.

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F;
[75-69-4]; R-11

(2) Seawater

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 97-106.

VARIABLES:

T/K = 273 - 305

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

t/°C	Bunsen coefficient, α/dimensionless	t/°C	Bunsen coefficient, α/dimensionless
7.4	0.411 ± 0.001 (6)	17.9	0.247 ± 0.002 (9)
7.9	0.391 ± 0.003 (5)	18.0	0.233 ± 0.006 (11)
10.0	0.331 ± 0.005 (6)	19.7	0.231 ± 0.002 (11)
10.2	0.343 ± 0.004 (10)	20.2	0.212 ± 0.002 (6)
10.4	0.344 ± 0.002 (7)	20.7	0.218 ± 0.001 (7)
10.5	0.352 ± 0.004 (10)	25.2	0.177 ± 0.002 (6)
12.3	0.313 ± 0.003 (9)	25.5	0.175 ± 0.001 (6)
15.0	0.276 ± 0.007 (10)	27.9	0.158 ± 0.001 (19)
15.1	0.274 ± 0.003 (9)	31.6	0.142 ± 0.001 (9)
15.2	0.274 ± 0.001 (8)		

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

COMPONENTS:

(1) Trichlorofluoromethane; CCl_3F;
[75-69-4]; R-11

(2) Seawater

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 1485-97.

VARIABLES:

T/K = 272 - 313

Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^2\ c_l\ P_l^{-1}$ /mol dm^{-3} atm^{-1}	t/°C	$10^2\ c_l\ P_l^{-1}$ /mol dm^{-3} ath^{-1} atm
-0.77	2.8152	4.79	1.9601
-0.77	2.7588	4.79	1.9607
-0.52	2.7263	4.81	1.8770
-0.52	2.6985	4.82	1.9773
-0.45	2.7107	4.84	1.9318
-0.43	2.7065	9.19	1.5302
-0.37	2.7110	9.19	1.5293
-0.37	2.7056	9.19	1.5330
4.79	1.9706	9.19	1.5372
4.79	1.9446	9.19	1.5727

(continued)

AUXILIARY INFORMATION

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 ^{63}Ni 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:

(1) Trichlorofluoromethane; CCl_3F; [75-69-4]; R-11

(2) Seawater

ORIGINAL MEASUREMENTS:

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

Deep-Sea Res. 1985, *32*, 1485-97.

VARIABLES:

T/K = 272 - 313

Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

t/°C	$10^2\ c_1\ P_1^{-1}$ /atm mol dm^{-3}	t/°C	$10^2\ c_1\ P_1^{-1}$ /atm mol dm^{-3}
9.19	1.5404	29.55	1.6182
20.43	0.8648	29.55	0.6042
20.44	0.8868	29.55	0.6037
20.44	0.8792	29.55	0.6020
20.44	0.8749	39.90	0.4280
20.44	0.8788	39.91	0.4301
20.44	0.8780	39.93	0.4299
29.53	0.6085	39.93	0.4357
29.53	0.6031	39.93	0.4281

COMPONENTS:	EVALUATOR:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. January 1993.

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:

$$\text{Solubility } [100\, w_1] = 3.4653 - 0.0230285\,(T/\text{K}) + 3.91621 \times 10^{-5}\,(T/\text{K})^2$$

The equation represents the combined data points which yield a standard deviation of 5.8×10^{-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 1. Tentative Solubility of Tetrachloromethane (1) in Water (2)

Temperature		Solubility	
°C	K	$100\, w_1$	$10^4\, x_1$
0	273.15	0.0970	1.137
5	278.15	0.0898	1.053
10	283.15	0.0846	0.9916
15	288.15	0.0813	0.9529
20	293.15	0.0800	0.9376
25	298.15	0.0813	0.9529
30	303.15	0.0832	0.9752
35	308.15	0.0878	1.029

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. January 1993.

CRITICAL EVALUATION: (continued)

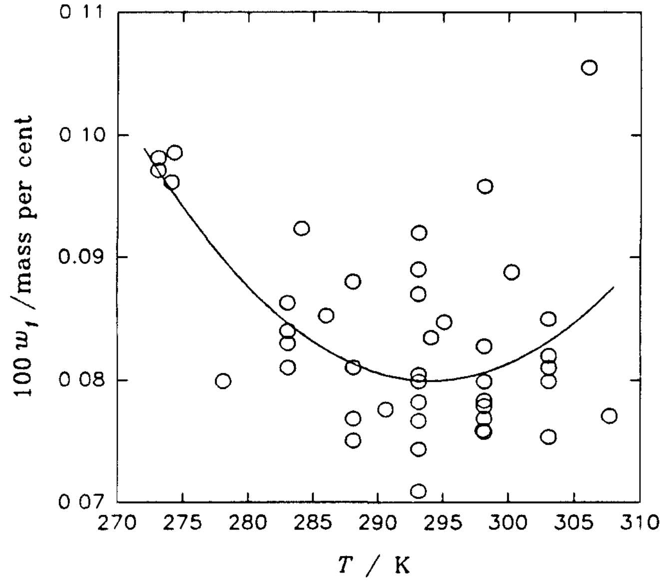

Figure 1. Solubility of Tetrachloromethane (1) in Water (2).

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:

$$\text{Solubility } [100\, w_2] = 0.301104 - 2.348078 \times 10^{-3}\, (T/\text{K}) + 4.607143 \times 10^{-6}\, (T/\text{K})^2$$

This equation yielded a standard deviation of 1.5 x 10^{-3} in the 273 to 308 K temperature range.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Water; H_2O; [7732-18-5]	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 2. Recommended Solubility of Water (2) in Tetrachloromethane (1)

Temperature		Solubility	
°C	K	100 w_2	$10^4 x_2$
10	283.15	0.00558	4.762
15	288.15	0.00699	5.965
20	293.15	0.00864	7.372
25	298.15	0.01051	8.967
30	303.15	0.01261	10.757
35	308.15	0.01495	12.750

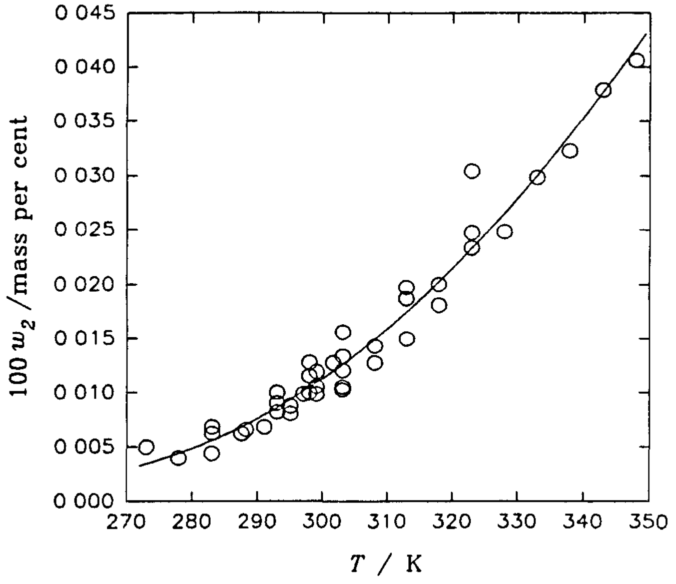

Figure 2. Solubility of Water (2) in Tetrachloromethane (1).

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(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K.
(2) Water; H_2O; [7732-18-5]	January 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:

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Correction?

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. January 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:

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COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Rex, A.

Z. Phys. Chem. 1906, *55*, 355-70.

VARIABLES:

T/K = 273 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
0	9.7×10^{-2}	9.7×10^{-2}	1.14
10	8.3×10^{-2}	8.3×10^{-2}	0.973
20	8.0×10^{-2}	8.0×10^{-2}	0.938
30	8.5×10^{-2}	8.5×10^{-2}	0.996

AUXILIARY INFORMATION

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.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Clifford, C. W.

J. Ind. Eng. Chem. 1921, *13*, 631-2.

VARIABLES:

T/K = 297 - 302

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^4\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
24.0	1.0×10^{-2}	8.53	5.55×10^{-4}
28.5	1.3×10^{-2}	11.09	7.22×10^{-4}

AUXILIARY INFORMATION

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 $CaCl_2$.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Clifford, C. W. *J. Ind. Eng. Chem.* 1921, *13*, 628.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.

J. Am. Chem. Soc. 1929, *51*, 2362-6.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25	7.7×10^{-2}	7.7×10^{-2}	9.02

AUXILIARY INFORMATION

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:

(1) Gross, P. M. *Z. Phys. Chem.* 1929, *6B*, 215.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

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

J. Am. Chem. Soc. 1930, *52*, 3568-73.

VARIABLES:

$T/K = 283 - 323$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
10	7.11×10^{-3}	7.11×10^{-3}	0.607
20	8.44×10^{-3}	8.44×10^{-3}	0.720

(continued)

AUXILIARY INFORMATION

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 CaH_2. The complete apparatus was placed in a water bath. The evolved hydrogen was measured volummetrically 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 % H_2O.
Temperature: ± 0.2 K (compiler).

REFERENCES:

(1) Rosenbaum, C. K. *Ph. D. Thesis*, Univ. of Wisconsin, Wisconsin, 1930.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

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

J. Am. Chem. Soc. 1930, *52*, 3568-73.

VARIABLES:

T/K = 283 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
30	1.09×10^{-2}	1.09×10^{-2}	0.930
40	1.52×10^{-2}	1.52×10^{-2}	1.30
50	2.37×10^{-2}	2.37×10^{-2}	2.02

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.; Saylor, J. H.

J. Am. Chem. Soc. 1931, *53*, 1744-51.

VARIABLES:

T/K = 288 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	1000 g_1/g_2	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
15	0.77	7.7×10^{-2}	9.02
30	0.81	8.1×10^{-2}	9.49

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_2SO_4 and NaOH solution, dried and fractionated before use.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: ± 2.5 %.
Temperature: ± 0.02 K.

REFERENCES:

(1) Gross, P. M. *J. Am. Chem. Soc.* 1929, *51*, 2362.
(2) Saylor, J. H. *Ph. D. Thesis*, Duke University, Durham, 1930.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Bell, R. P.

J. Chem. Soc. 1932, 2905-11.

VARIABLES:

$T/K = 288 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
15	6.35×10^{-2}	3.96×10^{-3}	3.38
20	7.67×10^{-2}	4.81×10^{-3}	4.10
25	9.35×10^{-2}	5.90×10^{-3}	5.03

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 α-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:	± 4.4 % mean.
Temperature:	± 0.02 K.

REFERENCES:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas, 1936, *55*, 407-11.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^4\ x_1$	100 w_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
30	0.955	8.15×10^{-2}	5.3×10^{-4}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Niini, A.

Suomen Kemistilehti 1938, *11a*, 19-20.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^5 x_1$ (compiler)	100 w_2	$10^4 x_2$ (compiler)
20	7.1×10^{-2}	8.32	5.0×10^{-3}	4.27

AUXILIARY 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°C and n_D = 1.4608 at 20°C.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: ± 20 %.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Fox, J. J.; Martin, A. K.

Proc. Roy. Soc. London, Ser. A, 1940, *174*, 234-62.

VARIABLES:

T/K = 291

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^4 x_1$ (compiler)
18.3	6.9×10^{-3}	6.9×10^{-3}	5.89

AUXILIARY 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: ± 0.2 K (compiler).

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Staverman, A. J.

Recl. Trav. Chim. Pays-Bas, 1941, *60*, 836-41.

VARIABLES:

T/K = 273 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^5 x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
0	0.50×10^{-2}	42.8	2.77×10^{-4}
25	1.16×10^{-2}	99.1	6.44×10^{-4}
30	1.58×10^{-2}	135.0	8.77×10^{-4}

AUXILIARY INFORMATION

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:

(1) Staverman, A. J. *Ph. D. Thesis*, Univ. of Leiden, Leiden, Belgium, 1938.

COMPONENTS:

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

(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:

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^4 x_1$ (compiler)
25	5.43×10^{-4}	9.78×10^{-3}	8.34

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 1 to 15 volume ratio mixture of water and tetrachloromethane was introduced into an equilibration 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:

(1) Eidinoff, M. L.; Joris, G. G.; Taylor, H. S.; Urey, H. C., Eds., *Production of Heavy Water*, McGraw-Hill, New York, 1955, p. 129.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

McGovern, E. W.

Ind. Eng. Chem. 1943, *35*, 1230-9.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_2$	$10^4\ x_2$ (compiler)
0	9.8×10^{-2}	1.15	-	-
10	8.4×10^{-2}	0.984	0.65×10^{-2}	5.55
20	8.0×10^{-2}	0.938	0.92×10^{-2}	7.85
25	8.0×10^{-2}	0.938	1.30×10^{-2}	11.09
30	8.0×10^{-2}	0.938	1.35×10^{-2}	11.52

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); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Powell, J. F.

Brit. J. Industr. Med. 1945, *2*, 212-6.

VARIABLES:

$T/K = 293 - 310$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Ostwald coefficient, L/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	1.05	8.05×10^{-2}	9.44
37	0.45	6.82×10^{-2}	7.99

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/mim. 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:

(1) Habgood, S.; Powell, J. F. *Brit. J. Industr. Med.* 1944, *1*, 39.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

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

Ind. Eng. Chem. 1948, *40*, 1491-3.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ V_1/V_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25.0	0.10	0.159	1.86

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium was established through repeated shaking and centrifuging of a tetrachloromethane and water mixture in a stoppered 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 Hanaslick 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: ± 1 K (compiler).

REFERENCES:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

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

Ind. Eng. Chem. 1949, *41*, 2627-8.

VARIABLES:

$T/K = 298 - 333$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ V_1/V_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25.0	0.10	0.159	1.86
60	0.10	0.159	1.86

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:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Chitwood, B. G.

Adv. in Chem. Ser., Am. Chem. Soc., 1952, *7*, 91-9.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^5\ x_1$ (compiler)	$10^6\ w_1M_1^{-1}/mol\ g^{-1}$ (compiler)
25	8.0×10^{-2}	9,38	5.20

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) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Donahue, D. J.; Bartell, F. E.

J. Phys. Chem. 1952, *56*, 480-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^5\ x_1$	$100\ w_1$ (compiler)	$10^4\ x_2$	$100\ w_2$ (compiler)
25	9.7	8.28×10^{-2}	8.3	9.73×10^{-3}

AUXILIARY INFORMATION

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: ± 0.1 K.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]	Rotariu, G. J.; Fraga, D. W.; Hildebrand, J. H. *J. Am. Chem. Soc.* 1952, *74*, 5783.
VARIABLES: T/K = 298	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	100 V_1/V_s	10^4 x_1 (compiler)
25	1.0×10^{-2}	1.6×10^{-2}	8.53

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.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]	Eberius, E. *Wasserbestimmung mit Karl-Fischer-Lösung*, Verlag Chemie, GMBH, Weinheim, 1954, p. 67.
VARIABLES: T/K = 293	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^3 x_1 (compiler)	10^6 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	0.012 ± 0.003	1.02	6.66

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.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Greinacher, E.; Lüttke, W.; Mecke, R.

Z. Elektrochem. 1955, *59*, 23-31.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	n_1/V_2/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	7.5	8.48 × 10^{-3}	7.24

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of water and tetrachloromethane 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) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Fitzgerald, M. E.; Griffing, V.; Sullivan, J.

J. Chem. Phys. 1956, *25*, 926-33.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	n_1/V_2/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	5.8	8.9 × 10^{-2}	1.04

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Desnoyer, M.

Dosage de l'Eau dans les Solvants Organiques par Absorption Infra-Rouge et Mesure des Constantes Dielectriques, Centre D'Etudes Nucleaires de Saclay, Report No. 1254, Saclay, France, June 23, 1959.

VARIABLES:

T/K = 299

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^4 x_1 (compiler)	10^6 $w_1M_1^{-1}$/mol g^{-1} (compiler)
26	1.01×10^{-2}	8.62	5.61

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).

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Zielinski, A. Z.

Chem. Stosowana 1959, *3*, 377-84.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	ρ_1/kg m^{-3}	10^3 x_1 (compiler)	100 w_1 (compiler)
25	1.54	8.24	9.72×10^{-2}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of water in the organic phase was determined by the Karl Fischer titration method (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) Distilled (compiler).
(2) Gliwice Chemicals, pure grade, used as received.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Mitchell, J.; Smith, D. M. *Aquametry: A Treatise on Metrhods for the Determination of Water*, Wiley, New York, 1952, pp. 73 and 260.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Tettamanti, K.; Nogradi, M.; Sawinsky, J.

Period. Polytech., Chem. Eng. 1960, *4*, 201-18.

VARIABLES:

$T/K = 293$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^5\ x_1$ (compiler)	$100\ w_2$	$10^4\ x_2$ (compiler)
20	7.0×10^{-2}	8.20	1.0×10^{-2}	8.53

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 weighted 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.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Liu, J.-L.; Huang, T.-C.

Scientia Sinica (Peking) 1961, *10*, 700-10.

VARIABLES:

$T/K = 288 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$1000\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
15	0.755	7.54×10^{-2}	8.837
20	0.748	7.47×10^{-2}	8.755
25	0.762	7.61×10^{-2}	8.919

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 H_2SO_4, NaOH, and water, dried over $CaCl_2$, and fractionated.
(2) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Johnson, J. R.; Christian, S. D.; Affsprung, H. E.

J. Chem. Soc. 1965, 1-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	$10^4 x_1$ (compiler)
25.0	8.7	9.89×10^{-3}	8.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method of establishing the water and tetrachloromethane solution equilibrium in a thermostat has been reported elsewhere (ref. 1). The concentration of water in the tetrachloromethane phase was determined using a Beckman KF-3 aquameter. For all measurements, 50 ml samples were analyzed.

SOURCE AND PURITY OF MATERIALS:

(1) Distilled (compiler).
(2) Source not given. Purified by distillation in an Oldershaw column before use.

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

REFERENCES:

(1) Christian, S. D.; Affsprung, H. E.; Johnson, J. R.; Worley, J. D. *J. Chem. Educ.* 1963, *40*, 419.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Johnson, J. R.; Cristian, S. D.; Affsprung, H. E.

J. Chem. Soc. A, 1966, 77-8.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	$10^4 x_1$ (compiler)
25.0	8.7	9.89×10^{-3}	8.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Samples of water and tetrachloromethane mixtures were equilibrated in a constant temperature waterbath. The solute isopiestic apparatus has been described elsewhere (ref. 1). The water solubilities were determined using a Beckman Model KF-3 Aquameter.

SOURCE AND PURITY OF MATERIALS:

(1) Distilled (compiler).
(2) Source not given, reagent grade, distilled in an Oldershaw column before use.

ESTIMATED ERRORS:

Solubility:	$\pm 0.3 \times 10^{-3}$.
Temperature:	± 0.1°C.

REFERENCES:

(1) Christisn, S. D.; Affsprung, H. E.; Johnson, J. R.; Worley, J. D. *J. Chem. Educ.* 1963, *40*, 419.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Johnson, J. R.

Self-Association and Hydration of Phenol in Several Organic Solvents, Ph. D. Thesis, Univ. of Oklahoma, Norman, Oklahoma, 1966.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_1/\text{mol m}^{-3}$	$100\ w_1$ (compiler)	$c_2/\text{mol m}^{-3}$	$100\ w_2$ (compiler)
25	5.1	7.8×10^{-2}	8.7	9.89×10^{-3}

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; H_2O; [7732-18-5]

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Grigsby, R. D.

Self-Association and Hydration of N-Methylacetamide in Carbon Tetrachloride, Ph. D. Thesis, Univ. of Oklahoma, Norman, Oklahoma, 1966.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_1/\text{mol m}^{-3}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)	Method used:
25	9.8	1.8×10^{-2}	1.53	coulometric
25	8.8	1.6×10^{-2}	1.36	total pressure

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:

(1) Grigsby R. D.; Christian, S. D.; Affsprung, H. R. *J. Phys. Chem.* 1968, *72*, 2465.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Christian, S. D.; Affsprung, H. E.; Hunter, W. J. A.; Gillam, W. S.; McCoy, W. H.

Solute Properties of Water, U. S. Office of Saline Water Research and Development Program, Report No. 301 1968, p. 71, 79-81.

VARIABLES:

T/K = 288 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	n_1/V_2/mol m^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
15	5.9 ± 0.2	6.64×10^{-3}	5.66
25	8.7 ± 0.3	9.89×10^{-3}	8.44

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: See above.
Temperature: ± 0.1 K.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Högfeldt, E.; Fredlund, F.

Acta Chem. Scand. 1970, *24*, 1858-60.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	10	9.7×10^{-3}	8.28

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Samples of tetrachloromethane were shaken to equilibrium with pure water. The liquid mixture was centrifuged and the organic phase analyzed for water following a modification of the Karl Fischer titration method.

SOURCE AND PURITY OF MATERIALS:

(1) Distilled (compiler).
(2) Source not given, 99.95 % pure, checked by VPC.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Simonov, V. D.; Pogulyai, V. E.; Shamsutdinov, T. M.

Russ. J. Phys. Chem. 1970, *44*, 1755-7.

VARIABLES:

T/K = 303 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\,x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
30	1.35×10^{-2}	1.15	7.49×10^{-4}
50	3.05×10^{-2}	2.60	1.69×10^{-3}

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 appearence 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: ± 0.5 K (compiler).

REFERENCES:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Simonov, V. D.; *et al.*

Dokl. Neftekim. Sekt., Bashkir. Respub. Pravl. Vses. Khim. Obshchest. 1971, 346-51.

VARIABLES:

T/K = 288 - 299

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1			$10^4\,x_1$		
	Alexeev	Fischer	Spectroscopy	Alexeev	Fischer	Spectroscopy
14.5	6.33×10^{-3}	-	6.30×10^{-3}	5.402	-	5.377

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

(1) Distilled.
(2) "KhCh" brand, treated with Na_2CO_3, dried with $CaCl_2$ and P_2O_5 and distilled before use.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.5 K.

REFERENCES:

(1) Alexeev, V. F. *Wied. Ann.* 1886, *28*, 305.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Simonov, V. D.; *et al.*

Dokl. Neftekim. Sekt., Bashkir. Respub. Pravl. Vses. Khim. Obshchest. 1971, 346-51.

VARIABLES:

T/K = 288 - 299

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

t/°C	100 w_1			10^4 x_1		
	Alexeev	Fischer	Spectroscopy	Alexeev	Fischer	Spectroscopy
18	7.00×10^{-3}	7.20×10^{-3}	7.10×10^{-3}	5.974	6.144	6.059
22	8.85×10^{-3}	8.90×10^{-3}	8.90×10^{-3}	7.551	7.594	7.594
24	9.12×10^{-3}	-	10.10×10^{-3}	7.782	-	8.617
26	10.70×10^{-3}	10.60×10^{-3}	-	9.129	9.043	-

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

Russ. J. Phys. Chem. 1971, *45*, 488-90.

VARIABLES:

T/K = 288 - 333

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	1000 g_1/g_2	100 w_1 (compiler)	10^5 x_1 (compiler)
15	0.81	8.1×10^{-2}	9.49
30	0.45	4.5×10^{-2}	5.27
45	0.25	2.5×10^{-2}	2.93
60	0.14	1.4×10^{-2}	1.64

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 periodicallty (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:

(1) Treger, Yu. A.; Flid, R. M.; Spektor, S. S. *Russ. J. Phys. Chem.* 1964, *38*, 253.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Water; H_2O; [7732-18-5]	Karger, B. L.; Chatterjee, A. K.; King, J. W. *Tech. Report No. 3*, Dept. of Chem., Northeastern Univ., Boston, Mass., May 10, 1971.
VARIABLES:	**PREPARED BY:**
T/K = 286	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Partition coefficient[1], K_L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
12.5	1.9	0.106	1.24

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

AUXILIARY INFORMATION

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_L) was obtained from the slope of the straight line plot of V_N/A_L vs. V_L/A_L.

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; H_2O; [7732-18-5] (2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]	Glasoe, P. K.; Schultz, S. D. *J. Chem. Eng. Data* 1972, *17*, 66-8.
VARIABLES:	**PREPARED BY:**
T/K = 288 - 318	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
15	6.2 ± 0.1	6.97×10^{-3}	5.95
25	8.6 ± 0.3	9.78×10^{-3}	8.35
30	9.3 ± 0.3	1.06×10^{-2}	9.08
35	11.4 ± 0.3	1.31×10^{-2}	11.2
45	15.6 ± 0.8	1.82×10^{-2}	15.5

AUXILIARY INFORMATION

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:

(1) Wernimont, G.; Hopkinson, F. J. *Ind. Eng. Chem., Anal. Ed.* 1943, 272.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

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

Russ. J. Phys. Chem. 1972, *46*, 311-2 (VINITI No. 3739-71).

VARIABLES:

$T/K = 288 - 299$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^4\ x_1$ (compiler)	$100\ w_2$	$10^4\ x_2$ (compiler)
15	6.76×10^{-3}	7.92	-	-
18	-	-	7.10×10^{-3}	6.12
20	7.95×10^{-3}	9.31	-	-
22	-	-	8.30×10^{-3}	7.08
26	9.76×10^{-3}	11.43	1.20×10^{-2}	10.24

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:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D.

Tr. Mosk. Khim.-Tekhnol. Inst. 1972, 183-6.

VARIABLES:

$T/K = 298 - 373$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Distribution coefficient[1], D_L/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25.0	29200	0.00439	0.514

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

(continued)

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 ^{36}Cl 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)

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D.

Tr. Mosk. Khim.-Tekhnol. Inst. 1972, 183-6.

VARIABLES:

$T/K = 298 - 373$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

$t/°C$	Distribution coefficient[1], D_L/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
50.1	9670	0.0364	4.26
70.0	4100	0.1687	19.79
90.0	1960	0.637	75.01
96.2	1500	0.983	116.09
100.0	1380	1.179	139.52

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D.

Tr. Mosk. Khim.-Tekhnol. Inst. 1974, 55-6.

VARIABLES:

$T/K = 298 - 343$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

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

where α = Distribution Coefficient

At the normal boiling point of CCl_4, 349.79 K, $\alpha = 120$, the activity coefficient, $\gamma_1 = 296$, and the mole fraction of (1) at saturation, $x_1 = 3.378 \times 10^{-3}$ (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:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Goldman, S.

Can. J. Chem. 1974, *52*, 1668-80.

VARIABLES:

$T/K = 283 - 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_1/\text{mol m}^{-3}$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
10	5.23	0.942×10^{-2}	8.04
15	6.05	1.09×10^{-2}	9.30
20	7.47	1.34×10^{-2}	11.4
25	8.87	1.60×10^{-2}	13.6
30	10.35	1.86×10^{-2}	15.8
35	12.38	2.23×10^{-2}	19.0
40	14.33	2.58×10^{-2}	22.0

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 $CaCl_2$ and distilled under dry nitrogen, density = 1.5826 g/cc at 25°C.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Simonov, V. D.; Shamsutdinov, T. M; Pogulyai, V. E.; Popova, L. N.

Russ. J. Phys. Chem. 1974, *48*, 1573-5.

VARIABLES:

$T/K = 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^5\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
40	2.50×10^{-2}	2.93	1.97×10^{-2}	1.68

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The synthetic method of Alexejew was used. Details are found elsewhere (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:

(1) Simonov, V. D.; Popova, L. N.; Shamsutdinov, T. M.; Pogulyai, V. I.; Memina, F. A. *Symp. Doklay Neftekhimicheskoi Sektsii, Ufa*, 1971, No. 6.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

McConnell, G.; Ferguson, D. M.; Pearson, C. R.

Endeavour 1975, *34*, 13-8.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^4\ g_1/g_2$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	7.85	7.85×10^{-2}	9.19

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); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Pearson, C. R.; McConnell, G.

Proc. Roy. Soc. B, 1975, *189*, 305-32.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	785	7.85×10^{-2}	9.20

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Kirchnerova, J.

Ph. D. Thesis, McGill Univ., Montreal, Quebec, April 1975, 280 pp.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
25	8.7	9.96×10^{-3}	8.50

AUXILIARY INFORMATION

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.

SOURCE AND PURITY OF MATERIALS:

(1) Distilled and deionized.
(2) Fisher Scientific Co., spectroanalyzed grade, further purified by extraction with H_2SO_4, dried and redistilled, 00.78 % pure.

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Kirchnerova, J.; Cave, G. C. B.

Can. J. Chem. 1976, *54*, 3909-16.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	10^4 x_1 (compiler)	100 w_1 (compiler)
25.0	8.7	8.5	9.96×10^{-3}

AUXILIARY INFORMATION

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).

SOURCE AND PURITY OF MATERIALS:

(1) Distilled and deionized.
(2) Fisher - C199, washed with H_2SO_4 and K_2CO_3 solutions and finally with water. Dried over silica gel and fractionally distilled. Purity was better than 99.8 %.

ESTIMATED ERRORS:

Solubility: ± 0.2 c_1 std. dev.
Temperature: ± 0.1 K.

REFERENCES:

(1) Kirchnerova, J. *Ph. D. Thesis*, McGill Univ., Montreal, Quebec, 1975.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Sato, A.; Nakijima, T.

Arch. Envir. Health 1979, *34*, 69-75.

VARIABLES:

T/K = 310

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Distribution coefficient[1], D_L/dimensionless	$100\,w_1$ (compiler)	$10^5\,x_1$ (compiler)
37	0.25	3.78×10^{-2}	4.43

[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:

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

ESTIMATED ERRORS:

Solubility: ± 0.04 std. dev.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Freed, V. H.; Chiou, C. T.; Schmedding, D.; Kohnert, R.

Environ. Health Perspect. 1979, *30*, 75-80.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\,w_1$	$100\,w_1$ (compiler)	$10^5\,x_1$ (compiler)
25	800	8.0×10^{-2}	9.38

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:

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

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.5 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Aref'eva, R. P.; Korenman, I. M.; Gorokhov, A. A.

USSR Patent 672 548, July 5, 1979, 3 pp. (CA. 91:113256k).

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1 V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	0.87 ± 0.03	8.72×10^{-2}	1.02

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).

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Coca, J.; Diaz, R. M.; Pazos, C.

Fluid Phase Equilib. 1980, *4*, 125-36.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^5\ x_1$ (compiler)	100 w_2	$10^4\ x_2$ (compiler)
25	7.0×10^{-2}	8.20	1.0×10^{-2}	8.53

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The mutual solubility data were determined by the method described by Othmer *et al.* (ref. 1). Ten cm^3 of tetrachloromethane was added to water from a buret and agitated until the solution became turbid. The appearance of the turbidity indicated the formation of a second phase. The solubility was calculated from 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 (compiler).

REFERENCES:

(1) Othmer, D. F.; White, R. E.; Trueges, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Ksiazczak, A.; Buchowski, H.

Fluid Phase Equilib. 1980, *5*, 131-40.

VARIABLES:

$T/K = 323$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^4\ x_l$	$100\ w_l$ (compiler)	$100\ w_l M_l^{-1}/mol\ g^{-1}$ (compiler)
50	21	2.46×10^{-2}	1.365×10^{-3}

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 $1/\Delta P$ versus V_g/V_l.

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); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, Univ. of East Anglia, Norwich, U. K., July 1980, 375 pp.

VARIABLES:

$T/K = 283 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_l$ (compiler)	$10^5\ x_l$ (compiler)
10	0.75 ± 0.06	6.54×10^{-2}	7.66
15	0.90 ± 0.07	6.84×10^{-2}	8.02
20	1.05 ± 0.07	7.28×10^{-2}	8.53
25	1.30 ± 0.10	7.24×10^{-2}	8.48

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements involved repeated equilibrations 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 equilibrations.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C.

Environ. Sci. Techn. 1980, *14*, 1227-9.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	$10^5 x_1$ (compiler)
25	4.92	7.58×10^{-2}	8.88

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility:	± 2.5 % std. dev.
Temperature:	± 0.3 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Veith, G. D.; Macek, K. J.; Petrucelli, S. R.; Carroll, J.

Proc. 3rd Ann. Symp. on Aquatic Toxicology, ASTM Publ. 707, Philadelphia, 1980, 116-29.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$n_1 V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	$10^5 x_1$ (compiler)
20	5.01	7.71×10^{-2}	9.04

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 1 K.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Wu, X.

Huaxue Shiji 1981, 221-4.

VARIABLES:

$T/K = 278 - 348$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/^\circ C$	$10^6 w_1$	$100 w_1$ (compiler)	$10^4 x_1$ (compiler)
5	42	0.42×10^{-2}	3.59
10	46	0.46×10^{-2}	3.93
15	67	0.67×10^{-2}	5.72
20	92	0.92×10^{-2}	7.85
25	109	1.09×10^{-2}	9.30
30	123	1.23×10^{-2}	10.5
35	144	1.44×10^{-2}	12.3
40	190	1.90×10^{-2}	16.2
45	201	2.01×10^{-2}	17.1
50	232	2.32×10^{-2}	19.8
55	250	2.50×10^{-2}	21.3
60	299	2.99×10^{-2}	25.5
65	324	3.24×10^{-2}	27.6
70	380	3.80×10^{-2}	32.4
75	408	4.08×10^{-2}	34.7

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_2SO_4 solutions and distilled water before dried on molecular sieve.

ESTIMATED ERRORS:

Solubility:	± 28 std. dev.
Temperature:	± 1 - 2 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Leighton, D. T.; Calo, J. M.

J. Chem. Eng. Data 1981, *26*, 382-5.

VARIABLES:

$T/K = 274 - 300$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Distribution coefficient[1], D_L/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
1.0	412.1	9.611×10^{-2}	1.127
1.3	412.4	9.866×10^{-2}	1.157
11.0	719.5	9.238×10^{-2}	1.083
13.0	859.5	8.533×10^{-2}	1.000
21.0	1280.3	8.358×10^{-2}	0.9796
22.0	1319.4	8.488×10^{-2}	0.9948
27.2	1571.4	8.899×10^{-2}	1.043

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 5 μL 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: ± 3.4 %.
Temperature: ± 0.5 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; *et al.*

Volatilization of Organic Pollutants from Water, U. S. EPA Report 600/3-82-019, Athens, Georgia, 1982 (PB 82-230939).

VARIABLES:

$T/K = 293 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	c_1/mol m^{-3}	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)	$100\ w_2$ (compiler)	$10^4\ x_2$
20	5.20	8.00×10^{-2}	9.376	-	-
25	5.10	7.85×10^{-2}	9.200	8.20×10^{-3}	7.0

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:

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

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 1.0 K.

COMPONENTS:

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

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Ohtsuka, K.; Kazama, K.

Sen'i Seihin Shohi Kagaku Kaishi 1982, *22*, 197-201.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	0.22	1.4×10^{-2}	1.19

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

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

Tellus 1983, *35B*, 170-6.

VARIABLES:

T/K = 278 - 306

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
5	0.4864	8.006×10^{-2}	9.383
10	0.5854	8.420×10^{-2}	9.869
15	0.7000	8.823×10^{-2}	10.34
20	0.8320	9.206×10^{-2}	10.79
25	0.9831	9.584×10^{-2}	11.23
33	1.2696	1.0554×10^{-1}	12.37

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

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

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:

(1) McAuliffe, C. D. *Chem. Techn.* 1971, *1*, 46.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Orlandini, M.; Fermeglia, M.; Kikic, I.; Alessi, P.

Chem. Eng. J. 1983, *26*, 245-50.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^4\,x_1$	$100\,w_1$ (compiler)	$10^4\,x_2$	$100\,w_2$ (compiler)
20	0.9	7.68×10^{-2}	7.1	8.322×10^{-3}

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 (C. Erba ATc/t) was equipped with a Shimadzu Chromatopac E-1A integrator. A stainless column packed with 100-120 mesh Chromosorb W DMCD coated with heptadecane nitrile was used for analysis.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stanford Univ., Stanford, CA., 1985, 306 pp.

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's Law Constant, H/dimensionless	ρ_1/kg m^{-3}	$100\,w_1$ (compiler)	$10^5\,x_1$ (compiler)
10	0.609	0.810	8.10×10^{-2}	9.493
20	0.980	0.784	7.84×10^{-2}	9.188
30	1.530	0.755	7.55×10^{-2}	8.848

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 direct 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); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Yoshioka, Y.; Ose, Y.; Sato, T.

Ecotoxicol. Envir. Saf. 1986, *12*, 15-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^7\ x_1$ (compiler)
20	2.6×10^{-3} [1]	2.6×10^{-4}	3.04

[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); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Lo, J. M.; Tseng, C. L.; Yang, J. Y.

Anal. Chem. 1986, *58*, 1596-7.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^5\ x_1$	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	8.0×10^{-2}	9.38	5.20×10^{-4}

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 (Tl) 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:	± 0.7×10^{-2} std. dev.
Temperature:	± 1.0 K (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Water; H_2O; [7732-18-5]	Gossett, J. M. *Environ. Sci. Tehn.* 1977, *21*, 202-8.
VARIABLES:	**PREPARED BY:**
T/K = 283 - 308	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's Law Constant, H/m^3 atm mol^{-1}	CV^1 %	100 w_1 (compiler)	10^4 x_1 (compiler)
10.0	1.32×10^{-2}	5.15	8.64×10^{-2}	1.013
17.5	2.11×10^{-2}	4.20	7.79×10^{-2}	0.912
24.8	3.04×10^{-2}	3.92	7.62×10^{-2}	0.893
34.6	4.60×10^{-2}	3.42	7.73×10^{-2}	0.906

[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; H_2O; [7732-18-5] (2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]	Kleeberg, H.; Klein, D.; Luck, W. A. P. *Chem.-Ing.-Techn.* 1987, *58*, 409-11.
VARIABLES:	**PREPARED BY:**
T/K = 298	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	9.3	1.68×10^{-2}	1.43

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); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants, EPA Technical Report, PB 87-212684, Cincinnati, OH., July 1987.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
24.85	3.02×10^{-2}	7.61×10^{-2}	8.92

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

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Techn.* 1979, *13*, 333.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

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

AFESC Tyndall Air Force Base, Report ESL-TR-86-66, *Vol. 1*, Florida, Sept. 1987, 86 pp (AD-A188 571).

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ w_1$	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
10	104	1.04×10^{-2}	1.218
20	146	1.46×10^{-2}	1.710
30	105	1.05×10^{-2}	1.230

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 Carbopack 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: ± 0.5 K (compiler).

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Vogel, A. I., rev. by Furniss, B. S.; *et al.*

Vogel's Textbook of Practical Organic Chemistry, 5th ed., Longman, London, 1989, p. 1442.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^5 x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25.0	8.0×10^{-2}	9.38	5.2×10^{-4}

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:

(1) Source not given. Analytical reagent, treated with KOH solution and dried by distillation.
(2) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

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

ORIGINAL MEASUREMENTS:

Wright, D. A.; Sandler, S. I.; DeVoll, D.

Environ. Sci. Techn. 1992, *26*, 1828-31.

VARIABLES:

$T/K = 293 - 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	γ^{∞}	$10^5 x_1$	100 w_1 (compiler)	100 $w_1M_1^{-1}$/mole g^{-1} (compiler)
20	12.200 ± 250	8.20	7.00×10^{-2}	4.55×10^{-4}
30	13.100 ± 100	7.63	6.51×10^{-2}	4.23×10^{-4}
40	13.100 ± 300	7.63	6.51×10^{-2}	4.23×10^{-4}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of tetrachloromethane (γ^{∞}) 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:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) MQ-Water

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stanford University, Stanford, CA., 1985, 306 pp.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	0.980	7.80×10^{-2}	9.145

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 direct 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: ± 0.5 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Municipal tap water (PASE)

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stanford University, Stanford, CA., 1985, 306 pp.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	0.958	7.996×10^{-2}	9.372

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 direct 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: ± 0.5 K.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Seawater

ORIGINAL MEASUREMENTS:

Liss, P. S.; Slater, P. G.

Nature 1974, *247*, 181-4.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant[1], H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
20	1.08	7.22×10^{-2}	8.46

[1] Obtained from [mass(1) cm^{-3}(air)/mass(1) cm^{-3}(seawater)].

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available except that the data originate elsewhere (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.
(2) Samples from Atlantic.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Lovelock, J. E. *Personal communication.*

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Seawater

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, Univ. of East Anglia, Norwich, U. K., July 1980, 375 pp.

VARIABLES:

$T/K = 283 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
10	0.82 ± 0.01	6.19×10^{-2}	7.25
15	0.95 ± 0.10	6.68×10^{-2}	7.83
20	1.21 ± 0.04	6.49×10^{-2}	7.61
25	1.43 ± 0.05	6.73×10^{-2}	7.89

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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.

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) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5] (2) Seawater	Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S. *Tellus* 1983, *35B*, 170-6.
VARIABLES:	**PREPARED BY:**
T/K = 278 - 306	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	$10^5 x_1$ (compiler)
5	0.7100	5.596×10^{-2}	6.557
10	0.8716	5.759×10^{-2}	6.748
15	1.0624	5.911×10^{-2}	6.927
20	1.2863	6.049×10^{-2}	7.088
25	1.5473	6.180×10^{-2}	7.242
33	2.0536	6.625×10^{-2}	7.763

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

$$\log_e H = -\frac{3230}{T(\mathrm{K})} + 11.27$$

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:

(1) McAuliffe, C. D. *Chem. Techn.* 1971, *1*, 46.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Calcium chloride; $CaCl_2$; [10043-52-4]

(3) Water; H_2O; [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:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
25	0.205	0.652	6.41×10^{-2}	7.66
	0.280	0.598	5.85×10^{-2}	7.03
	0.333	0.565	5.49×10^{-2}	6.64
	0.581	0.452	4.29×10^{-2}	5.31

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 H_2SO_4, NaOH and water; dried over $CaCl_2$ 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); CCl_4; [56-23-5]

(2) Hydrogen chloride; HCl; [7647-01-0]

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

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M. Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

Russ. J. Phys. Chem. 1971, *45*, 488-90.

VARIABLES:

T/K = 288 - 333
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

Concentration of HCl, 100 w_2	t/°C	1000 w_1	100 w_1 (compiler)	$10^5 x_1$ (compiler)
10	15	1.00	1.00×10^{-1}	12.35
	30	0.55	5.5×10^{-2}	6.79
	45	0.30	3.0×10^{-2}	3.70
	60	0.18	1.8×10^{-2}	2.22
20	15	1.25	1.25×10^{-1}	16.31
	30	0.74	7.4×10^{-2}	9.65
	45	0.40	4.0×10^{-2}	5.21
	60	0.23	2.3×10^{-2}	3.00

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic method was used for the determination of solubility. It involved the saturation of nitrogen with terachloromethane 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. *Russ. J. Phys. Chem.* 1964, *38*, 253.

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Lithium chloride; LiCl; [7447-41-8]

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

ORIGINAL MEASUREMENTS:

Liu, J.-L.; Huang, T.-C.

Scientia Sinica (Peking) 1961, *10*, 700-10.

VARIABLES:

T/K = 293
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
20	0.1867	0.717	7.13×10^{-2}	8.389
	0.3496	0.696	6.86×10^{-2}	8.108
	0.4352	0.676	6.69×10^{-2}	7.924
	0.7015	0.644	6.33×10^{-2}	7.541
	0.9765	0.609	5.94×10^{-2}	7.130

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 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.

SOURCE AND PURITY OF MATERIALS:

(1) Peking Chemical Factory, further purified by washing with H_2SO_4, NaOH and water; dried over $CaCl_2$ and fractionated.
(2) Merck reagent, mixed with HCl and recrystallized.
(3) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Magnesium sulfate; $MgSO_4$; [7487-88-9]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.

Z. phys. Chem. 1929, *6B*, 215-20.

VARIABLES:

$T/K = 298$
One concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_2/\text{mol dm}^{-3}$	$100\ g_1/g_3$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25	0.5	4.8×10^{-2}	4.8×10^{-2}	5.93

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 to 20 ml tetrachloromethane in 500 ml of an aqueous solution of $MgSO_4$ 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); CCl_4; [56-23-5]

(2) Magnesium sulfate; $MgSO_4$; [7487-88-9]

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

ORIGINAL MEASUREMENTS:

Liu, J.-L.; Huang, T.-C.

Sciencia Sinica (Peking) 1961, *10*, 700-10.

VARIABLES:

$T/K = 298$
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_2/\text{mol dm}^{-3}$	$\rho_1/\text{kg m}^{-3}$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25	0.199	0.637	6.21×10^{-2}	7.429
	0.318	0.572	5.50×10^{-2}	6.662
	0.433	0.522	4.97×10^{-2}	6.094
	0.537	0.487	4.58×10^{-2}	5.679

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 H_2SO_4, NaOH and water; dried over $CaCl_2$ 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); CCl_4; [56-23-5]

(2) Potassium chloride; KCl; [7447-40-7]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.

Z. phys. Chem. 1929, *6B*, 215-20.

VARIABLES:

T/K = 298
One concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	100 g_1/g_3	100 w_1 (compiler)	10^5 x_1 (compiler)
25	0.5	6.5×10^{-2}	6.5×10^{-2}	7.84

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 to 20 ml tetrachloromethane in 500 ml of an aqueous solution of KCl 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); CCl_4; [56-23-5]

(2) Potassium chloride; KCl; [7447-40-7]

(3) Water; H_2O; [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:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25	0.3032	0.698	6.89×10^{-2}	8.215
	0.4833	0.644	6.30×10^{-2}	7.586
	0.7232	0.608	5.89×10^{-2}	7.196
	0.9727	0.560	5.36×10^{-2}	6.646

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 potassium chloride solutions were determined using a Hilger spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Peking Chemical Factory, further purified by washing with H_2SO_4,NaOH and water; dried over $CaCl_2$ 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); CCl_4; [56-23-5]

(2) Potassium hydroxide; KOH; [1310-58-3]

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

ORIGINAL MEASUREMENTS:

Treadwell, W. D.; Köhl, A.

Helv. Chim. Acta 1926, *9*, 681-91.

VARIABLES:

T/K = 333
One concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
60	1.0	0.2	1.98×10^{-2}	2.41

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrium between a known volume of tetrachloromethane gas and KOH solution was established in an container under continuous shaking. The volume of tetrachloromethane not dissolved in the KOH solution was measured and the amount of dissolved gas was determined at the same time and conditions. A single measurement was done at each temperature.

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); CCl_4; [56-23-5]

(2) Potassium sulfate; K_2SO_4; [7778-80-5]

(3) Water; H_2O; [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:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
25	0.1323	0.660	6.49×10^{-2}	7.766
	0.3150	0.544	5.22×10^{-2}	6.433
	0.3518	0.507	4.84×10^{-2}	6.001

(continued)

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 potassium sulfate solutions were determined using a Hilger spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Peking Chemical Factory, further purified by washing with H_2SO_4, NaOH and water; dried over $CaCl_2$ 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); CCl_4; [56-23-5]

(2) Potassium sulfate; K_2SO_4; [7778-80-5]

(3) Water; H_2O; [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: (continued)

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^5\,x_1$ (compiler)
25	0.4516	0.464	4.37×10^{-2}	5.509
	0.5177	0.430	4.02×10^{-2}	5.124
	0.6034	0.388	3.60×10^{-2}	4.657

COMPONENTS:

(1) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

(2) Sodium chloride; NaCl; [7647-14-5]

(3) Water; H_2O; [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:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^5\,x_1$ (compiler)
25	0.2549	0.690	6.84×10^{-2}	8.099
	0.5025	0.642	6.30×10^{-2}	7.536
	0.6375	0.616	6.01×10^{-2}	7.229
	0.8383	0.578	5.58×10^{-2}	6.768
	0.9623	0.553	5.32×10^{-2}	6.486
	1.0250	0.541	5.19×10^{-2}	6.344

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 H_2SO_4, NaOH and water; dried over $CaCl_2$ 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); CCl_4; [56-23-5]

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

(3) Water; H_2O; [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:

t/°C	c_2/mol dm^{-3}	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^5 x_1$ (compiler)
25	0.130	0.657	6.47×10^{-2}	7.706
	0.230	0.593	5.76×10^{-2}	6.948
	0.380	0.491	4.69×10^{-2}	5.767
	0.464	0.450	4.26×10^{-2}	5.296
	0.564	0.401	3.75×10^{-2}	4.726

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 H_2SO_4, NaOH and water; dried over $CaCl_2$ and fractionated.

(2) Peking Chemical Factory, recrystallized twice before use.

(3) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Water-d$_2$; D_2O; [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:

t/°C	100 $w_1 M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	4.78×10^{-4}	9.57×10^{-3}	7.34

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: ± 0.1×10^{-5} avg. dev.

Temperature: ± 0.05 K.

REFERENCES:

(1) Eidinoff, M. L., Joris, G. G., Taylor, H. S., Urey, H. C., Eds. *Production of Heavy Water,* McGraw-Hill, New York, 1955, p. 129.

COMPONENTS:

(1) Water-d$_2$; D_2O; [7789-20-0]

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Epherre, P.; Roth, E.

Bull. Soc. Chim. Fr. 1968, 2291-2.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^5\ g_1/g_2$	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25	9	0.9×10^{-2}	6.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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: ± 0.4×10^{-5} g.

Temperature: ± 1 K (compiler).

COMPONENTS:

(1) Water-d_2; D_2O; [7789-20-0]

(2) Tetrachloromethane (carbon tetrachloride); CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

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

J. Chem. Eng. Data 1972, *17*, 66-8.

VARIABLES:

T/K = 288 - 308

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
15	5.7 ± 0.1	0.713×10^{-2}	5.47
25	7.5 ± 0.2	0.949×10^{-2}	7.28
30	8.4 ± 0.3	1.07×10^{-2}	8.21
35	10.3 ± 0.3	1.32×10^{-2}	10.13

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:

(1) Wernimont, G.; Hopkinson, F. J. *Ind. Eng. Chem.* 1943, *12*, 272.

COMPONENTS:	EVALUATOR:
(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4] (2) Water; H_2O; [7732-18-5]	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_1, of 1.618 at 298.15 K (ref. 1).

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

Temperature		Reported Solubility	
°C	K	100 w_1	$10^3 x_1$
20	293.15	2.099 (ref. 4)	2.352 (ref. 4)
24.85	298.00	1.821 (ref. 5)	2.035 (ref. 5)
25	298.15	1.618 (ref. 1)	1.805 (ref. 1)
30	303.15	0.3023 (ref. 2), 0.2972 (ref. 3)	0.3333 (ref. 2), 0.3277 (ref. 3)

REFERENCES:

1. Symons, J. M. et al. *Treatment Techniques for Controlling Trihalomethanes in Drinking Water*, U. S. EPA Report 600/2-81-156, Cincinnati, OH., 1981.
2. McNally, M. E.; Grob, R. L. *J. Chromatogr.* 1983, *260*, 23.
3. Ibid., 1984, *284*, 105.
4. Nicholson, B. C.; Maguire, B. P.; Bursill, D. B. *Environ. Sci. Technol.* 1984, *18*, 518.
5. Warner, H. P.; Cohen, J. M.; Ireland, J. C. *Determination of Henry's Law Constants of Selected Priority Pollutants*, U. S. EPA Technical Report, PB87-212684, Cincinnati, OH., July 1987.

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

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

ORIGINAL MEASUREMENTS:

Symons, J. M.; *et al.*

Treatment Techniques for Controlling Trihalomethanes in Drinking Water, U. S. EPA Report 600/2-81-156, Cincinnati, OH., 1981.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	9.5×10^{-2}	1.6179	1.805

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: ± 0.5 K.

REFERENCES:

(1) Werner, U. S. Environmental Protection Agency, Cincinnati, OH., *Personal Communication*, 1980.

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

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

ORIGINAL MEASUREMENTS:

McNally, M. E.; Grob, R. L.

J. Chromatogr. 1983, *260*, 23-32.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	3031.9	0.3023	3.333

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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. & 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., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

ESTIMATED ERRORS:

Solubility: ± 150 ppm std. dev.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

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

ORIGINAL MEASUREMENTS:

McNally, M. E.; Grob, R. L.

J. Chromatogr. 1984, *284*, 105-16.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g_1V_2^{-1}/kg\ m^{-3}$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	2.968	0.2972	3.276

AUXILIARY INFORMATION

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, PA., 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:

(1) McNally, M. E.; Grob, R. L. *J. Chromatogr.* 1983, *260*, 23.

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

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

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, $H/m^3\ atm\ mol^{-1}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	1.6×10^{-3}	2.099	2.352

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 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:	$\pm 0.2 \times 10^{-3}$ std. dev.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants, U. S. EPA Technical Report, PB87-212684, Cincinnati, OH., July 1987.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
24.85	2.12×10^{-3}	1.821	2.036

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: ± 6 % std. dev.

Temperature: ± 0.05 K.

REFERENCES:

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

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

(2) Milang water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	1.6×10^{-3}	2.099	2.353

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/dm^3, 140 mg $CaCO_3/dm^3$, 13 mg organic carbon/dm^3, 110 mg suspended solid/dm^3.

ESTIMATED ERRORS:

Solubility: Not specified.

Temperature: ± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

(2) Myponga water

ORIGINAL MEASUREMENTS:

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

Envinon. Sci. Technol, 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	1.5×10^{-3}	2.239	2.515

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) pH = 7.6, 370 mg salt/dm^3, 60 mg $CaCO_3/dm^3$, 10 mg organic carbon/dm^3.

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Bromodichloromethane; $CHBrCl_2$; [75-27-4]

(2) Myponga water + humic acid

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	1.5×10^{-3}	2.239	2.515

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) pH = 7.9, 20 mg humic acid/dm^3, 370 mg salt/dm^3, 68 mg $CaCO_3/dm^3$, 17 mg organic carbon/dm^3.

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:	EVALUATOR:
(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. January 1993.

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 exists 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 w_1, of 0.8124 at 298.15 K (ref. 1).

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

Temperature		Solubility	
°C	K	100 w_1	$10^4 x_1$
10	283.15	0.3040 (ref. 6)	2.637 (ref. 6)
20	293.15	0.6320 (ref. 4), 0.2375 (ref. 6)	5.498 (ref. 4), 2.059 (ref. 6)
24.85	298.00	1.423 (ref. 5)	12.470 (ref. 5)
25	298.15	0.8124 (ref. 1)	7.079 (ref. 1)
30	303.15	0.1049 (ref. 2), 0.2514 (ref. 3) 0.3132 (ref. 6)	0.9082 (ref. 2), 2.179 (ref. 3) 2.7168 (ref. 6)

REFERENCES:

1. Symons, J. M. et al. *Treatment Techniques for Controlling Trihalomethanes in Drinking Water*, U. S. EPA Report 600/2-81-156, Cincinnati, OH., 1981.
2. McNally, M. E.; Grob, R. L. *J. Chromatogr.* 1983, *260*, 23.
3. Ibid., 1984, *284*, 105.
4. Nicholson, B. C.; Maguire, B. P.; Bursill, D. B. *Environ. Sci. Technol.* 1984, *18*, 518.
5. Warner, H. P.; Cohen, J. M.; Ireland, J. C. *Determination of Henry's Law Constants of Selected Priority Pollutants*, U. S. EPA Technical Report, PB87-212684, Cincinnati, OH., July 1987.
6. Howe, G. B.; Mullins, M. E.; Rogers, T. N. *AFESC Tyndall Air Force Base*, Report ESL-TR-86-66, *Vol. 1*, Florida, Sept. 1987, 86 pp. (AD-A188 571).

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

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

ORIGINAL MEASUREMENTS:

Symons, J. M. *et al.*

Treatment Techniques for Controlling Trihalomethanes in Drinking Water, U. S. EPA Report 600/2-81-156, Cincinatti, OH., 1981.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant H/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	3.5×10^{-2}	0.8124	7.080

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are given elsewhere (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) Source and purity not given.
(2) Cincinatti tap water.

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.5 K.

REFERENCES:

(1) Werner, U. S. Environmental Protection Agency, Cincinatti, OH., *Personal communication*, 1980.

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

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

ORIGINAL MEASUREMENTS:

McNally, M. E.; Grob, R. L.

J. Chromatogr. 1983, *260*, 23-32.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
30	1049.9	0.1049	9.081

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Standard solutions were prepared in 100 cm^3 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 used as received.
(2) Distilled and run through two Barnstead purification cartridges.

ESTIMATED ERRORS:

Solubility:	± 36.4 ppm std. dev.
Temperature:	± 0.5 K (compiler).

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

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

ORIGINAL MEASUREMENTS:

McNally, M. E.; Grob, R. L.

J. Chromatogr. 1984, *284*, 105-16.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/g m^{-3}	100 w_1 (compiler)	10^4 x_1 (compiler)
30	2509	0.2514	2.179

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:

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

ESTIMATED ERRORS:

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

REFERENCES:

(1) McNally, M. E.; Grob, R. L. *J. Chromatogr.* 1983, *260*, 23.

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

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

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	8.7×10^{-4}	0.6320	5.498

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:	± 0.2×10^{-4} std. dev.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants, EPA Tech. Report PB87-212684, Cincinatti, OH., July 1987.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
24.85	7.83×10^{-4}	1.423	1.538

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:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. D. *Environ. Sci. Tehnol.* 1979, *13*, 333.

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

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

ORIGINAL MEASUREMENTS:

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

AFESC Tyndall Air Force Base, Report ESL-TR-86-66. *Vol. 1*, Florida, Sept. 1987, 86 pp. (AD-A188 571).

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^6 w_1	100 w_1 (compiler)	10^4 x_1 (compiler)
10	3040	0.3040	2.6368
20	2375	0.2375	2.0587
30	3132	0.3132	2.7168

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

250 cm^3 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:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

(2) Milang water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	8.5×10^{-4}	0.6469	5.632

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/dm^3, 140 mg $CaCO_3/dm^3$, 10 mg organic carbon/dm^3, 110 mg suspended solid/dm^3 .

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1]

(2) Myponga water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	8.0×10^{-4}	0.6873	5.984

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/dm^3, 60 mg $CaCO_3/dm^3$, 10 mg organic carbon/dm^3.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dibromochloromethane; $CHBr_2Cl$; [124-48-1] (2) Myponga water + humic acid	Nicholson, B. C.; Maguire, B. P.; Bursill, D. B. *Environ. Sci. Technol.* 1984, *18*, 518-21.
VARIABLES: T/K = 293	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	7.7×10^{-4}	0.7141	6.2191

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, 17 mg organic carbon/dm^3.

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

(2) Water; H_2O; [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:

$$\text{Solubility } [100\, w_1] = 2.371 - 0.01517\, (T/\text{K}) + 2.7808 \times 10^{-5}\, (T/\text{K})^2$$

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

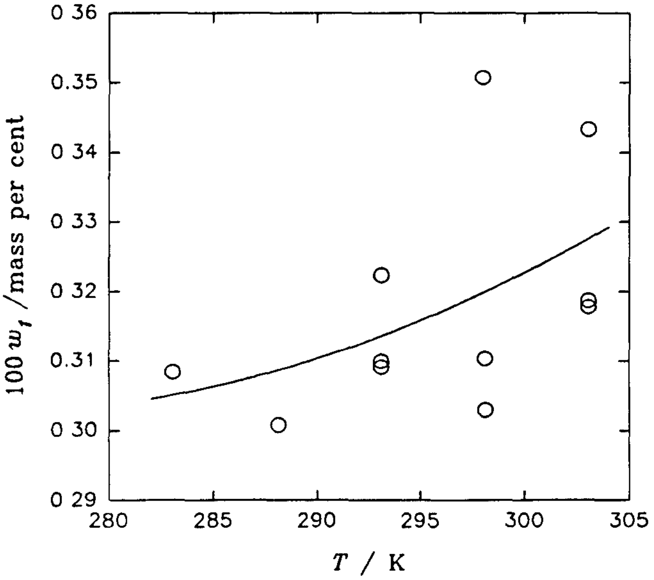

Figure 1. Solubility of Tribromomethane (1) in Water (2).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2] (2) Water; H_2O; [7732-18-5]	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)

Temperature		Solubility	
°C	K	$100\ w_1$	$10^4\ x_1$
10	283.15	0.305	2.18
15	288.15	0.309	2.21
20	293.15	0.314	2.24
25	298.15	0.320	2.29
30	303.15	0.328	2.34

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.

2. Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40*, 1491.

3. McNally, M. E.; Grob, R. L. *J. Chromatogr.* 1984, *284*, 105.

4. Wright, D. A.; Sandler, S. I.; DeVoll, D. *Environ. Sci. Technol.* 1992, *26*, 1828.

5. Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53*, 1744.

6. van Arkel, A. E.; Vles, S. E. *Recl. Trav. Chim. Pays-Bas* 1936, *55*, 407.

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

8. Symons, J. M. et al. *Treatment Techniques for Controlling Trihalomethanes in Drinking Water, U. S. EPA* Report 600/2-81-156, Cincinnati, OH., 1981.

9. Mackay, D. et al. *Volatilization of Organic Pollutants from Water*, U. S. EPA Report 600/2-82-019, Athens, Georgia, 1982, (PB 82-230939).

10. Nicholson, B. C.; Maguire, B. P.; Bursill, D. B. *Environ. Sci. Technol.* 1984, *18*, 518.

11. Munz, C. D. *Ph. D. Thesis*, Stamford University, Stamford, CA., 1985, 306 pp.

12. Warner, H. P.; Cohen, J. M.; Ireland, J. C. *Determination of Henry's Law Constants of Selected Priority Pollutants*, U. S. EPA Technical Report, PB87-212684, Cincinnati, OH., July 1987.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Squire, P. W.; Caines, C. M.

Pharm. J. 1905, *74*, 784-6.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	V_1/V_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	1.25×10^{-3}	0.361	2.582

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: Not specified.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.; Saylor, J. H.

J. Am. Chem. Soc. 1931, *53*, 1744-51.

VARIABLES:

T/K = 288 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	1000 g_1/g_2	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
15	3.01	0.301	2.15
30	3.19	0.319	2.28

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of tribromomethane 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., further purified by fractional freezing before use.
(2) Distilled.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Gross, P. M. *J. Am. Chem. Soc.* 1929, *51*, 2362.
(2) Saylor, J. H. *Ph. D. Thesis*, Duke University, Durham, 1930.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ n_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
30.0	1.26×10^{-3}	0.318	0.227

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); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

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

Ind. Eng. Chem. 1948, *40*, 1491-3.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	V_1/V_2	$100\ w_1$ (compiler)	$10^5\ x_1$ (compiler)
25.0	< 0.02	< 0.058	< 4.1

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:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

O'Connell, W. L.

Trans. Am. Inst. Mech. Eng. 1963, *226*, 126-32.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	0.311	0.310	2.22

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) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Symons, J. M. *et al.*

Treatment Techniques for Controlling Trihalomethanes in Drinking Water, U. S. EPA Report 600/2-81-156, Cincinnati, OH., 1981.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant H/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
25	2.4×10^{-2}	0.3107	2.221

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: ± 0.5 K.

REFERENCES:

(1) Werner, *U. S. Environmental Protection Agency*, Cincinnati, OH., Personal Communication, 1980.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Mackay, D. *et al.*

Volatilization of Organic Pollutants from Water, U. S. EPA Report 600/2-82-019, Athens, Georgia, 1982, (PB 82-230939).

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_1/mol\ m^{-3}$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)	$100\ w_2$ (compiler)	$10^3\ x_2$
25	12.0	0.3032	2.168	7.14×10^{-3}	1.0

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 dual flame ionization detector and an electron capture detector.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 1.0 K.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

(2) Water; H_2; [7732-18-5]

ORIGINAL MEASUREMENTS:

McNally, M. E.; Grob, R. L.

J. Chromatogr. 1984, *284*, 105-16.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g_1V_2^{-1}/g\ m^{-3}$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
30	3931	0.3933	2.814

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Standard tribromomethane 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, PA., U. S. A., purest grade available.
(2) Distilled and run through two Barnstead purification cartridges.

ESTIMATED ERRORS:

Solubility: ± 5.92 % std. dev.
Temperature: ± 0.5 K (compiler).

REFERENCES:

(1) McNally, M. E.; Grob, R. L. *J. Cromatogr.* 1983, *260*, 23.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	4.3×10^{-4}	0.3093	2.211

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:	$\pm$ 0.3 $\times$ 10^{-4} std. dev.
Temperature:	$\pm$ 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stamford University, Stamford, CA., 1985, 306 pp.

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant H/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
10	9.95×10^{-3}	0.3086	2.206
20	1.74×10^{-2}	0.3228	2.308
30	2.85×10^{-2}	0.3437	2.458

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility:	$\pm$ 3.9 %.
Temperature:	$\pm$ 0.5 K.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants, U. S. EPA Technical Report, PB-87-212684, Cincinnati, OH., July 1987.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m³ atm mol⁻¹	100 w_1 (compiler)	10^4 x_1 (compiler)
24.85	5.32×10^{-4}	0.3512	2.511

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:

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

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

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

ORIGINAL MEASUREMENTS:

Wright, D. A.; Sandler, S. I.; DeVoll, D.

Environ. Sci. Technol. 1992, *26*, 1828-31.

VARIABLES:

T/K = 293 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	γ^{∞}	100 w_1 (compiler)	10^4 x_1 (compiler)
20	3530 ± 260	0.396	2.83
35	3080 ± 425	0.454	3.25
50	4050 ± 220	0.345	2.47

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of tribromomethane (γ^{∞}) 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); $CHBr_3$; [75-25-2]

(2) Milang water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. **1984**, *18*, 518-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	4.6×10^{-4}	0.289	2.068

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/dm^3, 140 mg $CaCO_3$/dm^3, 13 mg organic carbon/dm^3, 110 mg suspended solid/dm^3.

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* **1979**, *13*, 333.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

(2) Myponga water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. **1984**, *18*(7), 518-521.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	4.1×10^{-4}	0.324	2.32

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/dm^3, 60 mg $CaCO_3$/dm^3, 10 mg organic carbon/dm^3 .

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* **1979**, *13*, 333.

COMPONENTS:

(1) Tribromomethane (bromoform); $CHBr_3$; [75-25-2]

(2) Myponga water + humic acid

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/m^3 atm mol^{-1}	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	4.3×10^{-4}	0.3093	2.173

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:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:	EVALUATOR:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	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 trichloromomethane (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:

$$\text{Solubility } [100\, w_1] = 12.5333 - 7.40557 \times 10^{-2}\, (T/\text{K}) + 1.16374 \times 10^{-4}\, (T/\text{K})^2$$

which shows a standard deviation of 5.6×10^{-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 trichloromomethane (1) in water (2) are presented in Table 1.

Table 1. Recommended Solubility of Trichloromethane (1) in Water (2)

Temperature		Solubility	
°C	K	$100\, w_1$	$10^3\, x_1$
0	273.15	0.988	1.503
5	278.15	0.938	1.427
10	283.15	0.895	1.361
15	288.15	0.857	1.303
20	293.15	0.825	1.254
25	298.15	0.798	1.212
30	303.15	0.778	1.182
35	308.15	0.763	1.159
40	313.15	0.755	1.147
45	318.15	0.752	1.142
50	323.15	0.755	1.147
55	328.15	0.763	1.159
60	333.15	0.778	1.182

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

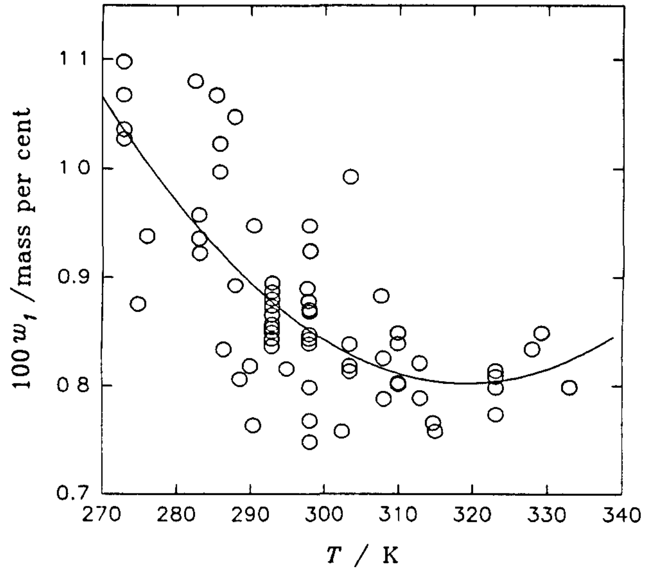

Figure 1. Solubility of Trichloromethane (1) in Water (2).

Part 2. The solubility of water (2) in trichloromomethane (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 trichloromomethane (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 trichloromomethane (1) between 263 and 323 K is as follows:

$$\text{Solubility } [100\, w_1] = 6.1195 \times 10^{-2} - 2.0623 \times 10^{-3}\, (T/\mathrm{K}) + 7.20879 \times 10^{-6}\, (T/\mathrm{K})^2$$

This equation represents the combined data with a standard deviation of 2.2×10^{-2} and a correlation coefficient of 0.916.

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

(continued next page)

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Water; H_2O; [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, $\log_{10} x_2$ 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 (2) 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)

Temperature		Solubility	
°C	K	100 w_1	$10^3 x_2$
-10	263.15	0.0177	1.172
-5	268.15	0.0265	1.753
0	273.15	0.0357	2.361
5	278.15	0.0453	2.994
10	283.15	0.0552	3.647
15	288.15	0.0655	4.324
20	293.15	0.0761	5.021
25	298.15	0.0871	5.744
30	303.15	0.0985	6.491
35	308.15	0.1102	7.258
40	313.15	0.1223	8.049
45	318.15	0.1347	8.859
50	323.15	0.1475	9.694

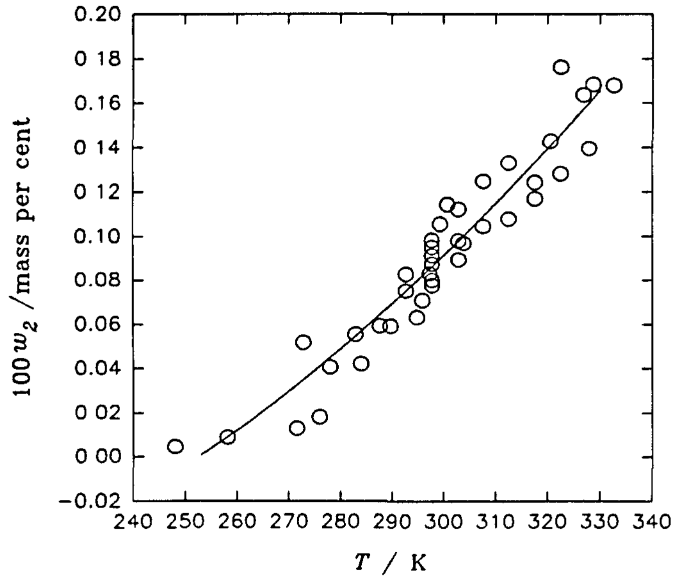

Figure 2. Solubility of Water (2) in Trichloromethane (1).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

Figure 3 shows the $\log_{10} x_2$ versus the reciprocal of absolute temperature behavior for comparison with the behavior shown in Figure 2.

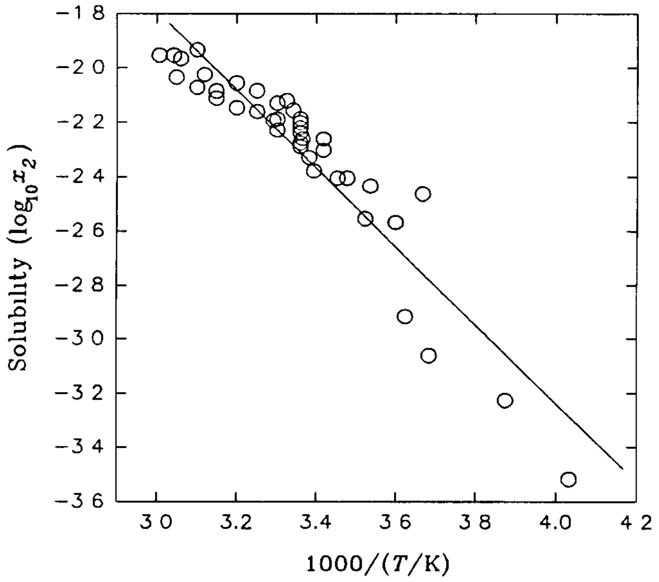

Figure 3. Solubility of Water (2) in Trichloromethane (1); $\log_{10} x_2$ versus 1000/T.

REFERENCES:

1. Herz, W. *Chem. Ber.* 1898, *31*, 2669-2672.

2. Salkowski, E. *Biochem. Z.* 1920, *107*, 191-201.

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(continued next page)

COMPONENTS:	EVALUATOR:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

REFERENCES:

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10. Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40*, 1491.
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COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Chancel, G.; Parmentier, F.

Compt. Rend. 1885, *100A*, 773-6.

VARIABLES:

T/K = 273 - 328

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
0.0	9.87	0.987	1.502
3.2	8.90	0.890	1.353
17.4	7.12	0.713	1.082
29.4	7.05	0.708	1.075
41.6	7.12	0.717	1.089
54.9	7.75	0.784	1.191

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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Herz, W.

Chem. Ber. 1898, *31*, 2669-72.

VARIABLES:

T/K = 295

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 V_1/V_2	100 w_1 (compiler)	100 V_2/V_1	100 w_2 (compiler)
22	0.420	0.620	0.152	0.102

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, d_4 = 1.4760 g/cm^3 at 22°C.
(2) Distilled (compiler), d_4 = 0.9980 g/cm^3 at 22°C.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Moore, B.; Roaf, H. E.

Proc. Roy. Soc., London 1904, *73*, 382-412.

VARIABLES:

T/K = 286

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
13	0.95	1.445	7.96×10^{-3}

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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Rex, A.

Z. Phys. Chem. 1906, *55*, 355-70.

VARIABLES:

T/K = 273 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
0	1.062	1.05	1.60
10	0.895	0.887	1.35
20	0.822	0.815	1.24
30	0.776	0.770	1.17

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of trichloromethane in water was determined in specially designed flasks with calibrated capillary 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); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	Antonov, G. N. *J. Chim. Phys.* 1907, *5*, 372-85.

VARIABLES:	PREPARED BY:
$T/K = 293$	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1M_1^{-1}/\text{mol g}^{-1}$ (compiler)
20	0.79	1.20	6.62×10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	Salkowski, E. *Biochem. Z.* 1920, *107*, 191-201.

VARIABLES:	PREPARED BY:
$T/K = 293$	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g_1V_2^{-1}/\text{kg m}^{-3}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	7.5	0.746	1.13

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 K (compiler).

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Clifford, C. W.

J. Ind. Eng. Chem. 1921, *13*, 631-2.

VARIABLES:

$T/K = 298 - 301$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1M_1^{-1}/\text{mol g}^{-1}$ (compiler)
24.5	0.084	0.554	4.66×10^{-3}
26.6	0.107	0.705	5.94×10^{-3}
27.8	0.116	0.764	6.44×10^{-3}

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:

(1) Clifford, C. W. *J. Ind. Eng. Chem.* 1921, *13*, 628.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Nicloux, M.; Scotti-Foglieni, L.

Ann. physiol. physicochim. biol. 1929, *5*, 434-82.

VARIABLES:

$T/K = 286 - 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Ostwald coefficient, L/dimensionless	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
13	12.9	0.974	1.48
20	7.7	0.787	1.20
25	7.0	0.877	1.33
30	6.2	0.944	1.44
37	3.8	0.753	1.14
40	3.5	0.772	1.17

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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

McCollum, J. L.

J. Pharmacol. Exper. Therap. 1930, *40*, 305-25.

VARIABLES:

T/K = 310

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 $g_1V_2^{-1}$/g cm^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
37.5	1.0	0.997	1.517

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A colorimetric method was used. A 2.5 g trichloromethane sample was pipetted into a centrifuge tube containing 20 cm^3 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; H_2O; [7732-18-5]

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Gibby, C. W.; Hall, J.

J. Chem. Soc. 1931, 691-3.

VARIABLES:

T/K = 248 - 327

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^4 x_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
-25	0.6×10^{-2}	4.0	3.33×10^{-4}
-15	0.9×10^{-2}	6.0	5.00×10^{-4}
-1	1.4×10^{-2}	9.3	7.77×10^{-4}
3	1.9×10^{-2}	12.6	1.05×10^{-3}
11	4.3×10^{-2}	28.4	2.39×10^{-3}
17	6.1×10^{-2}	40.3	3.39×10^{-3}
22	6.5×10^{-2}	42.9	3.61×10^{-3}
23	7.2×10^{-2}	47.5	4.00×10^{-3}
31	1.00×10^{-1}	65.9	5.55×10^{-3}
45	1.18×10^{-1}	77.7	6.55×10^{-3}
48	1.44×10^{-1}	94.7	8.00×10^{-3}
54	1.65×10^{-1}	108.3	9.16×10^{-3}

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 H_2SO_4, NaOH, and H_2O. Dried with Na_2CO_3 and refluxing with Mg_3N_2 before use.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 1 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Gross, P. M; Saylor, J. H.

J. Am. Chem. Soc. 1931, *53*, 1744-51.

VARIABLES:

$T/K = 288 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
15	0.852	1.28	0.845
30	0.771	1.16	0.765

AUXILIARY INFORMATION

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 H_2SO_4, Hg, and distilled water and fractionated before use.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: ± 1.0 %.
Temperature: ± 0.02 K.

REFERENCES:

(1) Gross, P. M. *J. Am. Chem. Soc.* 1929, *51*, 2362.
(2) Saylor, J. H. *Ph. D. Thesis*, Duke University, Durham, *1930*.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Evans, T. W.

Ind. Eng. Chem. Anal. Edit. 1936, *8*, 206-8.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
20	0.8	1.21	0.2	1.3

AUXILIARY INFORMATION

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 graduated to 0.05 cm^3 over a 5 cm^3 volume range. These bottles held approximately 50 cm^3. 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); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	van Arkel, A. E.; Vles, S. E. *Recl. Trav. Chim. Pays-Bas* 1936, *55*, 407-11.
VARIABLES:	PREPARED BY:
T/K = 303	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^2 x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
30.0	0.764	0.116	6.46×10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	De Minjer, C. H. *Doctoral Dissertation*, Technische Hoogeschool, Delft, 1939, 165 pp.
VARIABLES:	PREPARED BY:
T/K = 288	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^2 x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
15	0.20	1.31	1.11×10^{-2}

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 H_2SO_4 and K_2CO_3 solutions, followed by distillation before use.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Wilson, P. E. *J. Am. Chem. Soc.* 1921, *43*, 710.

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Staverman, A. J.

Recl. Trav. Chim. Pays-Bas 1941, *60*, 836-41.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1M_1^{-1}/mol\ g^{-1}$ (compiler)
0	5.29×10^{-2}	3.52	2.94×10^{-3}
25	9.32×10^{-2}	6.23	5.17×10^{-3}
30	1.130×10^{-1}	7.50	6.27×10^{-3}

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:

(1) Staverman, A. J. *Ph. D. Thesis*, Univ. of Leiden, Leiden, Belgium, 1938.

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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:

$t/°C$	$100\ w_1M_1^{-1}/mol\ g^{-1}$	$10^3\ x_1$ (compiler)	$100\ w_1$ (compiler)
25	4.88×10^{-3}	5.80	8.79×10^{-2}

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:	$\pm 0.1 \times 10^{-4}$ avg. dev.
Temperature:	± 0.05 K.

REFERENCES:

(1) Eidinoff, M. L.; Joris, G. G.; Taylor, H. S.; Urey, H. C., Eds. *Production of Heavy Water*, McGraw-Hill, New York, 1955, p. 129.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

McGovern, E. W.

Ind. Eng. Chem. 1943, *35*, 1230-9.

VARIABLES:

T/K = 273 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3 x_1$ (compiler)	100 w_2	$10^3 x_2$ (compiler)
0	1.02	1.55	-	-
10	0.91	1.38	-	-
20	0.82	1.25	-	-
25	0.79	1.20	0.097	6.39
30	0.77	1.17	0.100	6.59
40	0.74	1.12	0.135	8.88
50	0.76	1.15	-	-

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);
$CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Reinders, W.; De Minjer, C. H.

Recl. Trav. Chim. Pays-Bas 1947, *66*, 573-604.

VARIABLES:

T/K = 273 - 333

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^3 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
0	0.98	1.49	0.1	6.59
25	0.90	1.37	-	-
42	0.71	1.08	-	-
60	0.75	1.14	0.17	11.2

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 H_2SO_4 and K_2CO_3 solutions, followed by distillation before use.
(2) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichloromethane (chloroform);
$CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

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

Ind. Eng. Chem. 1948, *40*, 1491-3.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 V_1/V_2	10^3 x_1 (compiler)	100 w_1 (compiler)
25.0	0.90	2.01	1.32

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 returning the mixture 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:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Donahue, D. J.; Bartell, F. E.

J. Phys. Chem. 1952, *56*, 480-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^3 x_1$	$100 w_1$ (compiler)	$10^3 x_2$	$100 w_2$ (compiler)
25	1.2	0.790	5.0	7.58×10^{-2}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of trichloromethane and water was placed in a glass stoppered flask and was shaken intermittently for at last 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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Kudryavtseva, G. I.; Krutikova, A. D.

J. Appl. Chem. USSR. 1953, *26*, 1129-33.

VARIABLES:

$T/K = 293$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

$t/°C$	$100 w_1$	$10^3 x_1$ (compiler)	$100 w_2$	$10^2 x_2$ (compiler)
20	0.84	1.28	0.99	6.21

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:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Eberius, E.

Wasserbestimmung mit Karl-Fischer-Lösung, Verlag Chemie, GMBH, Weinheim, 1954, p. 67.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1 M_1^{-1}/mol\ g^{-1}$ (compiler)
20	0.084 ± 0.003	5.54	4.66×10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 50 g trichloromethane sample was shaken with pure water in a 100 cm^3 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).

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Zielinski, A. Z.

Chem. Stosowana 1959, *3*, 377-84.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$\rho_1/kg\ m^{-3}$	$10^3\ x_1$ (compiler)	$100\ w_1$ (compiler)
25	1.44	6.41	9.73×10^{-2}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of water in trichloromethane was determined by the Karl Fischer titration method (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) Distilled (compiler).
(2) Gliwice Chemicals, pure grade reagent, used as received.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Mitchell, J.; Smith, D. M. *Aquametry: A Treatise on Methods for the Determination of Water*, Wiley, New York, 1952, p. 73 and 260.

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Desnoyer, M.

Dosage de L'Eau dand les Solvants Organiques par Absorption Infra-Rouge et Mesure des Constantes Dielectriques, Centre D'Etudes Nucleaires de Saclay, Rept. No. 1254, Saclay, June 23, 1959.

VARIABLES:

$T/K = 299$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1M_1^{-1}$/mol g^{-1} (compiler)
26	8.6×10^{-2}	5.67	4.77×10^{-3}

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_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Tettamanti, K.; Nogradi, M.; Sawinsky, J.

Periodica Polytech. 1960, *4*, 201-18.

VARIABLES:

$T/K = 293$

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
20	0.82	1.25	7.0×10^{-2}	4.62

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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Conti, J. J.; Othmer, D. F.; Gilmont, R.

J. Chem. Eng. Data 1960, *5*, 301-7.

VARIABLES:

T/K = 298 - 329

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^3 x_1 (compiler)	100 w_2	10^3 x_2 (compiler)
25	0.75	1.139	8.0×10^{-2}	5.278
56.1	0.80	1.216	1.7×10^{-1}	11.16

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 concentra-tions were determined. The analytical techniques are described elsewhere (ref. 1).

SOURCE AND PURITY OF MATERIALS:

(1) U. S. P. grade. Washed with H_2SO_4 and K_2CO_3 solutions and then distilled. Only the center cut was used.

(2) Deionized, distilled twice before use.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Conti, J. J.; Othmer, D. F. *Unpublished data.*

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Ababi, V.; Popa, A.; Mihaila, Gh.

Analele Stiint. Univ. Al. I. Cuza Iasi. Sect. IC. Chem. 1964, *10*, 71-84.

VARIABLES:

T/K = 294

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
20.5	0.7	1.4	5.86×10^{-3}

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_D = 1.4454 at 20°.C.

(2) Distilled (compiler).

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Ababi, V.; Popa, A. *Analele Stiint. Univ. Al. I. Cuza Iasi. Sect. I,* 1960, *IV*, 929.

(2) Ibid., 1960, *VIII*, 233.

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Chistyakov, V. M.; Shapurova, V. V.

Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol. 1964, *7*, 349-50.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	10^3 x_1 (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
20	6.3×10^{-2}	4.16	3.5×10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Masterton, W. L.; Gendrano, M. C.

J. Phys. Chem. 1966, *70*, 2895-8.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	73.8	8.98×10^{-2}	5.92

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: ± 0.2×10^{-3} avg. dev.
Temperature: ± 0.05 K.

REFERENCES:

(1) Christian, S.; Affsprung, H.; Johanson, J. *J. Chem. Soc.* 1963, 1896.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Lowe, H. J.

in *Theory and Application of Gas Chromatography*, H. S. Kroman and S. R. Bender, Eds., Grune and Stratton, New York, 1968, p. 194-209.

VARIABLES:

T/K = 310

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
37	3.80	0.753	1.14

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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Okuda, Y.

Arch. Jap. Chir. 1968, *37*, 700-16.

VARIABLES:

T/K = 288 - 313

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
15	7.15 ± 2.03	0.5915	8.971
20	5.95 ± 1.35	0.6092	9.241
25	5.08 ± 0.83	0.6378	9.677
30	4.40 ± 0.53	0.6717	10.195
35	3.85 ± 0.40	0.7091	10.766
37	3.70 ± 0.39	0.7501	11.392
40	3.40 ± 0.34	0.7499	11.389

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:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	Lowe, H. J.; Hagler, K. in *Gas Chromatography, Biology and Medicine*, R. Poster, Ed., Churchill, London, 1969, p. 86-112.
VARIABLES:	PREPARED BY:
T/K = 310	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
37	3.91	0.788	1.197

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	Bachofen, H.; Farhi, L. E. *J. Appl. Physiol.* 1971, *30*, 136-9.
VARIABLES:	PREPARED BY:
T/K = 310	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
37	4.04	0.80	1.216

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: ± 0.06.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

(1) Trichloromethane (chloroform);
$CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

Russ. J. Phys. Chem. 1971, *45*, 488-90.

VARIABLES:

T/K = 288 - 333

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$1000\ g_1/g_2$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
15	4.82	0.480	7.27
30	3.20	0.319	4.83
45	2.05	0.205	3.10
60	1.30	0.130	1.96

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.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

REFERENCES:

(1) Treger, Yu. A.; Flid, R. M.; Spektor, S. S. *Russ. J. Phys. Chem.* 1964, *38*, 253.

COMPONENTS:

(1) Trichloromethane (chloroform);
$CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Karger, B. L; Chatterjee, A. K.; King, J. W.

Techn. Rept. No. 3, Department of Chemistry, Northeastern University, Boston, Mass., May 10, 1971.

VARIABLES:

T/K = 286

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Partition coefficient,[1] K_L/dimensionless	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
12.5	13.8	1.02	1.55

[1] Gas-liquid chromatographic parameter, from instrument calibration.

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_L) was calculated from the slope of the straight line plot of V_N/A_L versus V_L/A_L.

SOURCE AND PURITY OF MATERIALS:

(1) J. T. Baker Chemical Co., reagent grade.
(2) Distilled (compiler).

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Antropov, L. I.; Populyai, V. E.; Simonov, V. D.; Shamsutdinov, T. M.

Russ. J. Phys. Chem. 1972, *46*, 311-2 (VINITI No. 3739-71).

VARIABLES:

$T/K = 288 - 299$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
15	1.0	1.52	-	-
18	-	-	6.2×10^{-2}	4.09
22	-	-	6.5×10^{-2}	4.29
26	-	-	7.9×10^{-2}	5.21

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:

(1) Alexejev, W. *Ann. Phys. Chem.* 1886, *28*, 305.

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Ödberg, L.; Löfvenberg, A.; Högfeldt, E.; Fredlund, F.

J. Inorg. Nucl. Chem. 1972, *34*, 2605-16.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_1/\mathrm{mol\ m^{-3}}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	73.0	8.87×10^{-2}	5.849

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:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	McConnell, G.; Ferguson, D. M.; Pearson, C. R. *Endeavour* 1975, *34*, 13-8.
VARIABLES:	PREPARED BY:
$T/K = 293$	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	8200	0.813	1.24

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:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	Pearson, C. R.; McConnell, G. *Proc. Roy. Soc. B.* 1975, *189*, 305-32.
VARIABLES:	PREPARED BY:
$T/K = 293$	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	8200	0.813	1.24

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 ^{63}Ni electron capture detector.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.

J. Gen. Chem. USSR. 1977, *47*, 2230-4.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	67.5	0.807	8.02

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Trichloromethane was added from a microburet 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 saturation 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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Sato, A.; Nakijima, T.

Arch. Envir. Health 1979, *34*, 69-75.

VARIABLES:

T/K = 310

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Ostwald coefficient, L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
37	3.5	0.677	1.027

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 equilibrated air in the vessel was withdrawn using an airtight syringe and was injected into a gas chromatograph and analyzed. The height of the chromatogram peak was used to calculate the partition coefficient.

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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Freed, V. H.; Chiou, C. T.; Schmedding, D.; Kohnert, R.

Environ. Health Perspect 1979, *30*, 75-80.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6 w_1$	$100 w_1$ (compiler)	$10^4 x_1$ (compiler)
25	7950	0.795	1.208

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. Samples were removed for analysis at regular intervals. 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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Aref'eva, R. P.; Korenman, I. M.; Gorokhov, A. A.

USSR Patent 672 548, July 5, 1979, 3 pp. (CA. 91:113 256k).

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g_1 V_2^{-1}/kg\ m^{-3}$	$100 w_1$ (compiler)	$10^3 x_1$ (compiler)
20	12.7 ± .2	1.274	1.944

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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Coca, J.; Diaz, R. M.; Pozas, C.

Fluid Phase Equilibr. 1980, *4*, 125-36.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	100 w_1	$10^4 x_1$ (compiler)	100 w_2	$10^4 x_2$ (compiler)
25	1.19	1.814	8.0×10^{-2}	5.278

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The mutual solubility data were determined by the method as described by Othmer *et al.* (ref. 1). Ten cm^3 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:	± 0.5 K (compiler).

REFERENCES:

(1) Othmer, D. F.; White, R. E.; Trueges, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, Univ. of East Anglia, Norwich, U. K., July 1980, 375 pp.

VARIABLES:

$T/K = 293 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant H/dimensionless	100 w_1 (compiler)	$10^3 x_1$ (compiler)
20	0.112 ± 0.038	0.847	1.393
25	0.166 ± 0.100	0.699	1.149

AUXILIARY INFORMATION

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:	± 0.5 K (compiler).

COMPONENTS: (1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Hutchinson, T. C.; Hellebust, J. A.; Tam, D.; *et al.* *Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment*, Plenum Press, New York, 1980, p. 577-86.
VARIABLES: T/K = 298	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	7.95	0.7973	1.21

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:

(1) Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1977, *22*, 399.

COMPONENTS: (1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Veith, G. D.; Macek, K. J.; Petrucelli, S. R.; Carroll, J. *Proc. 3rd Ann. Symp. on Aquatic Toxicology*, ASTM Publ. 707, Philadelphia, 1980, p. 116-29.
VARIABLES: T/K = 293	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$n_1V_2^{-1}$/mol m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	61.7	0.732	1.11

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 1 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C.

Environ. Sci. Techn. 1980, *14*, 1227-9.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$n_1V_2^{-1}$/mol m^{-3}	$100\,w_1$ (compiler)	$10^3\,x_1$ (compiler)
25	60.5	0.719	1.09

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.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility: ± 4.3% std. dev.
Temperature: ± 0.3 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Symons, J. M.; et al.

Treatment Techniques for Controlling Trihalomethanes in Drinking Water, U. S. EPA Report 600/2-81-156, Cincinnati, OH., 1981.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant H/dimensionless	$100\,w_1$ (compiler)	$10^3\,x_1$ (compiler)
25	0.152	0.8205	1.256

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: ± 0.5 K.

REFERENCES:

(1) Warner, *U. S. Environmental Protection Agency*, Cincinnati, OH., Personal communication, 1980.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]	Wu, X. *Huaxue Shiji* 1981, 221-4.
VARIABLES:	**PREPARED BY:**
$T/K = 278 - 328$	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
5	417	0.0417	2.76
10	568	0.0568	3.75
15	606	0.0606	4.00
20	758	0.0758	5.00
25	872	0.0872	5.75
30	909	0.0909	5.99
35	1061	0.1061	6.99
40	1099	0.1099	7.24
45	1251	0.1251	8.23
50	1289	0.1289	8.48
55	1402	0.1402	9.22

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, H_2SO_4, and distilled water. Dried on molecular sieve before use.

ESTIMATED ERRORS:

Solubility: ± 72 std. dev.
Temperature: 1 - 2 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Leighton, D. T.; Calo, J. M.

J. Chem. Eng. Data 1981, *26*, 382-5.

VARIABLES:

$T/K = 275 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Distribution coefficient[1], D_L/dimensionless	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
1.9	68.9	0.8251	1.254
13.5	128.7	0.7846	1.192
15.7	146.7	0.7565	1.149
17.1	155.0	0.7676	1.166
22.0	194.5	0.7669	1.165
24.9	204.8	0.8297	1.261

[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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; et al.

Volatilization of Organic Pollutants from Water, U. S. EPA Report 600/3-82-019, Athens, Georgia, 1982 (PB 82-230 939).

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$\rho_1/kg\ m^{-3}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	7.95	0.7950	1.203

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.

COMPONENTS:

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

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Ohtsuka, K.; Kazama, K.

Sen'i Seihin Shohi Kagaku Kaishi 1982, *22*, 197-201.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.5	0.101	6.66

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was added gradually to 50 cm^3 trichloromethane in a flask which was then lowered into a thermostat bath. The flash 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).

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

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

Tellus 1983, *35B*, 170-6.

VARIABLES:

T/K = 293 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
20	0.1044	0.9845	1.498
25	0.1686	0.7456	1.132

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:

(1) McAuliffe, C. D. *Chem. Techn.* 1971, *1*, 46.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Orlandini, M.; Fermeglia, M.; Kikic, I.; Alessi, P.

Chem. Eng. J. 1983, *16*, 245-50.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^3\ x_1$	$10^3\ x_2$	100 w_1 (compiler)	100 w_2 (compiler)
20	1.23	5.17	0.809	0.0784

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of water and trichloromethane was agitated overnight and left at equilibrium for 24 hours. Three samples were withdrawn from each phase using a syringe and analyzed using gas chromatography. The gas chromatograph (C. Erba ATc/t) was equipped with a Shimadzu Chromatopac E-1A integrator. The stainless column was packed with 100 - 200 mesh Chromosorb W DMCD coated with heptadecane nitrile.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

Solubility:	Not specified.
Temperature:	± 0.1 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Lincoff, A. H.; Gossett, J. M.

in *Gas Transfer at Water Surfaces*, W. Brutsaert and G. H. Jirka, Eds., D. Reidel Publ. Co., Dordrecht, 1984, p. 11-25.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

EPICS Method

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	3.33×10^{-3}	0.7442	1.130

$$\log_e H = -\frac{4180}{T(\mathrm{K})} + 8.553$$

(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:	± 5 - 10 %.
Temperature:	± 0.1 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Lincoff, A. H.; Gossett, J. M.

in *Gas Transfer at Water Surfaces*, W. Brutsaert and G. H. Jirka, Eds., D. Reidel Publ. Co., Dordrecht, 1984, p. 11-25.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES: (continued)

Batch Air Stripping Method

t/°C	Henry's law constant, H/m³ atm mol⁻¹	100 w_1 (compiler)	$10^3 x_1$ (compiler)
20	3.04×10^{-3}	0.8152	1.239

$$\log_e H = -\frac{4322}{T(\mathrm{K})} + 8.956$$

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

McNally, M. E.; Grob, R. L.

J. Chromatogr. 1984, *284*, 105-16.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1 V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	$10^4 x_1$ (compiler)
30	2.524	0.2529	3.825

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:

(1) McNally, M. E.; Grob, R. L. *J. Chromatogr.* 1983, *260*, 23.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Techn. 1984, *18*, 518-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	3.0×10^{-3}	0.8257	1.255

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 extraction of the samples, the extracts 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: $\pm$ 0.1 × 10^{-3} std. dev.
Temperature: $\pm$ 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Techn.* 1979, *13*, 333.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stamford University, Stamford, CA., 1885, 306 pp.

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's Law Constant, H/dimensionless	ρ_1/kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
10	7.69×10^{-2}	8.750	0.8750	1.330
20	1.24×10^{-1}	8.320	0.8320	1.264
30	1.94×10^{-1}	7.880	0.7880	1.197

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 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 × 10^{-3} std. dev.
Temperature: $\pm$ 0.5 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Takano, J.; Ishihara, Y.; Yasuoka, T.; Mitsuzawa, S.

Nippon Kagaku Kaishi, 1985, 2116-9.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	7.77	0.7770	1.180
	9.33	0.9330	1.419
	6.33	0.6330	0.9604
	8.55	0.8550	1.300

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 1 cm^3 trichloromethane and 30 cm^3 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.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Lo, J. M.; Tseng, C. L.; Yang, J. Y.

Anal. Chem. 1986, *58*, 1596-7.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
25	0.82	1.25	6.87×10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A 5 cm^3 trichloromethane sample containing labeled complex cobalt(III) pyrrolidinecarbodithioate was placed together with 1000 cm^3 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 NaI (T1) 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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Barr, R. S.; Newsham, D. M. T.

Fluid Phase Equilibr. 1987, *35*, 189-205.

VARIABLES:

T/K = 293 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^3 x_1$	$100 w_1$ (compiler)	$10^3 x_2$	$100 w_2$ (compiler)
20	1.218	0.8016	5.06	0.0767
35	1.121	0.7382	8.29	0.126
50	1.099	0.7238	11.6	0.177

Mole fraction of trichloromethane (x_1) was calculated from the activity coefficient at infinite dilution (γ^∞) using the relation $x_1 = 1/\gamma^\infty$.

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 $CaCl_2$ solution controlled the partial pressure of water. The water concentration of the sample was determined using a Karl Fischer titration apparatus.

SOURCE AND PURITY OF MATERIALS:

(1) Koch Light Laboratories Ltd., used as received.

(2) Double distilled tap water.

ESTIMATED ERRORS:

Solubility: Not specified.

Temperature: ± 0.05 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Gossett, J. M.

Environ. Sci. Technol. 1987, *21*, 202-8.

VARIABLES:

T/K = 283 - 308

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's Law Constant, H/m^3 atm/mol^{-1}	CV[1] %	$100 w_1$ (compiler)	$10^3 x_1$ (compiler)
9.6	1.50×10^{-3}	6.16	1.0320	1.571
17.5	2.46×10^{-3}	1.96	0.8980	1.365
24.8	3.67×10^{-3}	3.75	0.8424	1.280
34.6	5.63×10^{-3}	3.76	0.8332	1.2662

[1] CV = coefficient of variation (= 100 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); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants U. S. EPA Techn. Rept. PB87-212684, Cincinnati, OH., July 1987.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
24.85	3.39×10^{-3}	0.9169	1.397

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:

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

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

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

AFESC Tyndall Air Force Base, Report ESL-TR-86-66, *Vol. 1*, Florida, Sept. 1987, 86 pp. (AD-A188 571).

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	10^6 w_1	100 w_1 (compiler)	10^4 x_1 (compiler)
10	3471	0.3471	5.2535
20	2963	0.2963	4.4827
30	3596	0.3596	5.4432

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

250 cm^3 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:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Vogel, A. I., rev. by Furniss, B. S.; *et al.*

Vogel's Textbook of Practical Organic Chemistry, 5th ed., Longman, London, 1989, p. 1442.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3 x_1$ (compiler)	100 $w_1 M_1^{-1}$/mol g^{-1} (compiler)
20.0	0.82	1.25	6.87 × 10^{-3}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility determination was done in small test tubes (e. g., 100 × 12 mm) to permit vigorous shaking of the trichloromethane and water mixture. During the experiment, 0.20 cm^3 trichloromethane was added to 3.0 cm^3 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 $CaCl_2$ before use.
(2) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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

ORIGINAL MEASUREMENTS:

Wright, D. A.; Sandler, S. I.; DeVoll, D.

Environ. Sci. Technol. 1992, *26*, 1828-31.

VARIABLES:

T/K = 293 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	γ^∞	$10^3 x_1$	100 w_1 (compiler)
20	818 ± 20	1.22	0.803
35	847 ± 30	1.18	0.777
50	862 ± 27	1.16	0.764

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A differential static cell equilibrium apparatus was used for measuring the infinite dilution activity coefficient of trichloromethane (γ^∞) in water. The degassed water cells were submerged in a thermostated water bath. Trichloromethane was injected into the mixture cell and a magnetic stirrer was turned on. The mixture in the cells was 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) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Milang water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m³ atm mol⁻¹	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	3.3×10^{-3}	0.7506	1.1407

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 mg salt/dm³, 140 mg $CaCO_3$/dm³, 15 mg organic carbon/dm³, 110 mg suspended solid/dm³.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) MQ-Water

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stamford University, Stamford, CA., 1985, 306 pp.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
20	0.244	0.4207	6.371

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 con-stant. 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 mg total organic carbon per dm³, 0.75 mg COD/dm³.

ESTIMATED ERRORS:

Solubility: ± 0.016 std. dev.
Temperature: ± 0.5 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Municipal tap water (PASE)

ORIGINAL MEASUREMENTS:

Munz, C. D.

Ph. D. Thesis, Stamford University, Stamford, CA., 1985, 306 pp.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
20	0.324	0.3174	4.803

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:

(1) J. T. Baker Chemicals Co., NJ., > 99.5 % purity.

(2) 10 mg total organic carbon per dm^3, 40 mg COD/dm^3.

ESTIMATED ERRORS:

Solubility: ± 0.020 std. dev.
Temperature: ± 0.5 K.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Myponga water

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, $H/m^3\ atm\ mol^{-1}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
20	2.9×10^{-3}	0.8542	1.299

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 mg salt/dm^3, 60 mg $CaCO_3$/dm^3, 10 mg organic carbon/dm^3.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Myponga water + humic acid

ORIGINAL MEASUREMENTS:

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

Environ. Sci. Technol. 1984, *18*, 518-21.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	3.1×10^{-3}	0.7991	1.2145

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/cm^3, 370 mg salt/dm^3, 68 mg $CaCO_3$/dm^3, 17 mg organic carbon/dm^3.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

REFERENCES:

(1) Mackay, D.; Shiu, W. Y.; Sutherland, R. P. *Environ. Sci. Technol.* 1979, *13*, 333.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Seawater

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, Univ. of East Anglia, Norwich, U. K., July 1980, 375 pp.

VARIABLES:

T/K = 283 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^4 x_1 (compiler)
10	0.112 ± 0.025	0.569	9.33
15	0.129 ± 0.039	0.614	10.07
20	0.161 ± 0.027	0.605	9.92
25	0.197 ± 0.057	0.603	9.89

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: ± 0.5 K (compiler).

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Seawater

ORIGINAL MEASUREMENTS:

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

Tellus 1983, *35B*, 170-6.

VARIABLES:

$T/K = 283 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
10	0.1046	0.6500	9.864
15	0.1309	0.6470	9.818
20	0.1624	0.6428	9.753
25	0.2001	0.6377	9.675

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

$$\log_e H = -\frac{3649}{T(\mathrm{K})} + 10.63$$

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 48° N to 65° S in the Atlantic in late 1981.

ESTIMATED ERRORS:

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

REFERENCES:

(1) McAuliffe, C. D. *Chem. Techn.* 1971, *1*, 46.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Cesium chloride; CsCl; [7647-17-8]

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

ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.

J. Gen. Chem. USSR, 1977, *47*, 2230-4.

VARIABLES:

T/K = 293
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	c_1/mol m^{-3}	100 w_1 (compiler)	$10^3 x_1$ (compiler)
20	0.5	-	-	-
	1.0	64.5	0.6828	1.221
	1.5	58.5	0.5830	1.143
	2.0	-	-	-
	2.5	56.0	0.5081	1.237
	3.0	52.5	0.4560	1.263

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); $CHCl_3$; [67-66-3]

(2) Hydrogen chloride; HCl; [7647-01-0]

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

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

Russ. J. Phys. Chem. 1971, *45*, 488-90.

VARIABLES:

T/K = 288 - 333

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

Solubility of $CHCl_3$ in 10 % HCl solution:

t/°C	$10^3\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
15	6.70	0.670	10.71
30	4.44	0.444	7.086
45	2.36	0.236	3.759
60	1.34	0.134	2.132

Solubility of $CHCl_3$ in 20 % HCl solution:

t/°C	$10^3\ w_1$	$100\ w_1$ (compiler)	$10^4\ x_1$ (compiler)
15	9.20	0.920	15.58
30	5.16	0.516	8.706
45	2.84	0.284	4.781
60	1.50	0.150	2.522

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:

(1) Treger, Yu. A.; Flid, R. M.; Spektor, S. S. *Russ. J. Phys. Chem.* 1964, *38*, 253.

COMPONENTS:

(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

(2) Lithium chloride; LiCl; [7447-41-8]

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

ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.

J. Gen. Chem. USSR, 1977, *47*, 2230-4.

VARIABLES:

T/K = 293
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	c_1/mol m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	0.5	66.8	0.7880	1.212
	1.0	64.5	0.7503	1.168
	1.5	60.0	0.6921	1.091
	2.0	58.5	0.6675	1.065
	2.5	56.0	0.6320	1.022
	3.0	52.0	0.5805	1.003

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); $CHCl_3$; [67-66-3]

(2) Potassium chloride; KCl; [7447-40-7]

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

ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.

J. Gen. Chem. USSR, 1977, *47*, 2230-4.

VARIABLES:

T/K = 293
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	c_1/mol m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	0.5	56.0	0.6535	1.021

(continued)

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:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Potassium chloride; KCl; [7447-40-7] (3) Water; H_2O; [7732-18-5]	Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I. *J. Gen. Chem. USSR*, 1977, *47*, 2230-4.
VARIABLES:	**PREPARED BY:**
T/K = 293 Concentration	A. L. Horvath

EXPERIMENTAL VALUES: (continued)

t/°C	c_2/mol dm^{-3}	c_1/mol m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	1.0	50.0	0.5692	0.9160
	1.5	41.0	0.4591	0.7610
	2.0	-	-	-
	2.5	29.2	0.3131	0.5542
	3.0	24.2	0.2546	0.4639

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Trichloromethane (chloroform); $CHCl_3$; [67-66-3] (2) Rubidium chloride; RbCl; [7791-11-9] (3) Water; H_2O; [7732-18-5]	Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I. *J. Gen. Chem. USSR*, 1977, *47*, 2230-4.
VARIABLES:	**PREPARED BY:**
T/K = 293 Concentration	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	c_1/mol m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	0.5	-	-	-
	1.0	58.5	0.6454	1.0920
	1.5	-	-	-
	2.0	46.0	0.4738	0.9049
	2.5	43.5	0.4635	0.8751
	3.0	39.7	0.3852	0.8449

AUXILIARY INFORMATION

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.

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); $CHCl_3$; [67-66-3]

(2) Sodium chloride; NaCl; [7647-14-5]

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

ORIGINAL MEASUREMENTS:

Pavlovskaya, E. M.; Charykov, A. K.; Tikhomirov, V. I.

J. Gen. Chem. USSR, *47*, 2230-4.

VARIABLES:

T/K = 293
Concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_2/mol dm^{-3}	c_1/mol m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	0.5	57.2	0.6707	1.0390
	1.0	51.0	0.5837	0.9236
	1.5	42.6	0.4791	0.7730
	2.0	37.6	0.4156	0.6850
	2.5	30.9	0.3361	0.5660
	3.0	25.8	0.2754	0.4742

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 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) Water-d_2; D_2O; [7789-20-0]

(2) Trichloromethane (chloroform); $CHCl_3$; [67-66-3]

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:

t/°C	100 $w_1 M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	4.15×10^{-3}	8.31×10^{-2}	4.93

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:

(1) Eidinoff, M. L.; Joris, G. G.; Taylor, H. S.; Urey, H. C., Eds., *Production of Heavy Water*, McGraw-Hill, New York, 1955, p. 129.

COMPONENTS:

(1) Triiodomethane (iodoform);
CHI_3; [75-47-8]

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

ORIGINAL MEASUREMENTS:

Dehn, W. M.

J. Am. Chem. Soc. 1917, *39*, 1399-404.

VARIABLES:

T/K = 293 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^6\ x_1$ (compiler)
20 - 25	1.0×10^{-1}	1.0×10^{-1}	4.57

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Excess triiodomethane in 5 cm^3 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 vaccum 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);
CHI_3; [75-47-8]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$m_1/mol\ kg^{-1}$	$100\ w_1$ (compiler)	$10^6\ x_1$ (compiler)
30	3×10^{-4}	1.18×10^{-2}	5.41

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); CHI_3; [75-47-8]

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

ORIGINAL MEASUREMENTS:

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

Ind. Eng. Chem. 1948, *40*, 1491-3.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25.0	< 0.2	< 0.02	< 4.6

AUXILIARY INFORMATION

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:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:	EVALUATOR:
(1) Bromochloromethane; CH_2BrCl; [74-97-5] (2) Water; H_2O; [7732-18-5]	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:

233 1. Tewari, Y. B.; Miller, M. M.; Wasik, S. P.; Martire, D. E. *J. Chem. Eng. Data* 1982, *27*, 451.

234 2. Miller, M. M.; Wasik, S. P.; Huang, T.-C.; Shiu, W.-Y.; Mackay, D. *Environ. Sci. Technol.* 1985, *19*, 522.

[illegible] 3. O'Connell, W. L. *Trans. Am. Ins. Mech. Eng.* 1963, *226*, 126.

COMPONENTS:

(1) Bromochloromethane; CH_2BrCl; [74-97-5]

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

ORIGINAL MEASUREMENTS:

O'Connell, W. L.

Trans. Am. Inst. Mech. Eng. 1963, *226*, 126-32.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$10^3\ x_1$ (compiler)	$100\ g_2/g_1$	$10^3\ x_2$ (compiler)
20	1.5	2.08	9.0×10^{-2}	6.43

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; CH_2BrCl; [74-97-5]

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

ORIGINAL MEASUREMENTS:

Tewari, Y. B.; Miller, M. M.; Wasik, S. P.; Martire, D. E.

J. Chem. Eng. Data 1982, *27*, 451-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$c_1/mol\ m^{-3}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25.0	125	1.646	2.325

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 a 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; CH_2BrCl; [74-97-5]

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

ORIGINAL MEASUREMENTS:

Miller, M. M.; Wasik, S. P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-9.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$n_1V_2^{-1}/\text{mol m}^{-3}$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	129.0	1.646	2.325

AUXILIARY INFORMATION

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:	EVALUATOR:
(1) Dibromomethane; CH_2Br_2; [74-95-3] (2) Water; H_2O; [7732-18-5]	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:

$$\text{Solubility } [100\, w_1] = 10.1890 - 0.06336789\,(T/\text{K}) + 1.10906 \times 10^{-4}\,(T/\text{K})^2$$

which produced a standard deviation of 4.4×10^{-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 1. Recommended Solubility of Dibromomethane (1) in Water (2)

Temperature		Solubility	
°C	K	$100\, w_1$	$10^3\, x_1$
0	273.15	1.155	1.209
5	278.15	1.144	1.198
10	283.15	1.138	1.191
15	288.15	1.138	1.191
20	293.15	1.144	1.198
25	298.15	1.155	1.209
30	303.15	1.171	1.226
35	308.15	1.194	1.251
40	313.15	1.221	1.279
45	318.15	1.254	1.313
50	323.15	1.293	1.356

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.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Dibromomethane; CH_2Br_2; [74-95-3] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

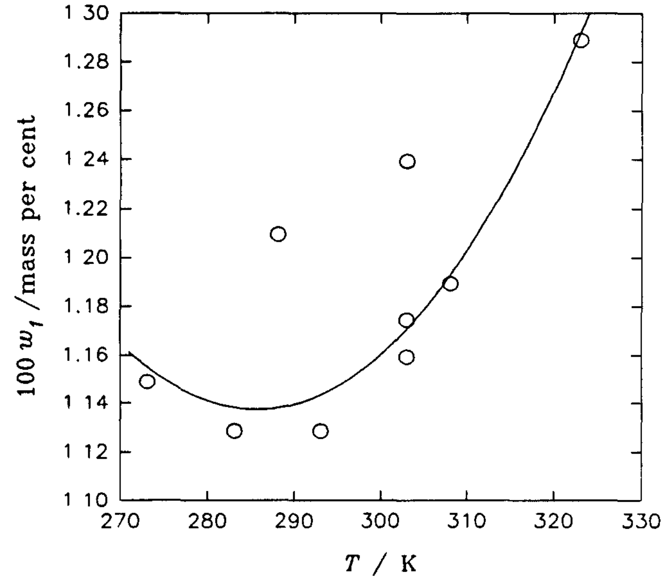

Figure 1. Solubility of Dibromomethane (1) in Water (2).

REFERENCES:

1. Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* 1948, *40*, 1491.

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

COMPONENTS:

(1) Dibromomethane; CH_2Br_2; [74-95-3]

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

ORIGINAL MEASUREMENTS:

Rex, A.

Z. Phys. Chem. 1906, *55*, 355-70.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
0	1.173	1.15	1.20
10	1.146	1.13	1.18
20	1.148	1.13	1.18
30	1.176	1.16	1.21

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

COMPONENTS:

(1) Dibromomethane; CH_2Br_2; [74-95-3]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.; Saylor, J. H.

J. Am. Chem. Soc. 1931, *53*, 1744-51.

VARIABLES:

$T/K = 288 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$1000\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
15	11.70	1.16	1.21
30	11.93	1.18	1.24

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of dibromomethane in 50 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., purified by fractionation through a Hempel column before use.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: ± 0.5 %.
Temperature: ± 0.02 K.

REFERENCES:

(1) Gross, P. M. *J. Am. Chem. Soc.* 1929, *51*, 2362.
(2) Saylor, J. H. *Ph. D. Thesis*, Duke University, Durham, 1930.

COMPONENTS:

(1) Dibromomethane; CH_2Br_2; [74-95-3]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	m_1/mol kg^{-1}	$10^2 x_1$	$100 w_1$ (compiler)
30.0	6.86×10^{-2}	0.123	1.174

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; CH_2Br_2; [74-95-3]

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

ORIGINAL MEASUREMENTS:

Botth, H. S.; Everson, H. E.

Ind. Eng. Chem. 1948, *40*, 1491-3.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$100 V_1/V_2$	$100 w_1$ (compiler)	$10^3 x_1$ (compiler)
25.0	0.70	1.71	1.80

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:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:

(1) Dibromomethane; CH_2Br_2; [74-95-3]

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

ORIGINAL MEASUREMENTS:

O'Connell, W. L.

Trans. Am. Inst. Mech. Eng. 1963, *226*, 126-32.

VARIABLES:

$T/K = 293 - 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
20	-	-	0.07	6.71
25	1.1	1.14	-	-

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) Dibromomethane; CH_2Br_2; [74-95-3]

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

ORIGINAL MEASUREMENTS:

Wright, D. A.; Sandler, S. I.; DeVoll, D.

Environ. Sci. Tech. 1992, *26*, 1828-31.

VARIABLES:

$T/K = 293 - 323$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	γ^∞	$10^3\ x_1$	$100\ w_1$ (compiler)
20	869 ± 45	1.15	1.10
35	801 ± 35	1.25	1.19
50	740 ± 32	1.35	1.29

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. Degassed 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) Source and purity not given.
(2) Distilled, filtered and deionized.

ESTIMATED ERRORS:

Solubility: See above.
Temperature: ± 0.05 K.

COMPONENTS:	EVALUATOR:
(1) Dichloromethane; CH_2Cl_2; [75-09-2] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION:

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 Treszczanovicz (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):

$$\text{Solubility } [100\, w_1] = 58.838 - 0.38224\, (T/\text{K}) + 6.3928 \times 10^{-4}\, (T/\text{K})^2$$

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 1. Recommended Solubility of Dichloromethane (1) in Water (2)

Temperature		Solubility	
°C	K	100 w_1	$10^3\, x_1$
0	273.15	2.126	4.587
5	278.15	1.977	4.260
10	283.15	1.860	4.004
15	288.15	1.766	3.799
20	293.15	1.722	3.703
25	298.15	1.701	3.657
30	303.15	1.712	3.681
35	308.15	1.754	3.773

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Dichloromethane; CH_2Cl_2; [75-09-2] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

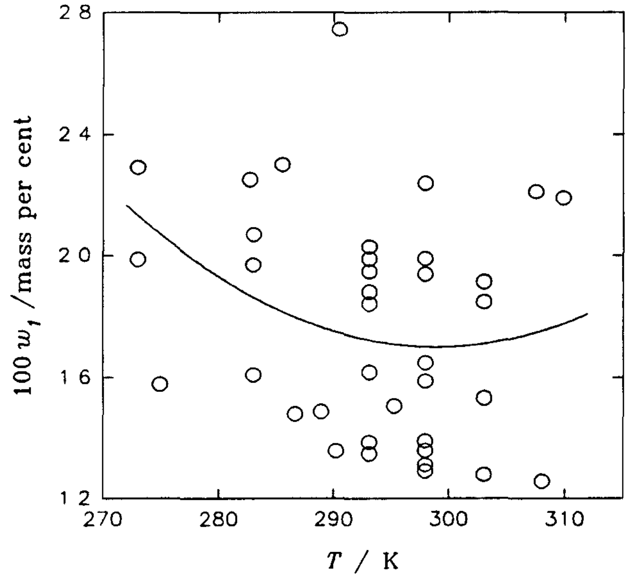

Figure 1. Solubility of Dichloromethane (1) in Water (2).

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 Terszczanowicz (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:

$$\log_{10} x_2 = 1.8214 - 1164.63/(T/\mathrm{K})$$

The equation represents the combined data with a standard deviation of 5.8 x 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)

COMPONENTS:	EVALUATOR:
(1) Dichloromethane; CH_2Cl_2; [75-09-2] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

Table 2. Recommended Solubility of Water (2) in Dichloromethane (1)

Temperature		Solubility	
°C	K	100 w_2	10^3 x_2
-20	253.15	0.0353	1.663
-15	258.15	0.0434	2.042
-10	263.15	0.0522	2.487
-5	268.15	0.0640	3.008
0	273.15	0.0768	3.612
5	278.15	0.0917	4.308
10	283.15	0.109	5.109
15	288.15	0.128	6.021
20	293.15	0.151	7.057
25	298.15	0.176	8.226
30	303.15	0.204	9.541
35	308.15	0.236	11.015
40	313.15	0.271	12.656

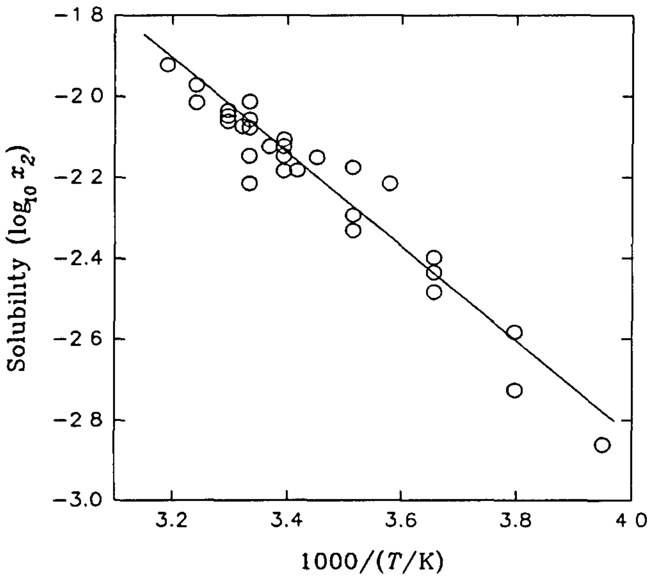

Figure 2. Solubility of Water (2) in Dichloromethane (1).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Dichloromethane; CH_2Cl_2; [75-09-2] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

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(continued next page)

COMPONENTS: (1) Dichloromethane; CH_2Cl_2; [75-09-2] (2) Water; H_2O; [7732-18-5]	EVALUATOR: A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

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COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Rex, A.

Z. Phys. Chem. 1906, *55*, 355-70.

VARIABLES:

T/K = 273 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	100 w_1 (compiler)	10^3 x_1 (compiler)
0	2.363	2.30	4.97
10	2.122	2.08	4.48
20	2.000	1.96	4.22
30	1.969	1.93	4.16

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; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Salkowski, E.

Biochem. Z. 1920, *107*, 191-201.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
20	12.24	1.211	2.59

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A volumetric method similar to that introduced by Alexejew 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).

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

$T/K = 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 x_1$	$m_1/\text{mol kg}^{-1}$ (compiler)	$100\ w_1$ (compiler)
30.0	0.416	0.232	1.931

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) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Bakowski, S.; Treszczanowicz, E.

Przemysl Chemiczny 1937, *21*, 204-6.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3 x_1$	$100\ w_2$	$10^3 x_2$
20	2.0	4.32	0.5	17.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water content of a liquid mixture was determined in a specially constructed apparatus which consisted of a 250 cm^3 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 cm^3.

SOURCE AND PURITY OF MATERIALS:

(1) Merck reagent, dried by means of $CaCl_2$ before use.
(2) Distilled (compiler).

ESTIMATED ERRORS:

Solubility: ± 0.01 cm^3.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Niini, A.

Suomen Kemistilehti 1938, *11A*, 19-20.

VARIABLES:

$T/K = 293$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^2\ x_2$ (compiler)
20	1.629	3.50	0.239	1.12

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 P_2O_5 and redistilled before use.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: ± 12 %.
Temperature: ± 0.5 K (compiler).

COMPONENTS:

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

(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Staverman, A. J.

Recl. Trav. Chim. Pays-Bas 1941, *60*, 836-41.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^5\ x_1$ (compiler)	$100\ w_1 M_1^{-1}/mol\ g^{-1}$ (compiler)
0	8.49×10^{-2}	400	4.71×10^{-3}
25	1.67×10^{-1}	788	9.27×10^{-3}
30	1.96×10^{-1}	925	10.90×10^{-3}

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:

(1) Staverman, A. J. *Ph. D. Thesis*, Univ. of Leiden, Leiden, Belgium, 1938.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

McGovern, E. W.

Ind. Eng. Chem. 1943, *35*, 1230-9.

VARIABLES:

T/K = 263 - 308

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3 x_1$ (compiler)	100 w_2	$10^3 x_2$ (compiler)
-10	-	-	0.056	2.63
0	2.00	4.31	0.079	3.71
10	1.62	3.48	0.110	5.17
20	1.40	3.00	0.150	7.03
25	1.32	2.83	0.198	9.27
30	1.29	2.76	0.200	9.36
35	1.27	2.72	0.228	10.66

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:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

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

Ind. Eng. Chem. 1948, *40*, 1491-3.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 V_1/V_2	100 w_1 (compiler)	$10^3 x_1$ (compiler)
25.0	2.60	3.32	7.23

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).

SOURCE AND PURITY OF MATERIALS:

(1) Commercial reagent, C. P. grade, used as received.
(2) Distilled.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Hanslick, R. S. *Ph. D. Thesis*, Columbia University, 1935.

COMPONENTS:

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

(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Davies, W.; Jagger, J. B.; Whalley, H. K.

J. Soc. Chem. Ind. (London) 1949, *68*, 26-31.

VARIABLES:

$T/K = 253 - 313$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1M_1^{-1}/\text{mol g}^{-1}$ (compiler)
-20	0.3×10^{-1}	1.4	1.66×10^{-3}
-10	0.4×10^{-1}	1.9	2.22×10^{-3}
0	0.7×10^{-1}	3.3	3.88×10^{-3}
10	1.0×10^{-1}	4.7	5.55×10^{-3}
20	1.4×10^{-1}	6.6	7.77×10^{-3}
30	1.9×10^{-1}	8.9	10.5×10^{-3}
40	2.6×10^{-1}	12.1	14.4×10^{-3}

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; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Donahue, D. J.; Bartell, F. E.

J. Phys. Chem. 1952, *56*, 480-4.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^3\ x_1$	$100\ w_1$ (compiler)	$10^2\ x_2$	$100\ w_2$ (compiler)
25	4.2	1.950	1.13	0.242

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:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Kudryavtseva, G. I.; Krutikova, A. D.

J. Appl. Chem. USSR. 1953, *26*, 1129-33.

VARIABLES:

T/K = 293

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^2\ x_2$ (compiler)
20	1.89	4.07	1.92	8.45

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The mutual solubility between dichloromethane and water was determined by titration from a microburet 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:	Not specified.
Temperature:	± 0.5 K (compiler).

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Maretic, M.; Sirocic, V.

Nafta (Zagreb) 1962, *13*, 126-31.

VARIABLES:

T/K = 298 - 346
P/mmHg = 750

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
25	1.4	3.00	0.2	9.36

t/°C	P/mmHg	$10^2\ x_1$	100 w_1 (compiler)
38.3	750	0.39	1.81
44.0	750	0.19	0.89
58.0	750	0.15	0.70
73.0	750	0.10	0.47

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined in a 50 cm^3 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 $CaCl_2$ and distilled. The middle fraction was used.
(2) Distilled.

ESTIMATED ERRORS:

Solubility:	± 0.2 % by mass.
Temperature:	± 2.0 K.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

du Pont de Nemours & Company,

Solubility Relationship of the Freon Fluorocarbon Compounds, Tech. Bull. *B-7*, Wilmington, Del., 1966, 16 pp.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
25	1.32	2.83	1.55 × 10^{-2}

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: ± 1 K (compiler).

REFERENCES:

(1) Sanders, P. A. *Handbook of Aerosol Technology*, 2^{nd} ed., Van Nostrand Reinhold Co., New York, 1979, p. 42.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Sabinin, V. E.; Kiya-Oglu, N. V.; Gorichnina, V. P.

J. Appl. Chem. USSR. 1970, *43*, 1788-90.

VARIABLES:

T/K = 293 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
20	0.6	1.28	0.15	7.03
30	2.6	6.63	0.19	8.89

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/cm³ and refractive index = 1.4233 at 20 °C.
(2) Distilled.

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

COMPONENTS:

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

(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Lees, F. P.; Sarram, P.

J. Chem. Eng. Data 1971, *16*, 41-4.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1M_1\,^{1}$/mol g^{1} (compiler)
25	0.13	6.10	7.2×10^{3}

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: ± 2 %.
Temperature: ± 0.1 K.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

Russ. J. Phys. Chem. 1971, *45*, 488-90.

VARIABLES:

T/K = 288 - 333

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$1000\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
15	25.00	2.44	5.28
30	15.60	1.54	3.31
45	8.80	0.872	1.86
60	5.30	0.527	1.12

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: ± 15 %.
Temperature: ± 0.05 K.

REFERENCES:

(1) Treger, Yu. A.; Flid, R. M.; Spektor, S. S. *Russ. J. Phys. Chem.* 1964, *38*, 253.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Karger, B. L.; Chatterjee, A. K.; King, J. W.

Tech. Rept. No: 3, Dept. of Chemistry, Northeastern Univ., Boston, Mass., May 10, 1971.

VARIABLES:

T/K = 286

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Partition coefficient[1], K_L/dimensionless	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
12.5	19.2	2.31	4.99

[1] Gas-liquid chromatographic parameter, from instrument calibration.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

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 & M flame ionization detector. The partition coefficient was obtained from the slope of the straight line plot of V_N/A_L versus V_L/A_L.

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: ± 0.5 K (compiler).

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Alexandrova, M. V.; Sadovnikova, L. V.; Martinov, W. W.

Sb. Nauchn. Tr., Ivanov. Energ. Inst. 1972, *14*, 146-54.

VARIABLES:

T/K = 293

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

t/°C	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
20	2.76	5.98	0.10	4.70

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used.

Solubility data were also reported for the ternary dichloromethane-water-acetic acid system.

SOURCE AND PURITY OF MATERIALS:

(1) Source not given. C. P. grade, used as received; n_D = 1.4242 at 20 °C.
(2) Distilled (compiler).

ESTIMATED ERRORS:

Solubility: Not specified.
Temperature: ± 0.1 K.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Antropov, L. I.; Populyai, V. E.; Simonov, V. D.; Shamsutdinov, T. M.

Russ. J. Phys. Chem. 1972, *46*, 311-2 (VINITI No: 3739-71).

VARIABLES:

T/K = 291 - 299

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3 x_1$ (compiler)	100 w_2	$10^3 x_2$ (compiler)
18	-	-	0.14	6.57
20	2.0	4.31	-	-
22	-	-	0.16	7.50
26	-	-	0.18	8.43

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:

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

ESTIMATED ERRORS:

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

REFERENCES:

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

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Sadovnikova, L. V.; Komarova, V. P.; Alexandrova, M. V.

Sb. Nauchn. Tr., Ivanov. Energ. Inst. 1972, *14*, 205-9.

VARIABLES:

T/K = 311

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3 x_1$ (compiler)	100 w_2	$10^3 x_2$ (compiler)
38	5.26	11.6	1.0×10^{-2}	0.47

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The titration method was used. The solubility was determined at the normal boiling point temperature. An ebuliometer 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:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Sadovnikova, L. V.; Komarova, V. P.; Alexandrova, M. V.; Serafimov, L. A.

Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. 1972, *15*, 1891-4.

VARIABLES:

T/K = 293

PREPARED BY:

Z. Maczynska

EXPERIMENTAL VALUES:

t/°C	100 w_1	$10^3\ x_1$ (compiler)	100 w_2	$10^3\ x_2$ (compiler)
19.85	2.76	5.98	0.1	5.0

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; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D.

Tr. Mosk. Khim.-Tekhnol. Inst. 1973, 183-6.

VARIABLES:

T/K = 298 - 373

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Distribution coefficient[1], D_L/dimensionless	100 w_1 (compiler)	$10^4\ x_1$ (compiler)
25.1	3920	0.0693	1.471
50.0	2480	0.2696	5.731
70.0	1650	0.7419	15.83
90.0	1240	1.6652	35.79
96.0	1130	2.1071	45.45
100	1080	2.4173	52.27

[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 ^{36}Cl labeled compound.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D.

Tr. Mosk. Khim.-Tekhnol. Inst. 1974, 55-6.

VARIABLES:

T/K = 280 - 310

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$$\log_{10} \alpha = \frac{547.33}{T(\mathrm{K})} - 1.0416$$

where α = Distribution Coefficient

At the normal boiling point of CH_2Cl_2, 313.15 K, $\alpha = 50.0$, the activity coefficient, $\gamma_1 = 67.0$, and the mole fraction of (1) at saturation, $x_1 = 3.953 \times 10^{-3}$ (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).

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

REFERENCES:

(1) Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D. *Tr. Mosk. Khim. Tekhnol. Inst.* 1973, 100.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

McConnell, G.; Ferguson, D. M.; Pearson, C. R.

Endeavour 1975, *34*, 13-8.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	13200	1.30	2.79

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of dichloromethane in water was determined using gas-liquid chromatography (GLC). The instrument was equipped with an electron capture detector. Where possible, identification was confirmed by using 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:	± 0.2 K (compiler).

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Pearson, C. R.; McConnell, G.

Proc. Roy. Soc. B. 1975, *189*, 305-32.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
25	13200	1.320	2.84

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 ^{63}Ni electron capture detector.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Archer, W. L.; Stevens, V. L.

I&EC Prod. Res. Dev. 1977, *16*, 319-25.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
25	2.0	4.22	0.20	9.34

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:

(1) *News Release* from Dow Chemicals Co., U. S. A., dated October 23, 1975.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Sato, A.; Nakijima, T.

Arch. Envir. Health 1979, *34*, 69-75.

VARIABLES:

$T/K = 310$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Partition coefficient[1], K_L/dimensionless	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
37	7.2	2.2	4.75

[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 (compiler).

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Coca, J.; Diaz, R. M.; Pazos, C.

Fluid Phase Eqilibr. 1980, *4*, 125-36.

VARIABLES:

$T/K = 298$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_2$	$10^3\ x_2$ (compiler)
25	1.37	2.94	0.18	8.43

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 (compiler).

REFERENCES:

(1) Othmer, D. F.; White, R. E.; Trueges, E. *Ind. Eng. Chem.* 1941, *33*, 1240.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Hutchinson, T. C.; Hellebust, J. A.; Tam, D.; *et al.*

Hydrocarbons and Halogenated Hydrocarbons in the Aquatic Environment, Plenum Press, New York, 1980, p. 577-86.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	ρ_1/kg m^{-3}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
25	19.4	1.946	4.19

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:

(1) Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1977, 22, 399.

COMPONENTS:

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

(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Wu, X.

Huaxue, Shiji 1981, 221-4.

VARIABLES:

T/K = 278 - 308

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ w_1$	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
5	1313	0.1313	6.16
10	1440	0.1440	6.75
15	1525	0.1525	7.15
20	1609	0.1609	7.54
25	1779	0.1779	8.33
30	1948	0.1948	9.12
35	2075	0.2075	9.71

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:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Leighton, D. T.; Calo, J. M.

J. Chem. Eng. Data 1981, *26*, 382-5.

VARIABLES:

T/K = 275 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Partition coefficient[1], K_L/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
1.9	61.4	1.5871	3.409
13.5	111.5	1.4886	3.195
15.7	121.5	1.4904	3.199
17.1	141.6	1.3651	2.927
22.0	157.1	1.5144	3.251
24.9	161.9	1.6569	3.561

[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:

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

(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Ohtsuka, K.; Kazama, K.

Sen'i Seihin Shohi Kagaku Kaishi 1982, *22*, 197-201.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$g_1V_2^{-1}$/kg m^{-3}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	2.00	0.151	7.08

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was added gradually to 50 cm^3 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 JIS extra pure reagent, further purified by conventional methods before use.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Lincoff, A. H.; Gossett, J. M.

in *Gas Transfer at Water Surface*, by W. Brutsaert and G. H. Jirka, Eds., D. Reidel Publ. Co., Dordrecht, 1984, p. 17-25.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

EPICS Method:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	2.25×10^{-3}	1.7786	3.826

$$\log_e H = -\frac{4191}{T(\text{K})} + 8.200$$

Batch Air Stripping Method:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	$10^3\ x_1$ (compiler)
20	1.97×10^{-3}	2.0314	4.379

$$\log_e H = -\frac{4472}{T(\text{K})} + 9.035$$

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:	± 5 - 10 %.
Temperature:	± 0.1 K.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Gossett, J. M.

Environ. Sci. Technol. 1987, *21*, 202-8.

VARIABLES:

T/K = 283 - 308

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's Law Constant, H/m^3 atm mol^{-1}	CV[1] %	100 w_1 (compiler)	10^3 x_1 (compiler)
9.6	1.15×10^{-3}	19.2	2.2513	4.862
17.5	1.31×10^{-3}	19.9	2.7492	5.960
24.8	2.19×10^{-3}	17.4	2.1422	4.842
34.6	3.26×10^{-3}	2.37	2.2150	4.782

[1] CV = coefficient of variation (= 100 S.D./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:	± 0.1 K.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Warner, H. P.; Cohen, J. M.; Ireland, J. C.

Determination of Henry's Law Constants of Selected Priority Pollutants Cincinnati, OH., July 1987.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/m^3 atm mol^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
24.85	3.19×10^{-3}	1.599	3.436

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 dichloromethane 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. Dichloromethane 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, used as received. Stated purity > 99 %.

(2) Distilled and deionized.

ESTIMATED ERRORS:

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

REFERENCES:

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

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

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

AFESC Tyndall Air Force Base, Report ESL-TR-86-66, *Vol. 1,* Florida, Sept. 1987, 86 pp. (AD-A188 571).

VARIABLES:

T/K = 283 - 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10^6\ w_1$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
10	11092	1.1092	2.3736
20	13508	1.3508	2.8961
30	11211	1.1211	2.3993

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

250 cm^3 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 than 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:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Vogel, A. I., rev. by Furniss, B. S.; *et al.*

Vogen's Textbook of Practical Organic Chemistry, 5th ed., Longman, London, 1989, p. 1442.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1 M_1^{-1}$/mol g^{-1} (compiler)
25.0	1.30	2.79	1.53×10^{-2}

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 cm^3 dichloromethane was added to 3.0 cm^3 of water and shaked. 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; CH_2Cl_2; [75-09-2]

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

ORIGINAL MEASUREMENTS:

Wright, D. A.; Sandler, S. I.; DeVoll, D.

Environ. Sci. Technol. 1992, *26*, 1828-31.

VARIABLES:

$T/K = 283 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	γ^∞	$100\,w_1$ (compiler)	$10^3\,x_1$ (compiler)
10	235 ± 5	1.977	4.26
20	251 ± 14	1.849	3.98
30	250 ± 8	1.858	4.00

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A differential static cell equilibrium apparatus was used to measure the infinite dilution activity coefficient of dichloromethane (γ^∞) 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: ± 0.05 K.

COMPONENTS:

(1) Dichloromethane; CH_2Cl_2; [75-09-2]

(2) Hydrogen chloride; HCl; [7647-01-0]

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

ORIGINAL MEASUREMENTS:

Svetlanov, E. B.; Velichko, S. M.; Levinskii, M. I.; Treger, Yu. A.; Flid, R. M.

Russ. J. Phys. Chem. 1971, *45*, 488-90.

VARIABLES:

T/K = 288 - 333
HCl concentration

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

Solubility of CH_2Cl_2 in 10 % HCl solution:

t/°C	$10^3 w_1$	$100 w_1$ (compiler)	$10^3 x_1$ (compiler)
15	29.40	2.940	6.733
30	18.50	1.850	4.198
45	12.50	1.250	2.822
60	6.00	0.600	1.347

Solubility of CH_2Cl_2 in 20 % HCl solution:

t/°C	$10^3 w_1$	$100 w_1$ (compiler)	$10^3 x_1$ (compiler)
30	24.50	2.450	5.909
45	12.00	1.200	2.862
60	6.50	0.650	1.543

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. *Russ. J. Phys. Chem.* 1964, *38*, 253.

COMPONENTS:	EVALUATOR:
(1) Diiodomethane; CH_2I_2; [75-11-6] (2) Water; H_2O; [7732-18-5]	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:

1. Gross, P. M; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53*, 1744.
2. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1951, *73*, 5733.
3. van Arkel, A. E.; Vles, S. E. *Recl. Trav. Chim. Pays-Bas* 1936, *55*, 407.
4. O'Connell, W. L. *Trans. Am. Inst. Mech. Eng.* 1963, *226*, 126.
5. Hutchison, C. A.; Lyon, A. M. *Columbia University Report A-745*, July 1, 1943.

COMPONENTS:

(1) Diiodomethane; CH_2I_2; [75-11-6]

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

ORIGINAL MEASUREMENTS:

Gross, P. M.; Saylor, J. H.

J. Am. Chem. Soc. 1931, *53*, 1744-51.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	1000 g_1/g_2	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
30	1.24	0.124	8.35

AUXILIARY INFORMATION

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 $Na_2S_2O_3$ solution. washed with distilled water, dried, and fractionally frozen twice before use.
(2) Distilled.

ESTIMATED ERRORS:

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

REFERENCES:

(1) Gross, P. M. *J. Am. Chem. Soc.* 1929, *51*, 2362.
(2) Saylor, P. M. *Ph. D. Thesis*, Duke University, Durham, 1930.

COMPONENTS:

(1) Diiodomethane; CH_2I_2; [75-11-6]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	m_1/mol kg^{-1}	100 w_1 (compiler)	$10^5\ x_1$ (compiler)
30	4.6×10^{-3}	0.123	8.28

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Details are not available.

SOURCE AND PURITY OF MATERIALS:

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

ESTIMATED ERRORS:

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

COMPONENTS:

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

(2) Diiodomethane; CH_2I_2; [75-11-6]

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:

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
25	1.207×10^{-3}	2.174×10^{-2}	3.222

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:	± 1.5×10^{-5} avg. dev.
Temperature:	± 0.05 K.

REFERENCES:

(1) Eidinoff, M. L.; Jorris, G. G.; Taylor, H. S.; Urey, H. C., eds. "*Production of Heavy Water*," McGraw-Hill, New York, 1955, p. 129.

COMPONENTS:

(1) Diiodomethane; CH_2I_2; [75-11-6]

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

ORIGINAL MEASUREMENTS:

Andrews, L. J.; Keefer, R. M.

J. Am. Chem. Soc. 1951, *73*, 5733-6.

VARIABLES:

T/K = 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	c_1/mol m^{-3}	100 w_1 (compiler)	10^5 x_1 (compiler)
25.0	3.11	8.35×10^{-2}	5.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water was mixed with diiodomethanme 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:	± 0.5 K (compiler).

REFERENCES:

(1) Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71*, 3644.

COMPONENTS:

(1) Diiodomethane; CH_2I_2; [75-11-6]

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

ORIGINAL MEASUREMENTS:

O'Connell, W. L.

Trans. Am. Inst. Mech. Eng. 1963, *226*, 126-32.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	100 g_1/g_2	100 w_1 (compiler)	$10^5 x_1$ (compiler)
20	0.124	0.124	8.34

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-d_2; D_2O; [7789-20-0]

(2) Diiodomethane; CH_2I_2; [75-11-6]

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:

t/°C	100 $w_1M_1^{-1}$/mol g^{-1}	100 w_1 (compiler)	$10^3 x_1$ (compiler)
25	1.017×10^{-3}	2.04×10^{-2}	2.721

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: $\pm 0.3 \times 10^{-5}$ avg. dev.
Temperature: ± 0.05 K.

REFERENCES:

(1) Eidinoff, M. L.; Joris, G. G.; Taylor, H. S.; Urey, H. C., Eds., "*Production of Heavy Water*," McGraw-Hill, New York, 1955, p. 129.

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

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

EVALUATOR:

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

March 1993.

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:

$$\text{Solubility } [100\,w_1] = 19.0036 - 0.11723\,(T/\text{K}) + 1.95356 \times 10^{-4}\,(T/\text{K})^2$$

This regression equation was established using the combined data from (refs. 4 - 8), which yielded a standard deviation of 4.3×10^{-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)

Temperature, °C	K	Solubility, $100\,w_1$	$10^3\,x_1$
0	273.15	1.557	2.003
5	278.15	1.510	1.942
10	283.15	1.472	1.893
15	288.15	1.444	1.856
20	293.15	1.425	1.831
25	298.15	1.417	1.821
30	303.15	1.418	1.822
35	308.15	1.430	1.838
40	313.15	1.450	1.864

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Iodomethane; CH_3I; [74-88-4] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, U.K. March 1993.

CRITICAL EVALUATION: (continued)

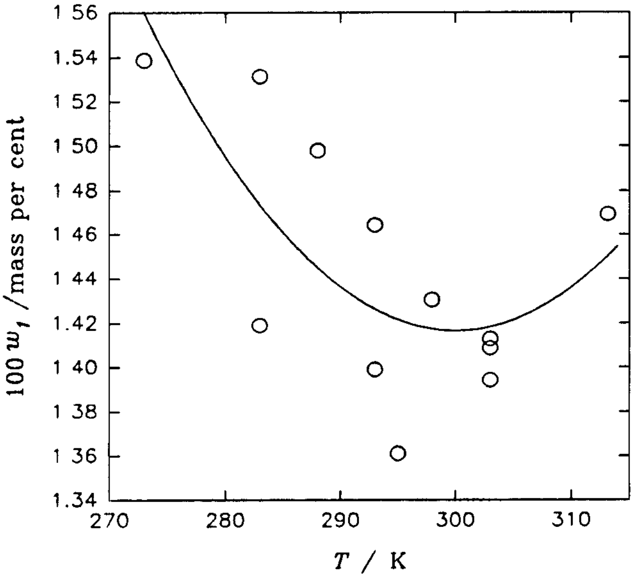

Figure 1. Solubility of Iodomethane (1) in Water (2).

REFERENCES:

293 1. Glew, D. N. *Ph. D. Thesis*, University of Cambridge, Cambridge, U. K. 1952, 245 pp.

29[illegible].5 2. Balls, P. W. *Ph. D. Thesis*, University of East Anglia, Norwich, U. K. July 1980, 375 pp.

297 3. Liss, P. S.; Slater, P. G. *Nature* 1974, *247*, 181.

290 4. Rex, A. *Z. Phys. Chem.* 1906, *55*, 355.

29[illegible] 5. Führer, H. *Ber.* 1924, *57*, 510.

292 6. van Arkel, A. E.; Vles, S. E. *Recl. Trav. Chim. Pays-Bas* 1936, *55*, 407.

29[illegible] 7. Swain, C. G.; Thornton, E. R. *J. Am. Chem. Soc.* 1962, *84*, 822.

29[illegible] 8. Hunter-Smith, R. J.; Balls, P. W.; Liss, P. S. *Tellus*, 1983, *35B*, 170.

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

Rex, A.

Z. Phys. Chem. 1906, *55*, 355-70.

VARIABLES:

$T/K = 273 - 303$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ g_1/g_2$	$100\ w_1$ (compiler)	$10^3\ x_1$ (compiler)
0	1.565	1.540	1.981
10	1.446	1.425	1.831
20	1.419	1.400	1.793
30	1.429	1.409	1.811

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 before use, b.p. = 42.8 °C.
(2) Distilled.

ESTIMATED ERRORS:

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

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

Fühner, H.

Ber. 1924, *57*, 510-5.

VARIABLES:

$T/K = 295$

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$100\ w_1$	$10^3\ x_1$ (compiler)	$100\ w_1 M_1^{-1}/\text{mol g}^{-1}$ (compiler)
22	1.362	1.75	9.59×10^{-3}

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:

(1) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

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

Recl. Trav. Chim. Pays-Bas 1936, *55*, 407-11.

VARIABLES:

T/K = 303

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	m_1/mol kg^{-1}	100 w_1 (compiler)	10^3 x_1 (compiler)
30	0.101	1.413	1.816

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) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

Glew, D. N.

Ph. D. Thesis, University of Cambridge, Cambridge, U. K. 1952, 245 pp.

VARIABLES:

T/K = 273 - 323

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	P_1/c_1 /dm^3 mmHg mol^{-1}	Henry's law constant, H/m^3 atm mol^{-1} (compiler)	100 w_1 (compiler)	10^3 x_1 (compiler)
0.01	1274	1.676×10^{-3}	8.47	11.61
5.04	1686	2.218×10^{-3}	6.40	8.60
10.20	2160	2.842×10^{-3}	4.99	6.62
15.12	2730	3.592×10^{-3}	3.95	5.19
19.95	3380	4.447×10^{-3}	3.19	4.16
24.93	4060	5.342×10^{-3}	2.66	3.46
29.93	4730	6.224×10^{-3}	2.29	2.97
34.91	5540	7.290×10^{-3}	1.96	2.53
39.87	6380	8.395×10^{-3}	1.70	2.19
44.88	7160	9.421×10^{-3}	1.52	1.96
49.76	8040	10.58×10^{-3}	1.36	1.75

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 turnings.
(2) Gas free, deionizes by ion exchange resin.

ESTIMATED ERRORS:

Solubility: ± 0.5 %.
Temperature: ± 0.2 K.

REFERENCES:

(1) Glew, D. N.; Moelwyn-Hughes, E. A. *Faraday Discussion Chem. Soc.* 1953, 150.

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

Swain, C. G.; Thornton, E. R.

J. Am. Chem. Soc. 1962, *84*, 822-6.

VARIABLES:

T/K = 303 - 313
Pressure

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	P_1/c_1 $/dm^3$ mmHg mol^{-1}	Henry's law constant, H/m^3 atm mol^{-1} (compiler)	100 w_1 (compiler)	10^3 x_1 (compiler)
29.44	4880	6.421×10^{-3}	1.397	1.793
29.45	4900	6.447×10^{-3}	1.392	1.788
40.34	6850	9.013×10^{-3}	1.478	1.900
40.35	6920	9.105×10^{-3}	1.463	1.881

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 determined 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:	± 3 %.
Temperature:	± 0.01 K.
Pressure:	± 0.05 mmHg.

REFERENCES:

(1) Brown, H. C.; Taylor, M. D.; Gerstein, M. *J. Am. Chem. Soc.* 1944, *66*, 431.

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

Balls, P. W.

Ph. D. Thesis, University of East Anglia, Norwich, U. K., July 1980, 375 pp.

VARIABLES:

T/K = 283 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
10	0.12 ± 0.04	1.464	1.882
15	0.15 ± 0.05	1.829	1.829
20	0.17 ± 0.03	1.514	1.947
25	0.20 ± 0.04	1.539	1.979

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:	± 0.5 K (compiler).

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

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

ORIGINAL MEASUREMENTS:

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

Tellus 1983, *35B*, 170-6.

VARIABLES:

T/K = 283 - 298

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	10^3 x_1 (compiler)
10	0.1147	1.5317	1.971
15	0.1425	1.4982	1.927
20	0.1757	1.4645	1.883
25	0.2151	1.4308	1.839

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

$$\log_e H = -\frac{3541}{T(\mathrm{K})} + 10.34$$

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:

(1) McAuliffe, C. D. *Chem. Techn.* 1971, *1*, 46.

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

(2) Seawater

ORIGINAL MEASUREMENTS:

Liss, P. S.; Slater, P. G.

Nature 1974, *247*, 181-4.

VARIABLES:

T/K = 293

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	Henry's law constant, H/dimensionless	100 w_1 (compiler)	100 $w_1M_1^{-1}$/mol g^{-1} (compiler)
20	0.24	1.093	7.7×10^{-3}

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) Lovelok, J. E. *Personal communication.*

COMPONENTS:

(1) Iodomethane; CH_3I; [74-88-4]

(2) Water-d_2; D_2O; [7789-20-0]

ORIGINAL MEASUREMENTS:

Swain, C. G.; Thornton, E. R.

J. Am. Chem. Soc. 1962, *84*, 822-6.

VARIABLES:

T/K = 303 - 313

PREPARED BY:

A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	P_1/c_1 /dm³ mmHg mol⁻¹	Henry's law constant, H/m³ atm mol⁻¹ (compiler)	100 w_1 (compiler)	10³ x_1 (compiler)
29.43	5450	7.171×10^{-3}	1.131	1.611
29.45	5340	7.026×10^{-3}	1.154	1.645
40.34	7420	9.763×10^{-3}	1.231	1.755
40.35	7450	9.803×10^{-3}	1.226	1.748

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. *J. Am. Chem. Soc.* 1944, *66*, 822.

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