SOLUBILITY DATA SERIES

Editor-in-Chief
A. S. KERTES

Volume 20

HALOGENATED BENZENES, TOLUENES AND PHENOLS WITH WATER

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PERGAMON PRESS

OXFORD · NEW YORK · TORONTO · SYDNEY · FRANKFURT

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FOREWORD

*If the knowledge is
undigested or simply wrong,
more is not better*

How to communicate and disseminate numerical data effectively in chemical science and technology has been a problem of serious and growing concern to IUPAC, the International Union of Pure and Applied Chemistry, for the last two decades. The steadily expanding volume of numerical information, the formulation of new interdisciplinary areas in which chemistry is a partner, and the links between these and existing traditional subdisciplines in chemistry, along with an increasing number of users, have been considered as urgent aspects of the information problem in general, and of the numerical data problem in particular.

Among the several numerical data projects initiated and operated by various IUPAC commissions, the *Solubility Data Project* is probably one of the most ambitious ones. It is concerned with preparing a comprehensive critical compilation of data on solubilities in all physical systems, of gases, liquids and solids. Both the basic and applied branches of almost all scientific disciplines require a knowledge of solubilities as a function of solvent, temperature and pressure. Solubility data are basic to the fundamental understanding of processes relevant to agronomy, biology, chemistry, geology and oceanography, medicine and pharmacology, and metallurgy and materials science. Knowledge of solubility is very frequently of great importance to such diverse practical applications as drug dosage and drug solubility in biological fluids, anesthesiology, corrosion by dissolution of metals, properties of glasses, ceramics, concretes and coatings, phase relations in the formation of minerals and alloys, the deposits of minerals and radioactive fission products from ocean waters, the composition of ground waters, and the requirements of oxygen and other gases in life support systems.

The widespread relevance of solubility data to many branches and disciplines of science, medicine, technology and engineering, and the difficulty of recovering solubility data from the literature, lead to the proliferation of published data in an ever increasing number of scientific and technical primary sources. The sheer volume of data has overcome the capacity of the classical secondary and tertiary services to respond effectively.

While the proportion of secondary services of the review article type is generally increasing due to the rapid growth of all forms of primary literature, the review articles become more limited in scope, more specialized. The disturbing phenomenon is that in some disciplines, certainly in chemistry, authors are reluctant to treat even those limited-in-scope reviews exhaustively. There is a trend to preselect the literature, sometimes under the pretext of reducing it to manageable size. The crucial problem with such preselection - as far as numerical data are concerned - is that there is no indication as to whether the material was excluded by design or by a less than thorough literature search. We are equally concerned that most current secondary sources, critical in character as they may be, give scant attention to numerical data.

On the other hand, tertiary sources - handbooks, reference books and other tabulated and graphical compilations - as they exist today are comprehensive but, as a rule, uncritical. They usually attempt to cover whole disciplines, and thus obviously are superficial in treatment. Since they command a wide market, we believe that their service to the advancement of science is at least questionable. Additionally, the change which is taking place in the generation of new and diversified numerical data, and the rate at which this is done, is not reflected in an increased third-level service. The emergence of new tertiary literature sources does not parallel the shift that has occurred in the primary literature.

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With the status of current secondary and tertiary services being as briefly stated above, the innovative approach of the *Solubility Data Project* is that its compilation and critical evaluation work involve consolidation and reprocessing services when both activities are based on intellectual and scholarly reworking of information from primary sources. It comprises compact compilation, rationalization and simplification, and the fitting of isolated numerical data into a critically evaluated general framework.

The *Solubility Data Project* has developed a mechanism which involves a number of innovations in exploiting the literature fully, and which contains new elements of a more imaginative approach for transfer of reliable information from primary to secondary/tertiary sources. *The fundamental trend of the Solubility Data Project is toward integration of secondary and tertiary services with the objective of producing in-depth critical analysis and evaluation which are characteristic to secondary services, in a scope as broad as conventional tertiary services.*

Fundamental to the philosophy of the project is the recognition that the basic element of strength is the active participation of career scientists in it. Consolidating primary data, producing a truly critically-evaluated set of numerical data, and synthesizing data in a meaningful relationship are demands considered worthy of the efforts of top scientists. Career scientists, who themselves contribute to science by their involvement in active scientific research, are the backbone of the project. The scholarly work is commissioned to recognized authorities, involving a process of careful selection in the best tradition of IUPAC. This selection in turn is the key to the quality of the output. These top experts are expected to view their specific topics dispassionately, paying equal attention to their own contributions and to those of their peers. They digest literature data into a coherent story by weeding out what is wrong from what is believed to be right. To fulfill this task, the evaluator must cover *all* relevant open literature. No reference is excluded by design and every effort is made to detect every bit of relevant primary source. Poor quality or wrong data are mentioned and explicitly disqualified as such. In fact, it is only when the reliable data are presented alongside the unreliable data that proper justice can be done. The user is bound to have incomparably more confidence in a succinct evaluative commentary and a comprehensive review with a complete bibliography to both good and poor data.

It is the standard practice that the treatment of any given solute-solvent system consists of two essential parts: I. Critical Evaluation and Recommended Values, and II. Compiled Data Sheets.

The Critical Evaluation part gives the following information:

   (i)   a verbal text of evaluation which discusses the numerical
         solubility information appearing in the primary sources located in
         the literature. The evaluation text concerns primarily the quality
         of data after consideration of the purity of the materials and
         their characterization, the experimental method employed and the
         uncertainties in control of physical parameters, the
         reproducibility of the data, the agreement of the worker's results
         on accepted test systems with standard values, and finally, the
         fitting of data, with suitable statistical tests, to mathematical
         functions;
  (ii)   a set of recommended numerical data. Whenever possible, the set of
         recommended data includes weighted average and standard deviations,
         and a set of smoothing equations derived from the experimental data
         endorsed by the evaluator;
 (iii)   a graphical plot of recommended data.

The Compilation part consists of data sheets of the best experimental data in the primary literature. Generally speaking, such independent data sheets are given only to the best and endorsed data covering the known range of experimental parameters. Data sheets based on primary sources where the data are of a lower precision are given only when no better data are available. Experimental data with a precision poorer than considered acceptable are reproduced in the form of data sheets when they are the only known data for a particular system. Such data are considered to be still suitable for some applications, and their presence in the compilation should alert researchers to areas that need more work.

The typical data sheet carries the following information:

(i)   components - definition of the system - their names, formulas and Chemical Abstracts registry numbers;

(ii)   reference to the primary source where the numerical information is reported. In cases when the primary source is a less common periodical or a report document, published though of limited availability, abstract references are also given;

(iii)   experimental variables;

(iv)   identification of the compiler;

(v)   experimental values as they appear in the primary source. Whenever available, the data may be given both in tabular and graphical form. If auxiliary information is available, the experimental data are converted also to SI units by the compiler.

Under the general heading of Auxiliary Information, the essential experimental details are summarized:

(vi)   experimental method used for the generation of data;

(vii)   type of apparatus and procedure employed;

(viii)   source and purity of materials;

(ix)   estimated error;

(x)   references relevant to the generation of experimental data as cited in the primary source.

This new approach to numerical data presentation, formulated at the initiation of the project and perfected as experience has accumulated, has been strongly influenced by the diversity of background of those whom we are supposed to serve. We thus deemed it right to preface the evaluation/compilation sheets in each volume with a detailed discussion of the principles of the accurate determination of relevant solubility data and related thermodynamic information.

Finally, the role of education is more than corollary to the efforts we are seeking. The scientific standards advocated here are necessary to strengthen science and technology, and should be regarded as a major effort in the training and formation of the next generation of scientists and engineers. Specifically, we believe that there is going to be an impact of our project on scientific-communication practices. The quality of consolidation adopted by this program offers down-to-earth guidelines, concrete examples which are bound to make primary publication services more responsive than ever before to the needs of users. The self-regulatory message to scientists of the early 1970s to refrain from unnecessary publication has not achieved much. A good fraction of the literature is still cluttered with poor-quality articles. The Weinberg report (in 'Reader in Science Information', ed. J. Sherrod and A. Hodina, Microcard Editions Books, Indian Head, Inc., 1973, p. 292) states that 'admonition to authors to restrain themselves from premature, unnecessary publication can have little effect unless the climate of the entire technical and scholarly community encourages restraint...' We think that projects of this kind translate the climate into operational terms by exerting pressure on authors to avoid submitting low-grade material. The type of our output, we hope, will encourage attention to quality as authors will increasingly realize that their work will not be suited for permanent retrievability unless it meets the standards adopted in this project. It should help to dispel confusion in the minds of many authors of what represents a permanently useful bit of information of an archival value, and what does not.

If we succeed in that aim, even partially, we have then done our share in protecting the scientific community from unwanted and irrelevant, wrong numerical information.

A. S. Kertes

PREFACE

This volume contains a comprehensive collection and critical evaluation of published solubility data for halogenated benzenes, halogenated toluenes, and halogenated phenols in water prior to 1983. In addition, the solubilities of water in some of the mentioned compounds are also included as well as the mutual solubilities between heavy water (D$_2$O) and some of the compounds. It should be readily apparent to the reader that there is a great scarcity of data available from the published literature on these systems. This is due primarily to the limited use of the organic compounds in commercial quantities.

All halogenated benzenes, toluenes, and phenols are liquids or solids at room temperature. Consequently, this volume is concerned entirely with the solubility behavior for condensed systems only (solid or liquid solutes in liquid solvents). For several of the compounds considered, only one single measured solubility value is available. It is particularly noteworthy, for example, that only one source (1) has provided the only reported data for solubilities in water of almost the entire series of halogenated, substituted phenols. As the critical evaluators often observe, further experimental investigations are needed for an improvement of the reported solubilities and for an extension of the solubilities over wider temperature ranges. Of course, higher temperature (above the normal boiling point of water) and higher pressure (above atmospheric pressure) solubility data are extremely scarce and available for only a very few systems.

The evaluators for this volume have often been faced with the difficult task of examining and evaluating the reliability of a single solubility with only a limited description of the experimental procedures used for the measurement. In such cases, the evaluator's experience in the techniques of measurement has proved invaluable. Also, some of the reported solubility data are several decades old. However, despite the dated experimental techniques, these published measurements have been found to be no less reliable than those of more recent investigations. Consequently, a recently reported result of a solubility measurement has not automatically become the most reliable or recommended value. In every case, efforts have been made to provide the most reliable and realistic solubility value regardless of the period of origin.

Because of their nature, mixtures of water and halogenated benzenes, halogenated toluenes, and halogenated phenols at room temperature over a wide range of proportions form two distinct phases, one aqueous rich and the other organic rich. However, at higher temperatures and at high pressures, the mutual solubilities usually increase significantly as shown, for example, in Figure 1 for 1,4-difluorobenzene in water system (from the reported work of Jockers and Schneider (2)). With changing temperature and pressure, the two liquid phases generally become identical at a critical, or consolute, point. With changing pressure, the critical solution temperature will change, forming a critical solution line. However, applied pressure exerts only a small effect on the critical temperature.

Systems containing halogen derivatives of benzenes, toluenes, and phenols with water are classified as non-regular type solutions. Consequently, those theories and relationships which were developed by J. H. Hildebrand and his co-workers over several decades for explaining solubility behavior are not generally useful for such systems. However, for the organic rich phase, where the less-well-behaved and more non-ideal water molecules are in very low concentrations, the solubility can be correlated against Absolute temperature by means of the equation:

$$\log x(2) = A - B/T$$

where: $x(2)$ = mole fraction solubility of water in the organic phase
T = Absolute temperature
A,B = Adjustable constants

That is, for water as the solute, the logarithm of its mole fraction composition is a linear (straight line) function of the reciprocal of the Absolute temperature (3-6). This linearity of the solubility behavior indicates that the organic-rich phase may approach the random distribution of molecules in solution which is one of the basic assumptions in the regular solution theory as detailed by Hildebrand and Scott (7). However, the strictly straight line correlation given above is not always followed for a wide temperature interval, e.g., from the triple point to the critical point. Even so, for the solubility of water in the halogenated benzenes, toluenes, and phenols, a good fit can be anticipated in the temperature range between the triple point of the solvent and the normal boiling point of water (373.15 K).
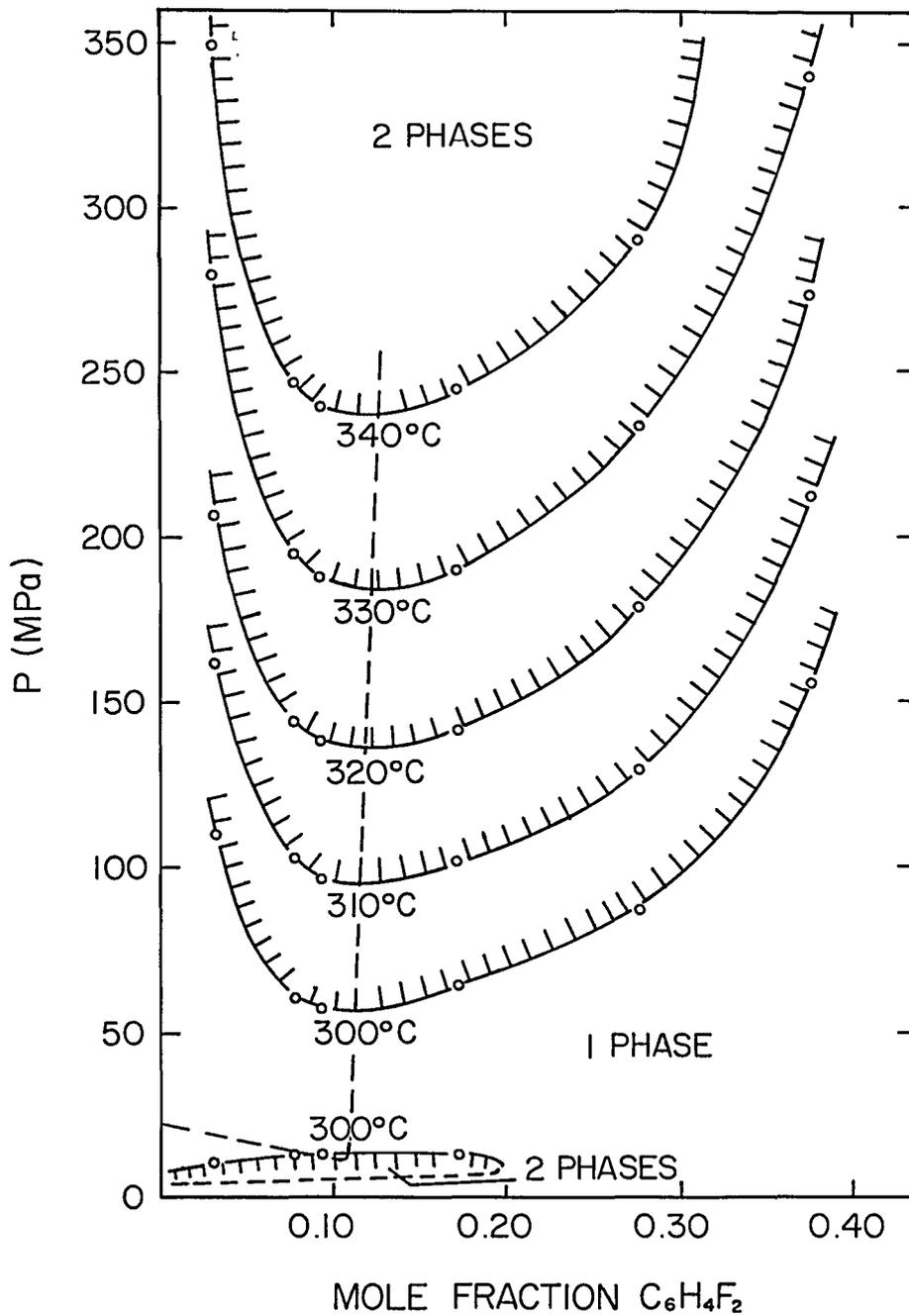
Figure 1.   Solubility behavior of 1,4-difluorobenzene and water versus pressure
           and temperature (2).

Since each system has been treated separately in the evaluation procedure, it is appropriate here in the Introduction to present the general behavior of the evaluated solubilities of water in the various organic constituents as a function of temperature. These relationships are shown in Figure 2 as the logarithm of mole fraction solubility versus the reciprocal of Absolute temperature. It can be seen that, despite the similarity of the organic solvents, the solubility curves do not show any sort of strict regularity. However, according to Horvath (8), some relatively simple pattern of behavior such as parallel straight lines should be expected. It is clear from Figure 2 that, for example, the solubility curve for iodobenzene shows a slope which differs from the remaining system. Indeed, further studies are needed as additional solubility data become available.

One very simple and practical relationship has been found to be quite useful for solubility data correlation. A plot of the logarithm of solubility in water expressed as molarity against the solute molar volume at 25°C follows a simple linear behavior and such plots may be used to check reported solubility data (9-11). The great advantage of this procedure is that the only information required is the density of the solute at 25°C which is relatively easy to measure when not available in standard references. Such a relation, which was reported by Horvath (8), has been used in this volume and is shown in Figure 3 for eight halogenated benzenes. However, the values shown in the figure do not include the recently reported measurements by Yalkowsky et al. (12).

The utility of the logarithm of molar saturation versus molar volume correlation was recognized in its application to the evaluation of the solubility of 1,3-dibromobenzene in water where the two independently determined measurements were in conflict. The solubility data for eighteen of the substances reported by Yalkowsky et al., including the 1,3-dibromobenzene, were correlated as shown in Figure 4. This graph suggests that the errors for the measured solubilities may, in fact, not agree well with the ± 10 percent which was reported by Yalkowsky (13) for the measurements. The graph suggests also that the reported solubility of 1,3-dibromobenzene in water may be too high in relation to the other solubilities reported by Yalkowsky et al.

It is, of course, relevant to consider the existence of trends and regularities observed in the behavior of physical parameters and properties, such as their thermodynamic constants and hydrophobic interactions, as determined from solubility measurements involving groups of compounds. In the case of solution enthalpies, for example, Gill et al. (14) have investigated their positive linear dependence with temperature for slightly soluble aromatic compounds. The calorimetric enthalpy of solution determinations for slightly soluble aromatic compounds over a temperature interval provide a very useful relationship for the temperature dependence of the solubility in water. The heat capacity change derived from the enthalpy of solution varies slightly with temperature (over limited, but reasonable, ranges of temperature). Consequently, thermodynamic expressions can provide useful descriptions of the temperature dependence of solubilities.

The curve for solubility versus temperature for all liquid aromatic hydrocarbons shows a minimum for zero heat of solution. This temperature minimum is calculated from the equation:

$$\Delta H^{\infty}_{soln} (T) = \Delta H^{\infty}_{soln} (T_o) + \Delta C^{\infty}_{p,soln} (T - T_o)$$

by use of the condition: $\Delta H^{\infty}_{soln} (T) = 0$ at $T = T_{min}$

so that: $T_{min} = T_o - \Delta H^{\infty}_{soln} (T_o)/\Delta C^{\infty}_{p,soln}$

In other words, the minimum solubility temperatures, T_{min}, for liquid aromatic hydrocarbons in water are calculated from the measured solution enthalpies at $T_o = 298.15$ K, $\Delta H^{\infty}_{soln} (T_o)$ and the heat capacity change at $T_o = 298.15$ K, $\Delta C^{\infty}_{p,soln}$.

The minimum solubility phenomenon is a characteristic of the solubility versus temperature curves in the 285 through 320 K range for liquid aromatic hydrocarbon in water systems. This minimum is illustrated in the cases of 1,2-dichlorobenzene, 1,3-dichlorobenzene, and chlorobenzene in water where solubilities have been reported over wide ranges of temperature.

The solubility in water behavior for 1,4-dichlorobenzene has been evaluated in two parts, one below and the other above the normal melting point (326.25 K) of the compound. This is necessary because of the distinct break in the solubility versus temperature behavior at the compound melting point. Here it is important to note that the solubility versus
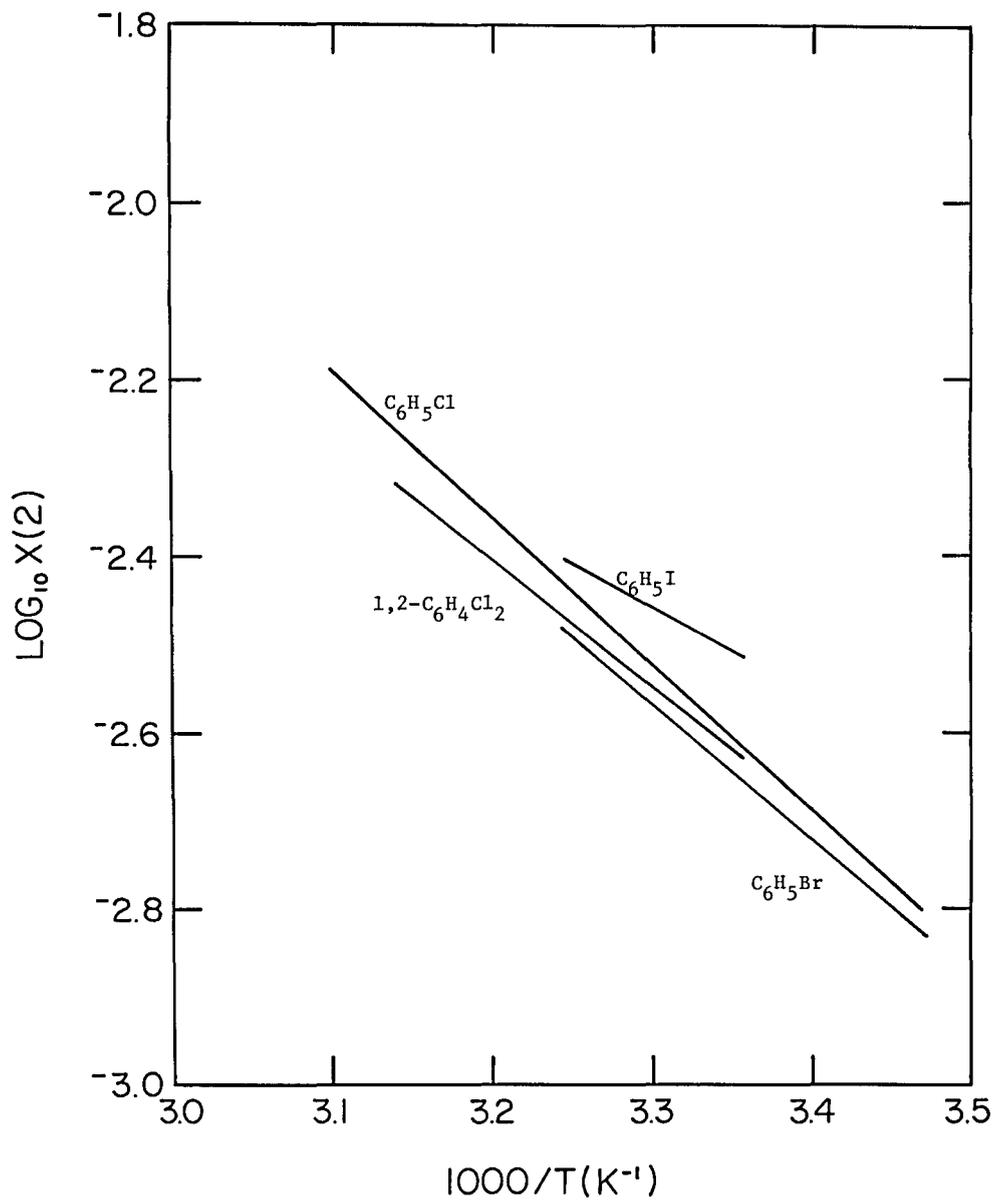
Figure 2. Logarithm of mole fraction water versus the reciprocal of Absolute temperature for the solubility of water in selected halogenated aromatic solvents.
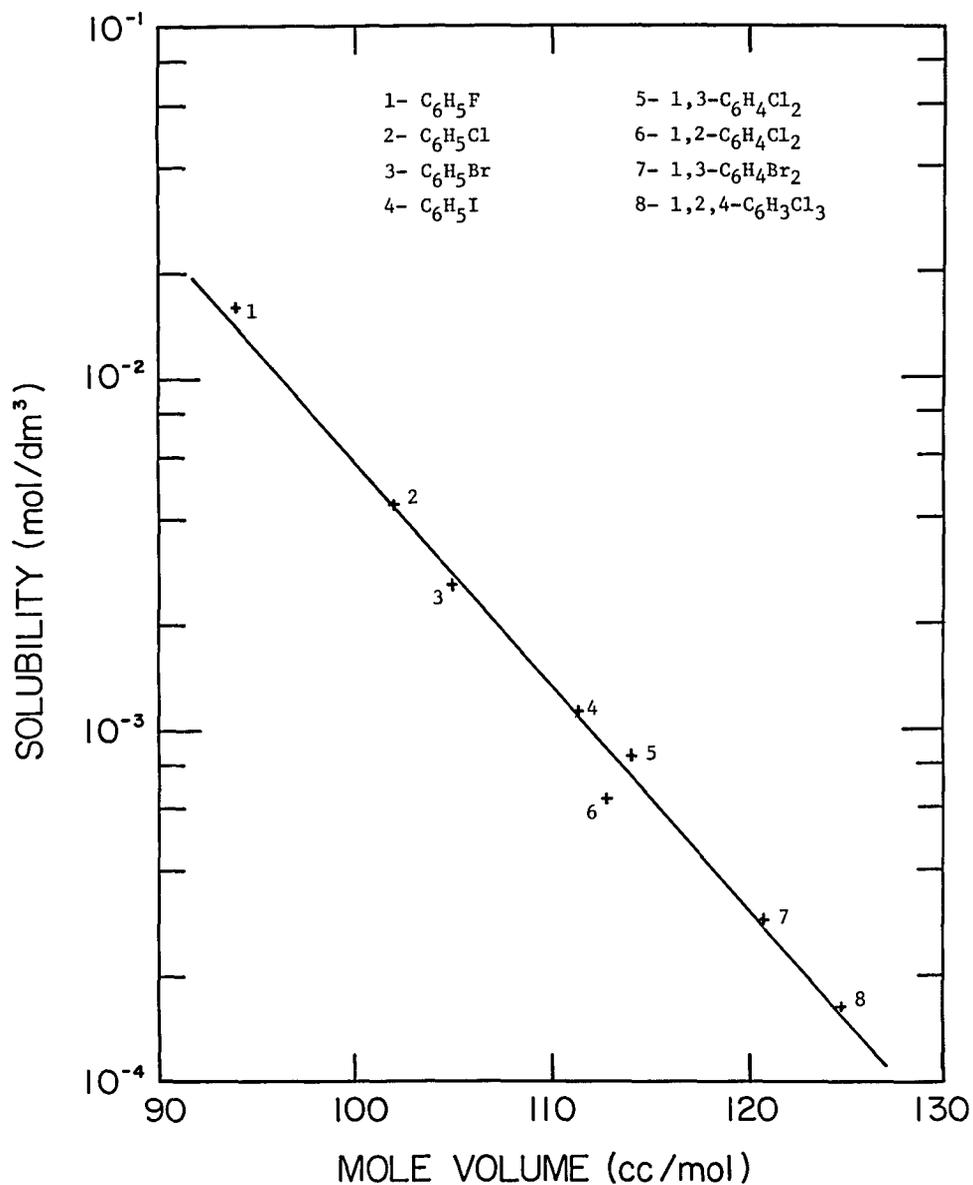
Figure 3. Logarithm of saturation molarity versus solute molar volume at 25°C for selected halogenated benzenes in water.

Correlation equation:

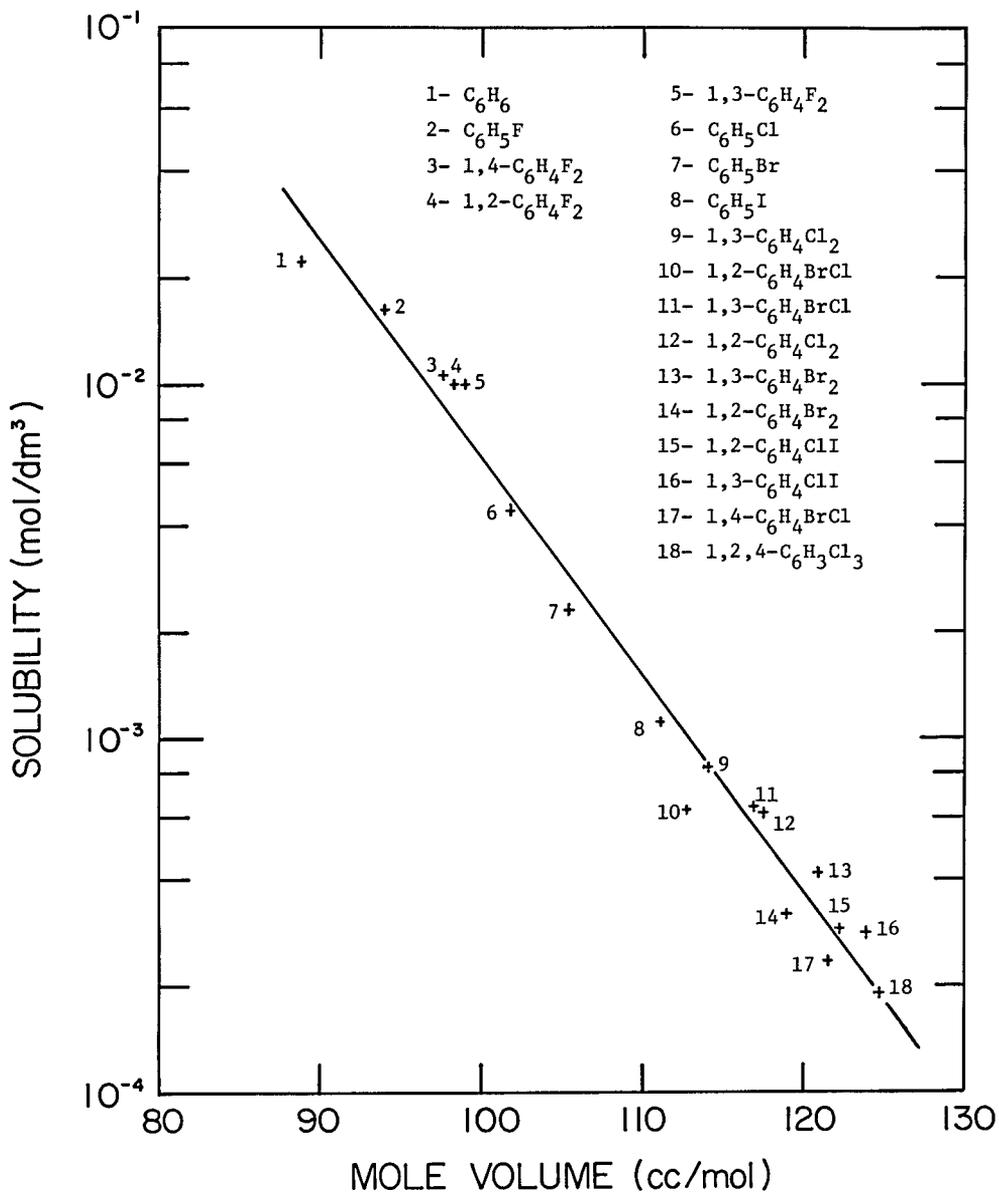$$\log_{10}S_1 (\text{mole/dm}^3) = 4.17442 - 6.40668 \times 10^{-2} \, \bar{V}_{25°C}(\text{cc/mol})$$

Figure 4. Logarithm of saturation molarity versus solute molar volume at 25°C
for selected aromatics in water as reported by Yalkowsky et al. (13).

Correlation equation:

$$\log_{10}S_1(\text{mol/dm}^3) = 3.94385 - 6.15067 \times 10^{-2} \, \bar{V}_{25°C}(\text{cc/mol})$$

Table I. Conversion Factors between Solubility Units

To \\ From	Bunsen coeff. B_2	Ostwald coeff. O_2	Technical coeff. T_2	Kuenen coeff. K_2	Weight Percent W_2	Mole Fraction X_2
Bunsen coefficient, B_2	1	$\dfrac{273.15\, O_2}{T}$	$\dfrac{d\, T_2}{0.9678}$	$d\, K_2$	$\dfrac{22415\, z\, d\, W_2}{(100-W_2)\, M\, P}$	$\dfrac{22415\, z\, d\, X_2}{(1-X_2)\, M_L\, P}$
Ostwald coefficient, O_2	$\dfrac{T\, B_2}{273.15}$	1	$\dfrac{d\, T\, T_2}{264.35}$	$\dfrac{d\, T\, K_2}{273.15}$	$\dfrac{22415\, z\, d\, T\, W_2}{273.15(100-W_2)\, M\, P}$	$\dfrac{22415\, z\, d\, T\, X_2}{273.15(1-X_2)\, M_L\, P}$
Technical coefficient, T_2	$\dfrac{0.9678\, B_2}{d}$	$\dfrac{264.35\, O_2}{d\, T}$	1	$0.9678\, K_2$	$\dfrac{0.9678 \cdot 22415\, z\, W_2}{(100-W_2)\, M\, P}$	$\dfrac{0.9678 \cdot 22415\, z\, X_2}{(1-X_2)\, M_L\, P}$
Kuenen coefficient, K_2	$\dfrac{B_2}{d}$	$\dfrac{273.15\, O_2}{d\, T}$	$\dfrac{T_2}{0.9678}$	1	$\dfrac{22415\, z\, W_2}{(100-W_2)\, M\, P}$	$\dfrac{0.9678 \cdot 22415\, z\, X_2}{(1-X_2)\, M_L\, P}$
Weight percent, W_2	$\dfrac{100}{1 + \dfrac{22415\, z\, d}{M\, P\, B_2}}$	$\dfrac{100}{1 + \dfrac{22415\, z\, d\, T}{273.15\, M\, P\, O_2}}$	$\dfrac{100}{1 + \dfrac{22415\, z\, 0.9678}{M\, P\, T_2}}$	$\dfrac{100}{1 + \dfrac{22415\, z}{M\, P\, K_2}}$	1	$\dfrac{100}{1 + \dfrac{(1-X_2)M_L}{M\, X_2}}$
Mole fraction, X_2	$\dfrac{1}{1 + \dfrac{22415\, z\, d}{M_L\, P\, B_2}}$	$\dfrac{1}{1 + \dfrac{22415\, z\, d\, T}{273.15\, M_L\, P\, O_2}}$	$\dfrac{1}{1 + \dfrac{22415\, z\, 0.9678}{M_L\, P\, T_2}}$	$\dfrac{1}{1 + \dfrac{22415\, z}{M_L\, P\, K_2}}$	$\dfrac{W_2/M}{\dfrac{W_2}{M} + \dfrac{100 - W_2}{M_L}}$	1

d = density of liquid solvent [g/ml], z = compressibility factor of gaseous solute, T = absolute temperature [K], P = partial pressure of solute [atm], M = molecular weight of solute, M_L = molecular weight of solvent.

temperature curves for the solid aromatic hydrocarbons such as 1,4-dichlorobenzene do not pass through minima around ambient temperature. Thus, the heats of solution do not become zero in this temperature range.

While the theory of isotope effects upon physical properties of compounds has developed considerably during the last three decades, some areas of understanding still involve qualitative descriptions despite a large number of investigations. In this connection, a large amount of work on the physicochemical properties of heavy water and its effect upon other properties has been done (15). The objective of various studies has been the establishment of the effects of nuclear masses upon intermolecular bond energies and upon the physical properties of liquids relative to their molecular structure, temperature, pressure, and chemical behavior (16).

The solubilities of ordinary water and heavy water have been determined in 29 organic liquids and in all cases the heavy water was found less soluble than the ordinary water (17). This can be explained simply by the difference in the total molecular surface areas. With increasing temperature, the solubility differences decrease markedly.

In the case of the solubility of liquid organics in ordinary water and in heavy water, there is good indication that the dissolving power of heavy water is less than that of ordinary water under the same conditions (18). As they do for solubilities of ordinary water and heavy water in organics, the isotopic effects decrease in extent with increasing temperature for organic liquid solubilities in the two solvents. With respect to the mutual solubilities of halogenated benzenes, toluenes, and phenols with ordinary water and heavy water, the available data do not show exceptions or unusual irregularities. In all cases, the usual behavior, as described above, is observed.

The solubility data found in the literature have been reported in various units. While the users of solubility data very often prefer mole fraction or weight percentage concentration units, others have been employed. As a convenience, the appropriate conversion factors between the various concentration units are presented in Table I from Horvath (19). Also, it should be pointed out that some original measurement conversions have been made in order to present the reported data in currently used concentration units. However, no assumed parameters have been involved in these conversions. In addition, the actual reported values have been used to calculate concentrations in two other concentration units. These values are reported routinely to one more significant figure than the measured value to aid the user in further calculations. One should not assume that these calculated concentration values have any greater precision than the originally measured values. Care has been taken to identify the reported concentration values throughout the volume.

Finally, it should be indicated that the halogenated compounds have been organized according to the Hill System. The heavy water follows the ordinary water.

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March 1984

LIQUID-LIQUID SOLUBILITY: INTRODUCTORY INFORMATION

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The Solubility Data Series is made up of volumes of comprehensive and critically evaluated solubility data on chemical systems in clearly defined areas. Data of suitable precision are presented on data sheets in a uniform format, preceded for each system by a critical evaluation if more than one set of data are available. In those systems where data from different sources agree sufficiently, recommended values are proposed. In other cases, values may be described as "tentative" or "rejected".

This volume is primarily concerned with liquid-liquid systems, but a limited number or related solid-liquid and multicomponent (organic-water-salt) systems have been included where it was 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 artifical 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. Such data have not been found for systems in this volume. Generally, however, data on reported miscibility gap regions and upper and lower critical solution temperatures are included where appropriate and when available.

TERMINOLOGY

In this volume, a mixture (1,2) or a solution (1,2) refers to a single liquid phase containing components 1 and 2. In a mixture, no distinction is made between solvent and solute.

The solubility of a substance is the relative proportion of 1 in a mixture which is saturated with respect to component 1 at a specified temperature and pressure. (The term "saturated" implies the existence of equilibrium with respect to the processes of mass transfer between phases.)

QUANTITIES USED AS MEASURES OF SOLUBILITY

Mole fraction of component 1, x_1 or $x(1)$:

$$x_1 = n_1/\sum_i n_i = \frac{m_1/M_1}{\sum(m_i/M_i)}$$

where n_i is the amount of substance (number of moles) of component i, m_i is the mass of substance i and M_i is its molar mass.

Mole per cent of component 1 is $100x_1$

Mass fraction of component 1, w_1

$$w_1 = m_1/\sum_i m_i$$

where m_i is the mass of component i.

Mass per cent of component 1 is $100w_1$, and may be described as g(1)/100g in which the 100g without a subscript means that it is mass of solute relative to solution and not to solvent. The equivalent terms "weight fraction" and "weight per cent" are not used. The mole fraction solubility is related to the mass fraction solubility in a binary system by

$$x_1 = \frac{w_1/M_1}{w_1/M_1 + (1 - w_1)/M_2}$$

Amount of substance concentration of component i in a solution of volume V,

$$c_i = n_i/V$$

is expressed in units of mol L^{-1}. The terms "molarity" and "molar" and the unit symbol M are not used. However, the unit mol(1)/dm^3 is used frequently rather than "molarity" (where the dm^3 without a subscript means solution and not solvent volume). Within the range of experimental errors usually encountered in reported solubility measurements, this unit may be taken as equal to "molarity".

Mass ratio is frequently used for a two-component solution in the form g(1)/g(2), mg(1)/g(2), etc. The term "parts per million" (ppm) is not used, but may be expressed as mg(1)/kg or g(1)/10^{6}g, etc.

Molality of component 1 in component 2 is often used in solid-liquid systems defined as $m_1 = n_1/n_2M_2$, but is not used in liquid-liquid systems where the distinction between "solute" 1 and "solvent" 2 is inappropriate. The term molality alone in inadequate, and the units (mol kg(2)$^{-1}$, mmol kg(2)$^{-1}$) must be stated.

Mole fractions 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.

ORDERING OF SYSTEMS

It is necessary to establish a method of ordering chemical compounds, to be used for the lists of saturating components which define each chemical system. This order is also used for ordering systems within volumes.

The systems are ordered first on the basis of empirical formula according to the Hill system (ref. 2). The organic compounds, within each Hill formula are ordered as follows:

(i) by degree of unsaturation, then

(ii) by order of increasing chain length in the parent hydrocarbon, then

(iii) by order of increasing chain length of hydrocarbon branches, then

(iv) numerically by position of unsaturation, then

(v) numerically by position by substitution, then

(vi) alphabetcially by IUPAC name.

For 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 (^{2}H) compounds immediately follow the corresponding ^{1}H compounds.

GUIDE TO THE COMPILATIONS AND EVALUATIONS

The format used for the compilations and evaluations has been discussed in the Forward. Additional information on the individual sections of each sheet is now provided in the folowing.

"*Components*". Each component is listed by its IUPAC name (ref. 1), chemical formula according to the Hill system, and Chemical Abstracts Registry Number. Also included are the "Chemical Abstracts" name if this differs from the IUPAC name, and trivial name or names if appropriate. IUPAC and common names are cross-referenced to "Chemical Abstracts" names in the System Index.

"*Original Measurements*". References are expressed in "Chemical Abstracts" style, journal names being abbreviated, and if necessary transliterated, in the form given by the "Chemical Abstracts Service Source Index" (CASSI). In the case of multiple entries (for example translations) an asterisk indicates the publication used for the data compilation.

"*Variables*". Ranges of variations of temperature, pressures, etc. are indicated here.

"*Prepared by*". The compiler is name here.

"*Experimental Values*". Components are described as (1) and (2), as defined in "Components". The experimental data are presented in the units in the original paper. Thus the temperature is expressed t/°C or t/°F as in the original, and conversion to T/K is made only in the critical evaluation. However, the author's units are expressed according to IUPAC recommendations (ref. 3,4) as far as possible.

In addition, compiler-calculated values of mole fractions and/or mass per cent are included if the original data do not use these units. 1975 or 1977 atomic weights (ref. 5) are used in such calculations. If densities are reported in the original paper, conversions from concentrations to mole fractions are included in the compilation sheets, 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.

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.

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.

"*Methods*". An outline of the method is presented, reference being made to sources of further detail if these are cited in the original paper. "Chemical Abstracts" abbreviations are often used in this text.

"*Source and Purity of Materials*". For each component, referred to as (1) and (2), the following information (in this order and in abbreviated form) is provided if it is available in the original papers:

> source and specification
>
> method of preparation
>
> properties
>
> degree of purity

"*Estimated Error*". If this information was omitted by the authors, and if the necessary data are available in the paper, 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, the type of apparatus, and other relevant information. Methods used by the compilers for reporting estimated errors are based on the papers of Ku and Eisenhart (ref. 6).

"*References*". These are the references (usually cited in the original paper) which the compiler considers particularly useful in discussing the method and material.

"*Evaluator*". The information provided here is the name of the evaluator, the evaluator's affiliation, and the date of the evaluation.

"*Critical Evaluation*". The evaluator aims, to the best of his or her ability, to check that the compiled data are correct, to assess their reliability and quality, to estimate errors where necessary, and to recommend numerical values. The summary and critical review of all the data supplied by the compiler include the following information:

(a) *Critical text*. The evaluator produces a text evaluating *all* the published data for the particular system being discussed, reviewing their merits or shortcomings. Only published data (including theses and reports) are considered, and even some of the published data may only be referred to in this text if it is considered that inclusion of a data compilation sheet is unjustified.

(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 in the compilation sheets, stating the limits within which it should be used.

(c) *Graphical summary*. This may be provided in addition to tables and/or fitting equations.

(d) *Recommended values.* Data are *recommended* if the results of at least two independent experimental groups are available and are in good agreement, and if the evaluator has no doubt as to the adequacy and reliability of the experimental and computational procedures used.

Data are reported as *tentative* if only one set of measurements is available, or if the evaluator is uncertain of the reliability of some aspect of the experimental or computational method but judges that it should cause only minor error, or if the evaluator considers some aspect of the computational or experimental method undesirable but believes the data to have some value in those instances when an approximate value of the solubility is needed.

Data determined by an inadequate method or under ill-defined conditions are *rejected*, the reference being included in the evaluation together with a reason for its rejection by the evaluator.

(e) *References.* All pertinent references are listed here, including all those publications appearing in the accompanying compilation sheets and also those which have been rejected and not compiled.

(f) *Units.* The final recommended values are reported in SI units (ref. 3). It should be noted that in most cases the rounded absolute temperature values (e.g. 298 K) actually refer to 298.15 K, etc., although very few solubilities are known with such precision that the differences are significant.

Continuation Sheets. These are used for both compilations and evaluations, and include sections listing the "Components" and also the "Original measurement" or "Evaluator" as well as the word "continued". Compilation continuation sheets may include a section headed "Comments and/or Additional Data".

REFERENCES

1. Regaudy, J.; Klesney, S. P. *Nomenclature of Organic Chemistry (IUPAC)*, ("The Blue Book"), Pergamon, Oxford, 1979.

2. Hill, E. A. *J. Am. Chem. Soc.* 1900, *22*, 478.

3. Whiffen, D. H., ed. *Manual of Symbols and Terminology for Physicochemical Quantities and Units* (IUPAC), ("The Green Book"), Pergamon, Oxford, 1979; *Pure Appl. Chem.* 1979, *51*, 1.

4. McGlashan, M. L. *Physicochemical Quantities and Units*, 2nd ed. Royal Institute of Chemistry, London, 1971.

5. IUPAC Commission on Atomic Weights, *Pure Appl. Chem.* 1976, *47*, 75; 1979, *51*, 405.

6. Ku, H. H. and Eisenhart, C., in Ku, H. H., ed. *Precision Measurement and Calibration*, NBS Special Publication 300, Vol. 1, Washington, D. C., 1969.

COMPONENTS:	EVALUATOR:
(1) Hexachlorobenzene; C_6Cl_6; [118-74-1] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku September 1982

CRITICAL EVALUATION:

Little is known about the solubility of hexachlorobenzene in water at normal temperatures despite the fact that large quantities of this compound are used commercially. In recent times, however, toxicologists and environmental chemists have begun to study the aqueous solubilities of chlorinated aromatic hydrocarbons in connection with pollution analyses. Currently, solubility data for this compound at ordinary temperatures exist in two published papers. A third work reports the solubility of hexachlorobenzene at higher temperatures.

The work of Weil, Dure, and Quentin (1) discusses the determination of extremely small solubilities. Their saturation process was carried out by a chromatographic technique to avoid contamination on glass surfaces and formation of possible colloidal aggregates of the solute. In their procedure, Mg silica gel, overcoated with the solute, was eluted with water. However, the analytical procedure was not reported, a factor which makes it difficult to estimate the precision of the measured values. It is known that certain problems and complications arise in the course of the determination of solubilities of this magnitude. First of all, the effects of a third component (glass or silica gel) may be significant. Also, the purity of the solvent (water) can exert a dominant influence on results in cases of highly diluted, saturated systems. In addition to distillation and deionization, the solvent should also be degassed, a procedure not done for the reported measurements. For such reasons, the values of Weil et al. may involve large absolute errors.

Hollifield (2) applied a nephelometric procedure for the estimation of the solubility of hexachlorobenzene in water. His analytical method involved the preparation of a standard curve by successive dilution of an acetone solution of the test substance with water. The turbidities of the solutions were measured nephelometrically. Extrapolation of this curve to an intensity of the reagent blank gave an estimate of the solubility in water. The solubility value reported for 297 ± 2 K was 110 µg(1)/kg. The method evidently gives rough estimates of the solubilities and it has the advantage of being rapid. The lack of precision in the procedure can be appreciated from a review of the reported solubility data which show deviations of several orders of magnitude from reported literature values. Consequently, these solubility values are not considered further in this evaluation.

Sharov (3) has reported the solubility of hexachlorobenzene in water at higher temperatures. Two variables (temperature and pressure) make a comparison with other solubility data difficult. Only the value referred to 353 K was probably measured at normal pressure. Even so, its value of 10 mg(1)/kg(2) cannot be used to support the solubility value of Weil et al.

The following solubility value for hexachlorobenzene in water is based upon the value reported by Weil et al. However, for the reasons stated, the value should be considered doubtful.

T/K	10^8 mol(1)/dm^3	10^6 g(1)/kg	$10^{10}x(1)$
298.15	1.8	5.0	3.2

<div align="center">REFERENCES</div>

1. Weil, L.; Dure, G.; Quentin, K-E. *Wasser Abwasser Forsch.* <u>1974</u>, *7*, 169-75.

2. Hollifield, H.C. *Bull. Environ. Contam. Toxicol.* <u>1979</u>, *23(4/5)*, 579-86.

3. Sharov, V. G. *V. Sb. Dostizheniya Nauk-Neftekhim-Vam.* <u>1975</u>, 138-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexachlorobenzene; C_6Cl_6; [118-74-1] (2) Water; H_2O; [7732-18-5]	Weil, L.; Dure, G.; Quentin, K-E. *Wasser Abwasser Forsch.* 1974, 7, 169-75.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^6 g(1)/dm^3$ [a]	$10^8 mol(1)/dm^3$ [b]	$10^{10} x(1)$ [b]
25	5.0	1.76	3.17

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation process involved a chromatographic technique. A 600 mg Florisil powder sample (15.5% MgO, 84.0% SiO, 0.5% Na_2SO_4), 60/100 mesh, was overcoated with 10 mg solute in 10 ml acetone solution. After the acetone was removed by evaporation, the solid mixture was transferred to a column (5 mm diameter, 7 cm length) and the solute was eluted from the Mg silica gel coating with water. The organic solute was then extracted from the water solution. The procedure for determining the composition of the extracted sample was not specified.	C_6Cl_6: Source and purity not specified. H_2O: Twice distilled.
	ESTIMATED ERROR: Solubility: >20% (This evaluation is based on the table I in the original paper. In the table the effect of the ratio of the organic compound and Florisil was tested with five determinations in each case.) Temperature: ±0.2 K (evaluator).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Pentachlorobenzene; C_6HCl_5; [608-93-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

CRITICAL EVALUATION:

The solubility of pentachlorobenzene in water has been measured by Yalkowsky, Orr, and Valvani (1) and by Banerjee, Yalkowsky, and Valvani (2). The measurements differ primarily in the analytical procedures involved. The principal motivation for the studies was to obtain certain correlations for solubilities of halogenated benzenes in water.

In the former measurements (1), a conventional experimental procedure was employed. Commercial reagents without further purification were used for the measurements which were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (3), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The latter investigation (2) was based upon a radiochemical analysis. Although temperature regulation and time for equilibration seemed to have received sufficient attention, the result deviates far more than 10 percent from the value reported in (1). The accuracy of the latter measurements also depends upon the radiochemical purity of the substrate, a property which was not tested. The uncertainty of radiochemical purity may account in part for the deviation from the spectrophotometrically determined value.

The solubility of pentachlorobenzene in water is reported here as a tentative value based upon the spectrophotometric determinations (1):

T/K	$10^6 \text{mol}(1)/\text{dm}^3$	$10^4 g(1)/\text{kg}$	$10^8 x(1)$
298.15	2.2	5.52	3.95

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, *14(10)*, 1227-9.

3. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorobenzene; C_6HCl_5; [608-93-5] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^4 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^8 x(1)$ [a]
25	5.51	2.2	3.95

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	C_6HCl_5: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorobenzene; C_6HCl_5; [608-93-5] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Techn.* 1980, *14(10)*, 1227-9.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^8 x(1)$ [a]
25	1.332	5.32	9.613

a. Calculated by F. W. Getzen
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium was performed in sealed stainless steel centrifuge tubes with constant or intermittent shaking. The equilibrium was generally complete within 1 week. The mixture was then centrifuged for 60 minutes after which aliquots of the solution were removed for analysis either by a pipet or syringe. Liquid scintillation counting with ^{14}C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.	C_6HCl_5: Commercial reagent, the ^{14}C-labeled compound was purchased by NEN, the nonlabeled one by Aldrich. H_2O: Distilled water.

ESTIMATED ERROR:
Solubility: ±4.9% (std. deviation estimated by authors). Temperature: ±0.2 K (equilibration)   ±0.3 K (centrifugation).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The solubility of pentachlorophenol in water was first reported by Carswell and Nason (1) in 1938 in connection with their study of properties and uses of this compound. The determinations were done very rapidly and the method, the classical "synthetic" one, allowed the solubility measurements to be made at various temperatures. When the reported values are fit by linear regression to the logarithm of solubility versus the reciprocal of Absolute temperature, the following equation results:

$$\log_{10}(S_1(g(1))/kg) = (3.517 \pm 0.239) - (1589 \pm 74)/T \qquad [1]$$

The coefficient of correlation for equation [1] is 0.997. The calculated value for the solubility of pentachlorophenol from equation [1] is 0.0154 g(1)/kg at 298.15 K. As is evident, the magnitude of the standard error estimate is in the order of 6-7 percent.

Two other reports on the solubility of pentachlorophenol in water take into account the variation of the solubility with hydrogen ion activity. The earlier work published in 1955 by Blackman, Parke, and Garton (2) reported the pH value at which the solubility was measured. The later study by Toyota and Kuwahara (3) in 1967 provided the variation of solubility with pH in water, in aqueous KCl solutions, and in aqueous NH_4Cl solutions. Also provided in their work was an empirical equation for the solubility in water with respect to pH.

The ability of pentachlorophenol to protolyze in water makes the question of its solubility somewhat complicated. In order to establish the solubility behavior generally, one must measure solubilities with pH as one of the variables. The information provided in (2) and (3) is, however, too limited to allow further calculations in this respect. Thus, in reality, it is practical to evaluate and report only the total solubility of pentachlorophenol/phenoxide at the pH prevailing in the saturated solution. This total solubility can be compared with the value obtained from equation [1].

Some critical observations can be made concerning the measurements of Toyota and Kuwahara. First of all, no description of the sources and purities of reagents was provided. Also, the method of analysis was gravimetric based upon the assumption that the pentachlorophenol was insoluble at pH values lower than 3. That is, the saturation value was established by weighing the pentachlorophenol precipitated from a saturated solution with its pH suppressed below 3. Thus, the method rejected the solubility of pentachlorophenol at pH values lower than 3. Such a method permits the determination of total concentration of saturated solutions only at elevated pH values (from pH 6 and up; pH 5 seems too low). The accuracy of the method is not sufficient to determine the cosolute effects of urea, KCl, and NH_4Cl either. This can be seen clearly from the plots of $\log(s/s_0)$ versus the concentration of the cosolute. The complicated behavior is understandable in view of the fact that the cosolutes may have dissimilar effects on the phenol and the phenoxide ion. Therefore, the values must be discarded and the solubilities in water must be checked against other values available. Blackman et al. reported the total solubility of pentachlorophenol at pH 5.1. This hydrogen ion activity was established by the use of a phosphate buffer in amounts which may have been insufficient to affect the solubility. Therefore, this value can be taken as comparable with the value of Carswell and Nason provided the pH of the solution is taken to be in the range 4.5-5.5.

On the basis of the three solubilities available, 1.4×10^{-2} g(1)/kg from (1), a 9.6×10^{-3} g(1)/kg from (2), and 1.4×10^{-2} g(1)/kg from (3), the following is a tentative solubility value. (The last of these three values was calculated from the equation provided in (3) and it refers to 300 K.) Also, it must be emphasized that, as for any protolyzing solute, the solubility of pentachlorophenol in water is affected to a degree by changes in pH.

T/K	$10^5 mol(1)/dm^3$	$10^2 g(1)/kg$	$10^7 x(1)$
298.15	3.7	1.0	6.8

COMPONENTS:	EVALUATOR:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION: (Continued)

REFERENCES

1. Carswell, T. S.; Nason, H. K. *Ind. Eng. Chem.* 1938, *30(6)*, 622-6.

2. Blackman, G. E.; Park, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

3. Toyota, H.; Kuwahara, M. *Nippon Dojohiryogaku Zasshi* 1967, *38(2,3)*, 93-97.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5] (2) Water; H_2O; [7732-18-5]	Carswell, T. S.; Nason, H. K. *Ind. Eng. Chem.* 1938, *30(6)*, 622-6.

VARIABLES:	PREPARED BY:
Temperature: 0 - 70°C	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/kg$ [a]	$10^5 mol(1)/kg$ [b]	$10^7 x(1)$ [b]
0	0.5	1.9	3.4
27	1.8	6.76	12.2
50	3.5	13.1	23.7
62	5.8	21.8	39.2
70	8.5	31.9	57.5

a.   Reported (values given as percent (1) in original work).
b.   Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A known amount of pure pentachlorophenol was added to cold water. Then, the temperature was raised slowly with agitation until dissolution was complete.	C_5HCl_5O: Source and purity not specified. H_2O: No specifications given.

ESTIMATED ERROR:
Solubility: <6% (estimated by the evaluator on the basis of the smoothed curve of log c vs. 1/T, where c denotes solubility).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5]	Carswell, T. S.; Nason, H. K. *Ind. Eng. Chem.* <u>1938</u>, *30(6)*, 622-6.
(2) Water; H_2O; [7732-18-5]	

EXPERIMENTAL VALUES: Continued ...

Figure 1.   Solubility of pentachlorophenol in water versus Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	9.59	3.6	6.51

a.   Calculated by F. W. Getzen.
b.   Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The samples were equilibrated in a thermostat bath with intermittent shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	C_6HCl_5O: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two techniques of analysis).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5] (2) Potassium chloride; KCl; [7447-40-7] (3) Water; H_2O; [7732-18-5]	Toyota, H.; Kuwahara, M. *Nippon Dojohiryogaku Zasshi* 1967, *38(2,3)*, 93-97.
VARIABLES: pH, concentrations of KCl at 27°C	PREPARED BY: H. Ohtaki

EXPERIMENTAL VALUES:

All Measurements at 27°C

Initial pH = 5.0

$mol(KCl)/dm^3$	$10^2 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a,c]	pH [d]
1.0	1.68	6.3	1.13	5.32
0.50	2.32	8.7	1.56	5.45
0.20	1.65	6.2	1.12	5.25
0.10	2.08	7.8	1.41	5.34
0.05	3.20	12	2.17	5.28
0.02	2.16	8.1	1.46	5.20
0.0	3.20	12	2.17	5.35

Initial pH = 6.0

$mol(KCl)/dm^3$	$10 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a,c]	pH [d]
1.0	1.01	3.8	6.81	5.96
0.50	0.879	3.3	5.93	5.89
0.20	0.985	3.7	6.67	6.07

Continued ....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Pentachlorophenol and various amounts of NaOH and KCl were dissolved in water at 27°C and the solutions were left for 3 days with occasional stirring (once a day for 1 hour). Then, the undissolved pentachlorophenol was filtered off and the pH values of the filtrates were measured with a glass electrode. To each aliquot of the solutions was added hydrochloric acid to maintain their pH less than 3. The precipitates which resulted were aged and weighed.	Nothing specified.

ESTIMATED ERROR: No estimation was given for errors in the solubility measurements. However, the reported values of S/S° (S the solubility of pentachlorophenol in KCl solutions and S° its solubility in pure water) do not fall on a single smooth curve, but rather spread. Therefore, the errors may be estimated to be larger than 2-3%.

REFERENCES:

1. Nose, K.; Fukunaga, K. *Noyaku Seisan Gijutsu* 1952, *6*, 30.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5] (2) Potassium chloride; KCl; [7447-40-7] (3) Water; H_2O; [7732-18-5]	Toyota, H.; Kuwahara, M. *Nippon Dojohiryogaku Zasshi* <u>1967</u>, *38(2,3)*, 93-97.

EXPERIMENTAL VALUES: Continued ....

Initial pH = 6.0

mol(KCl)/dm^3	$10g(1)/dm^3$ [a]	$10^4mol(1)/dm^3$ [b]	$10^6x(1)$ [a,c]	pH [d]
0.10	1.17	4.4	7.94	6.00
0.05	1.39	5.2	9.38	5.95
0.02	1.54	5.8	10.5	5.98
0.0	0.613	2.3	4.15	5.70

Initial pH = 7.0

mol(KCl)/dm^3	$g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [a,c]	pH [d]
1.0	1.01	3.8	6.81	6.81
0.50	1.07	4.0	7.20	6.79
0.20	1.41	5.3	9.56	6.82
0.10	1.25	4.7	8.49	6.77
0.05	1.46	5.5	9.94	6.86
0.02	1.33	5.0	9.03	8.82
0.0	2.05	7.7	13.9	6.92

Initial pH = 8.0

mol(KCl)/dm^3	$10^{-1}g(1)/dm^3$ [a]	$10^2mol(1)/dm^3$ [b]	$10^3x(1)$ [a,c]	pH [d]
1.0	1.68	6.3	1.15	7.78
0.50	1.57	5.9	1.08	7.67
0.20	2.18	8.2	1.51	7.93
0.10	1.68	6.3	1.15	7.70
0.05	2.45	9.2	1.70	8.35
0.02	1.92	7.2	1.32	7.67
0.0	1.94	7.3	1.34	7.80

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated mole fraction based upon complete dissociation of KCl.
d. pH value of solution equilibrated with precipitate.

COMMENTS AND/OR ADDITIONAL DATA:

Solubilities of pentachlorophenol in water versus hydrogen ion activity, in the absence of KCl, at 27°C were measured and calculated. The stoichiometric amounts of dissolved pentachlorophenol were calculated from mass balance based upon incomplete dissociation. The dissociation constant was given as $K_p = [C_6Cl_5O^-][H^+]/[C_6Cl_5OH] = 3.2 \times 10^{-5}$ mol/dm^3. This value together with the activity of the hydrogen ion, $\{H^+\}$, as determined from pH measurements was incorporated in an equation for calculating the solubility:

$$S = \frac{1.796 \times 10^{-6}}{\{H+\}0.170} \left[1 + \frac{3.2 \times 10^{-5}}{\{H+\}} \right]$$

Observed and calculated values reported:

pH	5.0 $10^5mol(1)/dm^3$	6.0 $10^4mol(1)/dm^3$	7.0 $10^3mol(1)/dm^3$
Observed value:	4.05	6.05	8.85
Calculate value:	5.34	6.20	8.90

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5] (2) Ammonium chloride; NH_4Cl; [12125-02-9] (3) Water; H_2O; [7732-18-5]	Toyota, H.; Kuwahara, M. *Nippon Dojohiryogaku Zasshi* <u>1967</u>, *38(2,3)*, 93-97.

VARIABLES:	PREPARED BY:
pH, concentrations of NH_4Cl at 27°C	H. Ohtaki

EXPERIMENTAL VALUES:

All Measurements at 27°C

Initial pH = 5.0

$mol(NH_4Cl)/dm^3$	$10^2 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a,c]	pH [d]
1.0	0.8390	3.15	5.690	5.12
0.50	1.377	5.17	9.335	5.20
0.05	3.3161	12.45	22.472	5.41
0.0	3.0657	11.51	20.774	5.35

Initial pH = 5.5

$mol(NH_4Cl)/dm^3$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a,c]	pH [d]
0.05	6.153	2.31	4.170	5.73

Initial pH = 6.0

$mol(NH_4Cl)/dm^3$	$10 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a,c]	pH [d]
1.0	1.489	5.59	1.010	6.01
0.50	1.345	5.05	0.9120	6.05
0.30	2.9645	11.13	2.0099	6.19
0.20	2.650	9.95	1.797	6.14
0.0	0.5993	2.25	0.4061	5.70

Continued ....

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Pentachlorophenol and various amounts of NaOH and NH_4Cl were dissolved in water at 27°C and the solutions were left for 3 days with occasional sitrring (once a day for 1 hour). Then, the undissolved pentachlorophenol was filtered off and the pH values of the filtrates were measured with a glass electrode. To each aliquot of the solutions was added hydrochloric acid to maintain their pH less than 3. The precipitates which resulted were aged and weighed.	Nothing specified.

ESTIMATED ERROR: No estimation was given for errors in the solubility measurements. However, the reported values of S/S° (S the solubility of pentachlorophenol in KCl solutions and S° its solubility in pure water) do not fall on a single smooth curve, but rather spread. Therefore, the errors may be estimated to be larger than 2-3%.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentachlorophenol; C_6HCl_5O; [87-86-5] (2) Ammonium chloride; NH_4Cl; [12125-02-9] (2) Water; H_2O; [7732-18-5]	Toyota, H.; Kuwahara, M. *Nippon Dojohiryogaku Zasshi* 1967, *38(2,3)*, 93-97.

EXPERIMENTAL VALUES: Continued ....

Initial pH = 6.5

$mol(NH_4Cl)/dm^3$	$10g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [a,c]	pH [d]
1.0	2.352	0.883	1.595	6.46
0.50	3.9819	1.495	2.7005	6.50
0.10	5.966	2.24	4.045	6.40
0.0	6.233	2.34	4.226	6.52

Initial pH = 7.0

$mol(NH_4Cl)/dm^3$	$10g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [a,c]	pH [d]
1.0	2.9432	1.105	1.9967	6.97
0.50	5.114	1.92	3.469	6.98
0.30	7.777	2.92	5.275	7.03
0.20	8.736	3.28	5.926	7.10
0.10	11.13	4.18	7.553	6.86
0.05	14.76	5.54	10.01	6.92
0.0	20.40	7.66	13.85	6.92

Initial pH = 7.5

$mol(NH_4Cl)/dm^3$	$g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^4x(1)$ [a,c]	pH [d]
0.10	1.675	6.29	1.137	7.50

Initial pH = 8.0

$mol(NH_4Cl)/dm^3$	$g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [a,c]	pH [d]
1.0	0.3276	1.23	2.223	8.02
0.50	0.5780	2.17	3.920	8.00
0.30	0.6339	2.38	4.299	8.05
0.20	1.247	4.68	8.458	8.01
0.10	1.851	6.95	12.57	8.01
0.05	2.903	10.9	19.73	7.98
0.0	19.39	72.8	133.8	7.80

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated mole fraction based upon complete dissociation of NH_4Cl.
d. pH value of solution equilibrated with precipitate.

COMMENTS AND/OR ADDITIONAL DATA:

Solubilities of pentachlorophenol in water versus hydrogen ion activity, in the absence of NH_4Cl, at 27°C were measured and calculated. The stoichiometric amounts of dissolved pentachlorophenol were calculated from mass balance based upon incomplete dissociation. The dissociation constant was given as $K_D = [C_6Cl_5O^-][H^+]/[C_6Cl_5OH] = 3.2 \times 10^{-5}$ mol/dm^3. This value together with the activity of the hydrogen ion, $\{H^+\}$, as determined from pH measurements was incorporated in an equation for calculating the solubility:

$$S = \frac{1.796 \times 10^{-6}}{\{H^+\}^{0.170}} \left[1 + \frac{3.2 \times 10^{-5}}{\{H^+\}} \right]$$

Observed and calculated values reported:

pH	5.0	6.0	7.0
	$10^5mol(1)/dm^3$	$10^4mol(1)/dm^3$	$10^3mol(1)/dm^3$
Observed value:	4.05	6.05	8.85
Calculate value:	5.34	6.20	8.90

COMPONENTS:	EVALUATOR:
(1) 1,2,4,5-Tetrabromobenzene; $C_6H_2Br_4$; [636-28-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,2,4,5-tetrabromobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,2,4,5-tetrabromobenzene in water is reported here as a tentative value:

T/K	10^7 mol(1)/dm^3	10^5 g(1)/kg	$10^9 x(1)$
298.15	1.1	4.34	1.99

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4,5-Tetrabromobenzene; $C_6H_2Br_4$; [636-28-2] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^5 g(1)/dm^3$ [a]	$10^7 mol(1)/dm^3$ [b]	$10^9 x(1)$ [a]
25	4.33	1.1	1.99

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_2Br_4$: Commercial product (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2,3,4-Tetrachlorobenzene; $C_6H_2Cl_4$; [634-66-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,2,3,4-tetrachlorobenzene in water has been reported by Yalkowsky, Orr and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,2,3,4-tetrachlorobenzene in water is reported here as a tentative value:

T/K	10^5mol(1)/dm^3	10^3g(1)/kg	$10^7 x(1)$
298.15	2.0	4.33	3.61

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*,

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,3,4-Tetrachlorobenzene; $C_6H_2Cl_4$; [634-66-2] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	4.32	2.0	3.61

a. Calculated by F. W. Getzen.
b. Reported.

<div align="center">AUXILIARY INFORMATION</div>

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_2Cl_4$: Commercial product (Aldrich or Eastman), used as received. H_2O: Source and purity not reported.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2,3,5-Tetrachlorobenzene; $C_6H_2Cl_4$; [634-90-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

CRITICAL EVALUATION:

The solubility of 1,2,3,5-tetrachlorobenzene in water has been measured by Yalkowsky, Orr and Valvani (1) and by Banerjee, Yalkowsky, and Valvani (2). The measurements differ primarily in the analytical procedures involved. The principal motivation for the studies was to obtain certain correlations for solubilities of halogenated benzenes in water.

In the former measurements (1), a conventional experimental procedure was employed. Commercial reagents without further purification were used for the measurements which were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (3), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The latter investigation (2) was based upon a radiochemical analysis. Although temperature regulation and time for equilibration seemed to have received sufficient attention, the result deviates far more than 10 percent from the value reported in (1). The accuracy of the latter measurements also depends upon the radiochemical purity of the substrate, a property which was not tested. The uncertainty of radiochemical purity may account in part for the deviation from the spectrophotometrically determined value.

The solubility of 1,2,3,5-tetrachlorobenzene in water is reported here as a tentative value based upon the spectrophotometric determinations (1):

T/K	10^5mol(1)/dm^3	10^3g(1)/kg	10^7x(1)
298.15	1.6	3.46	2.89

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, 18(4), 351-3.

2. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, 14(10), 1227-9.

3. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,3,5-Tetrachlorobenzene; $C_6H_2Cl_4$; [634-90-2] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	3.45	1.6	2.89

a. Calculated by F. W. Getzen.
b. Reported.

<div align="center">AUXILIARY INFORMATION</div>

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_2Cl_4$: Commercial product (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.

	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,3,5-Tetrachlorobenzene; $C_6H_2Cl_4$: [643-90-8] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Techn.* <u>1980</u>, *14(10)*, 1227-9.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	4.016	1.86	3.361

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium was performed in sealed stainless steel centrifuge tubes with constant or intermittent shaking. The equilibrium was generally complete within 1 week. The mixture was then centrifuged for 60 minutes after which aliquots of the solution were removed for analysis either by a pipet or syringe. Liquid scintillation counting with ^{14}C-labeled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.	$C_6H_2Cl_4$: Commercial reagent, the ^{14}C-labeled compound was purchased by NEN, the nonlabeled by Aldrich. H_2O: Distilled water.

ESTIMATED ERROR:
Solubility: ±4.0% (std. deviation estimated by authors).   Temperature: ±0.2 K (equilibration), ±0.3 K (centrifugation).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2,4,5-Tetrachlorobenzene; $C_6H_2Cl_4$; [95-94-3]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,2,4,5-tetrachlorobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 $\pm$ 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of $\pm$ 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,2,4,5-tetrachlorobenzene in water is reported here as a tentative value:

T/K	10^6mol(1)/dm^3	10^4g(1)/kg	$10^8 x$(1)
298.15	2.8	6.06	5.06

REFERENCES

1.   Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2.   Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4,5-Tetrachlorobenzene; $C_6H_2Cl_4$; [95-94-3] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^4 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^8 x(1)$ [a]
25	6.05	2.8	5.06

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_2Cl_4$: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,3,4,6-Tetrachlorophenol; $C_6H_2Cl_4O$; [58-90-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

One study has been reported in the literature concerning the solubility of 2,3,4,6-tetrachlorophenol in water by Blackman, Parke, and Garton (1). Their concern was the relation of physical properties of certain substituted phenols to their physiological activities. In order to standardize the measuring conditions, they regulated the pH of all their saturated solutions to a value of 5.1 by the slight addition of a phosphate buffer. The electrolytic effects of this buffer addition on the equilibrium solubility can be neglected. However, the effects of pH changes upon the solubility are more complicated and should not be overlooked. In order to establish the solubility behavior generally, one must measure solubilities with pH as one of the variables. Such data, however, do not exist for 2,3,4,6-tetrachlorophenol. The only alternative here is to consider the total solubility of the compound in water, considering total solubility as the sum of the concentrations of the phenol and the phenolate ion. In the final analysis, the overall influence of pH upon the solubility is controlled by the acidity constant of the 2,3,4,6-tetrachlorophenol which was reported to be 5.3 by Blackman et al. Evidently the regulation of pH to a value of 5.1 in this case provides a higher concentration of the phenolate ion relative to the undissociated phenol as compared to that in a solution simply saturated with the pure phenol. Thus, the solubility value at the pH of 5.1 should have a somewhat higher value than that for the saturated solution of the pure phenol.

The information concerning the purity and further treatment of the reagents was also incomplete. The experimental procedures seem quite satisfactory however. The following solubility value based entirely upon the work reported by Blackman et al., must be considered as doubtful.

T/K	10^4mol(1)/dm^3	10g(1)/kg	$10^5 x(1)$
298.15	7.9	1.8	1.4

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3,4,6-Tetrachlorophenol; $C_6H_2Cl_4O$; [58-90-2] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	**PREPARED BY:** A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	1.83	7.9	1.43

a. Calculated by F. W. Getzen
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The samples were equilibrated in a thermostat bath with intermittent shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	$C_6H_2Cl_4O$: Not specified, probably a commercial product. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (estimated here on the basis of the reported results of the two techniques of analysis).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2,4-Tribromobenzene; $C_6H_3Br_3$; [615-54-3]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,2,4-tribromobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,2,4-tribromobenzene in water is reported here as a tentative value:

T/K	10^5mol(1)/dm^3	10^2g(1)/kg	$10^7x(1)$
298.15	3.2	1.01	5.78

REFERENCES

1.   Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2.   Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Tribromobenzene; $C_6H_3Br_3$; [615-54-3] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	1.01	3.2	5.78

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_3Br_3$: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,3,5-Tribromobenzene; $C_6H_3Br_3$; [626-39-1]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,3,5-tribromobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,3,5-tribromobenzene in water is reported here as a tentative value:

T/K	$10^6 mol(1)/dm^3$	$10^4 g(1)/kg$	$10^8 x(1)$
298.15	2.5	7.89	4.52

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Tribromobenzene; $C_6H_3Br_3$; [626-39-1] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^4 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^8 x(1)$ [a]
25	7.87	2.5	4.52

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_3Br_3$: Commercial product (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: ±10% (authors)
Temperature: ±1 K (authors).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4,6-Tribromophenol; $C_6H_3Br_3O$; [118-79-6] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku. November 1979.

CRITICAL EVALUATION:

The only two available published works concerning the solubility of 2,4,6-tribromophenol in water are old and information provided in these works concerning the methods of analysis is incomplete. Also, the purity of the reagents used in the measurements is open to question. However, the solubility value of 70 mg(1)/kg(2) at 288 K determined by Werner (1) in 1884 agrees quite well with the value of 76 mg(1)/kg(2) at 17-18°C measured by Ogston (2). (These concentrations have been established in the same units by assuming the density of the saturated solution to be 1.0 g/cm^3.)

It should be noted that the solubility of 2,4,6-tribromophenol in water is considerably dependent upon the acidity of the solution. Here, it is assumed that the solubility established refers to that of a solution having a pH value prevailing for saturated 2,4,6-tribromophenol in water.

The solubility of 2,4,6-tribromophenol in water is reported here as a doubtful value:

T/K	$10^4 mol(1)/dm^3$	$10^2 g(1)/kg$	$10^6 x(1)$
283.15	2.1	7.0	3.8

REFERENCES

1.   Werner, E. *Ann. Chim. Phys. Ser. G* <u>1884</u>, 572-3.

2.   Ogston, A. G. *J. Chem. Soc.* <u>1936</u>, *Part II*, 1713.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Tribromophenol; $C_6H_3Br_3O$; [118-79-6] (2) Water; H_2O; [7732-18-5]	Werner, E. *Ann. Chim. Phys. Ser. G* <u>1884</u>, 572-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [b]
15	7	2.1	3.8

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Information concerning the equilibration procedure was incomplete. The analysis was done by titration of the saturated solutions with a standard barium hydroxide solution.	$C_6H_3Br_3O$: Synthesized product, reported melting point 92°C. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Tribromophenol; $C_6H_3Br_3O$; [118-79-6] (2) Water; H_2O; [7732-18-5]	Ogston, A. G. *J. Chem. Soc.* <u>1936</u>, *Part II*, 1713.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
17-18	7.61	2.3	4.15

a.   Calculated by F. W. Getzen.
b.   Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
There were no specifications in the original paper about the experimental methods. Also, the temperature at which the measurements were made was not well defined.	$C_6H_3Br_3O$: Source and purity not specified. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2,3-Trichlorobenzene; $C_6H_3Cl_3$; [87-61-6]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,2,3-trichlorobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principla motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,2,3-trichlorobenzene in water is reported here as a tentative value:

T/K	10^4 mol(1)/dm^3	10^2 g(1)/kg	$10^6 x(1)$
298.15	1.7	3.09	3.07

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,3-Trichlorobenzene; $C_6H_3Cl_3$; [87-61-6] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	3.08	1.7	3.07

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_3Cl_3$: Commercial product (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.

	ESTIMATED ERROR:
	Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION:

The solubility of 1,2,4-trichlorobenzene in water has been measured by Meleshchenko (1), Yalkowsky et al. (2), and Chiou et al. (3). However, there appears to be a serious discrepancy between the three reported solubility values. According to the authors, the error estimates in their measurements were ± 8 percent for Meleshchenko, ± 10 percent for Yalkowsky et al., and ± 5 percent for Chiou et al. Consequently, in view of these uncertainties, the recommended solubility value must be taken as the arithmetical mean for the three reported measured values.

With reference to Figures 3 and 4 in the Introduction, the recommended solubility of 1,2,4-trichlorobenzene in water given below for 298.15 K is within an acceptable margin of expectation.

The single data point available for the solubility of water in 1,2,4-trichlorobenzene at 298.15 K by Eidinoff (4) is accepted as a tentative value.

T/K	$10^3 mol(1)/dm^3$	$10^2 g(1)/kg$	$10^4 x(1)$
298.15	3.05	3.79	3.82

T/K	$10^2 mol(2)/dm^3$	$10 g(2)/kg$	$10^3 x(2)$
298.15	1.63	2.02	2.03

REFERENCES

1. Maleshchenko, K. F. *Gigiena i Sanit.* 1960, *25(5)*, 54-57.

2. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

3. Chiou, C. T.; Schmedding, D. W.; Maines, M. *Environ. Sci. Technol.* 1982, *16(1)*, 4-10.

4. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M., Urey, H. C., Kirshenbaum, I., Eds.; McGraw-Hill: New York, 1955; Part II, Chapter 7, pp 129-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M., Urey, H. C., Kirshenbaum, I., Eds.; McGraw-Hill: New York, 1955; Part II, Chapter 7, pp 129-44.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [a]
25	2.0232	1.123	2.0340

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Addition of 2 ml H_2O to 100 ml $C_6H_3Cl_3$ in an equilibration flask was performed in a dry box. The closed flask was then placed in a water thermostat bath and the assembly was shaken for 90 min. The samples for analysis were taken with a sampling pipet while the equilibrium temperature was maintained. The water content in the sample was determined by a modified Karl Fischer titration.	$C_6H_3Cl_3$: Purified and dried before use. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: Average dev. ±0.00006 mol(1)/ kg. Temperature: ±0.05 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1] (2) Water; H_2O; [7732-18-5]	Maleshchenko, K. F. *Gigiena i Sanit.* <u>1960</u>, *25(5)*, 54-57.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [c]
19	3.0	1.65	2.98

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A 100 mg trichlorobenzene in 1 liter water mixture was shaken periodically for 5 days at 18-20°C. After filtration, a determined quantity of ether was added and extracted three times. The ether was evaporated and oxidation of the residue was accomplished with chlorosulphonic acid. The chlorine content was determined by iodometric titration.	$C_6H_3Cl_3$: Not specified. H_2O: Twice distilled before use.
	ESTIMATED ERROR: Solubility: ±8%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
(2) Water; H_2O; [7732-18-5]	

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	3.466	1.91	3.451

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1,2,4-trichlorobenzene in water was agitated at room temperature for about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. The determination was carried out in duplicate.	$C_6H_3Cl_3$: Aldrich commercial grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Schmedding, D. V.; Manes, M. *Environ. Sci. Technol.* 1982, *16(1)*, 4-10.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/^\circ C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	4.881	2.69	4.861

Note: The solubility was also reported in (1), as "unpublished results".

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2,4-trichlorobenzene was equilibrated with water in screwcapped bottles in a reciprocal shaker for 24 hours. After two days settling, samples were taken from the solution for analysis by gas chromatography. The chromatograph was equipped with a Ni[63] EC detector. Analyses were continued until a constant concentration was observed.	$C_6H_3Cl_3$: Not specified. H_2O: Distilled.

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

	REFERENCES: 1. Chiou, C. T. *Hazard Assess. Chem. Current Dev.* 1981, *1*, 117-53.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water-d_2; D_2O; [7789-20-0] (2) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, <u>1943</u>.
VARIABLES: One temperature	PREPARED BY: G. Jancso

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3mol(1)/kg$ [b]	$10^3x(1)$ [a]
25.0	1.999	9.98	1.808

a. Calculated by F. W. Getzen.
b. Reported (average of two experimental measurements).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

Between 25 and 100 ml 1,2,4-trichlorobenzene and 1 to 2 ml D_2O were placed in a flask and shaken for about 90 min. The thermostat water bath temperature was maintained within ±0.05°C. Then, a sample was removed and the amount of D_2O dissolved was determined by a modified Karl Fischer titration (1).
 	
The original report was unavailable; however, the method and the results were described in sufficient detail in (1). The solubility of H_2O in 1,2,4-trichlorobenzene was also determined and found to be 0.01123 mol(1)/kg. The average deviation for two experiments was ±0.00006 mol(1)/kg.
	$C_6H_3Cl_3$: Carefully purified and dried
	            before use. Source and method
	            not given.
	
	D_2O: Source not specified.

ESTIMATED ERROR:
Solubility: av. dev. ±2.1 x 10^{-5} mol
                D_2O/100 g solution.

Temperature: ±0.05 K.

REFERENCES:
1. Eidinoff, M. L. In "Production of Heavy
    Water", National Nuclear Energy Series
    Division III-Vol. 4F, Murphy, G. M.,
    Urey, H. C., Kirshenbaum, I., Eds.;
    McGraw-Hill: New York, <u>1955</u>; Part II,
    Chapter 7, pp 129-44.

COMPONENTS:	EVALUATOR:
(1) 1,3,5-Trichlorobenzene; $C_6H_3Cl_3$; [108-70-3]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,3,5-trichlorobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,3,5-trichlorobenzene in water is reported here as a tentative value:

T/K	10^5mol(1)/dm^3	10^3g(1)/kg	$10^7 x(1)$
298.15	3.6	6.55	6.51

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Trichlorobenzene; $C_6H_3Cl_3$; [108-70-3] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	6.53	3.6	6.51

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted with a small volume of methylene chloride which was then assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_3Cl_3$: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.

ESTIMATED ERROR:
  Solubility: ±10% (authors).
 	
  Temperature: ±1 K (authors).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4,5-Trichlorophenol; $C_6H_3Cl_3O$; [95-95-4]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The solubility 2,4,5-trichlorophenol in aqueous buffer solution has been reported by Blackman, Parke, and Garton (1) in 1954. The principal motivation of this study was to observe the relationships between physical properties and physiological activities of certain substituted phenols. The experimental conditions were standardized with respect to pH by the slight addition of a phosphate buffer to the test solutions. The final pH value of the saturated solutions was regulated to 5.1. Under saturation equilibrium conditions, however, the concentration of the buffer was relatively dilute having a concentration of about 6 mmol/dm³ relative to the added phosphate, KH_2PO_4.

The salt effect of the added buffer can be neglected, but the effect of the adjusted pH upon the acid dissociation equilibrium of the phenol must be given some consideration. The acidity constant for the 2,4,5-trichlorophenol was reported by Blackman et al. to have a magnitude in the order of 10^{-7}. Consequently, in the absence of the added buffer, the pH of the saturated solution should fall below the 5.1 value. Therefore, the adjustment of the pH to a value of 5.1 with the buffer should result in an increase in the concentration of the phenoxide ion relative to the undissociated phenol. This situation would result in a higher total solubility compared to the solution without the added buffer.

The authors did undertake tests of their method of analysis. They established the difference between the values measured by what they called "colorimetric" and "spectrophotometric" methods to be approximately 4 percent. However, the information concerning the purity of the reagents used was inadequate. Considering all such factors, the solubility of 2,4,5-trichlorophenol in water must be reported as a doubtful value.

The solubility of 2,4,5-trichlorophenol in water at a pH of 5.1 is reported here as a doubtful value:

T/K	10^3mol(1)/dm³	10g(1)/kg	$10^5 x(1)$
298.15	5.0	9.9	9.0

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-5-Trichlorophenol; $C_6H_3Cl_3O$; [95-95-4] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/cm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	9.48	4.8	8.68

a. Calculated by F. W. Getzen.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The samples were equilibrated in a thermostat bath with intermittent shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	$C_6H_3Cl_3O$: Source and purity not specified, probably a commercial reagent. H_2O: Distilled.

	ESTIMATED ERROR:
	Solubility: <5% (evaluated here on the basis of the reported results of the two techniques of analysis).

	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

Daccomo (1) has provided the first reported measurement of the solubility of 2,4,6-trichlorophenol in water. These measurements were made at least as early as 1885. They can be judged as somewhat unreliable for several reasons. First of all, the melting point of the substrate was 2-3 degrees below that reported later (69.5°C) in the "Handbook of Chemistry and Physics" (2). The measurements themselves were not described. However, it is porbable that the so-called "classical synthetic method" was applied. In this procedure, known amounts of solute and solvent are mixed and their miscibilities tested with temperature. The reported value of 0.85 g(1)/kg(2) at 298 K from three experimental points does not allow one to establish a reliable estimate of experimental errors.

Another value for the solubility of 2,4,6-trichlorophenol in water has been reported by Blackman, Parke, and Garton (3). Their determination was made at a solution pH of 5.1 through the slight addition of a phosphate buffer solution. Because the phenol in question has an acid pK value of 10.9 according to Blackman et al., the buffer solution pH evidently suppresses the ionization. This results in a decrease in concentration of the phenolate ion relative to the undissociated phenol. The net result is that the solubility should be suppressed somewhat for the buffered system relative to that for a system containing only the phenol itself in water. Converting the solubility value to the same units as those of Daccomo (using a solution density of 1.0 g/cm³), one obtains a value of 0.443 g(1)/kg(2) at the pH value of 5.1. This solubility value is quite possible, relative to the value provided by Daccomo, for the reasons indicated.

Since the variation of solubility with pH is not known in this case, only a doubtful value for the solubility of 2,4,6-trichlorophenol in water can be reported here. The value of Daccomo refers to a solution saturated with only the phenol at the pH which prevails for a saturated solution. Therefore, this value has been selected as the most appropriate saturation value at 298.15 K.

The solubility of 2,4,6-trichlorophenol in water is reported here as a doubtful value:

T/K	10^3mol(1)/dm^3	10g(1)/kg	$10^5x(1)$
298.15	2.2	4.3	4.0

REFERENCES

1. Daccomo, G. *Ber. Dtsch. Chem. Ges.* 1885, *18,* 1163-4.

2. "Handbook of Chemistry and Physics", 50th ed.; Weast, R. C., Ed.; CRC Press: Cleveland, Ohio, 1969; p C-426.

3. Blackman, G. E.; Park, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955 *54(1),* 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	4.34	2.2	3.98

a. Calculated by F. W. Getzen.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The samples were equilibrated in a thermostat bath with intermittent shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	$C_6H_3Cl_3O$: Not specified, probably a commercial product. H_2O: Distilled.

	ESTIMATED ERROR:
	Solubility: <5% (evaluated here on the basis of the reported results of the two techniques of analysis).

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2]	Daccomo, G. *Ber. Dtsch. Chem. Ges.* <u>1885</u>, *18*, 1163-4.
(2) Water; H_2O; [7732-18-5]	

VARIABLES:	PREPARED BY:
Temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [b]
11.2	5.10	2.581	4.653
25.4	8.58	4.341	7.828
96	24.3	12.28	22.17

a. Reported (parts(1) per 1000 parts(2) in original work).
b. Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

Continued ...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No specifications given. Probably the so-called synthetic method.	$C_6H_3Cl_3O$: Synthesized both from 2-chlorophenol and 4-chlorophenol, melting point 67°C.
	H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Trichlorophenol; $C_6H_3Cl_3O$; [88-06-2] (2) Water; H_2O; [7732-18-5]	Daccomo, G. *Ber. Dtsch. Chem. Ges.* <u>1885</u>, *18*, 1163-4.

EXPERIMENTAL VALUES: Continued ...
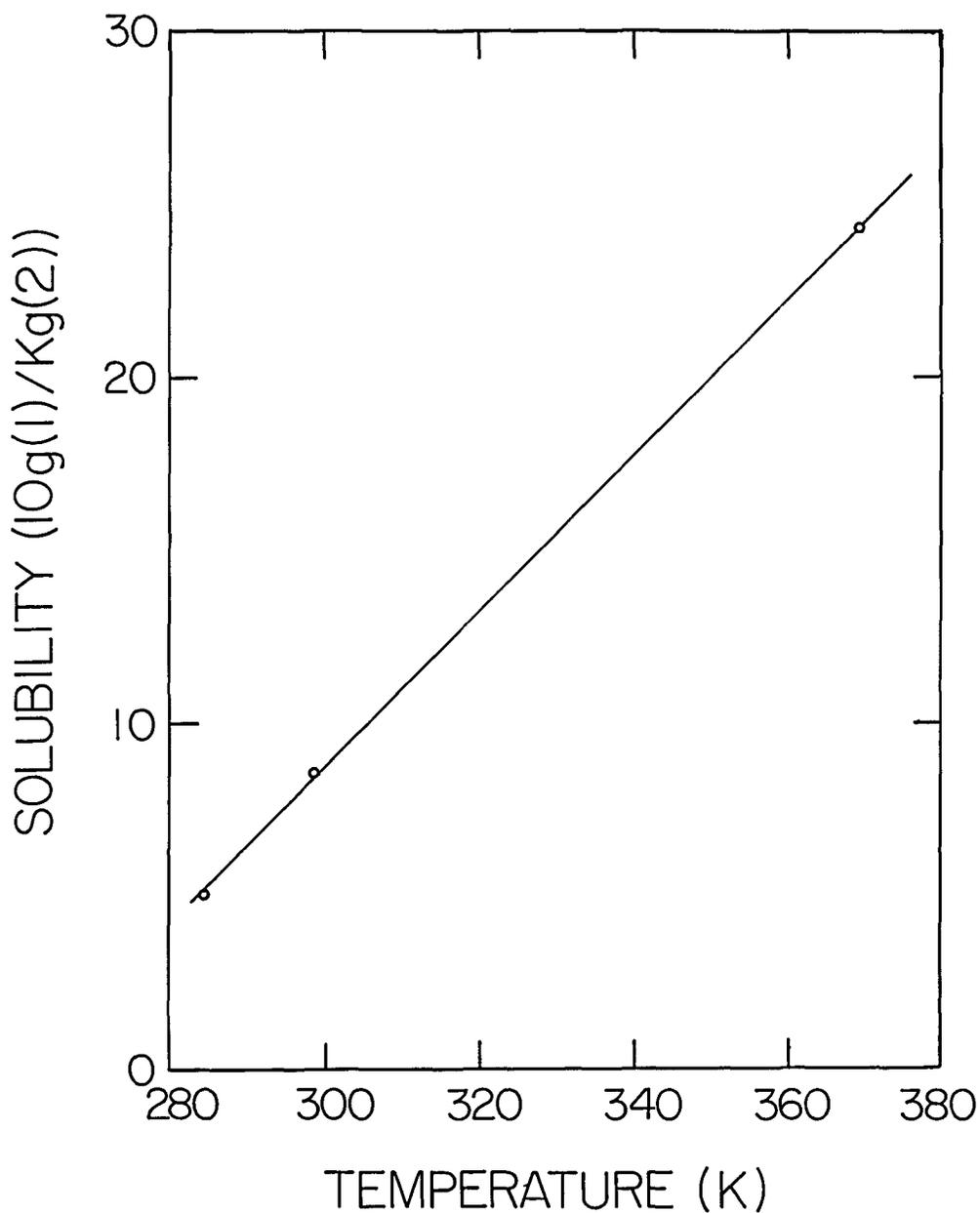
Figure 1.   Solubility of 2,4,6-trichlorophenol in water versus Absolute temperature.

COMPONENTS:	EVALUATOR:
(1) 1-Bromo-2-chlorobenzene; C_6H_4BrCl; [694-80-4] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979

CRITICAL EVALUATION:

The experimental results consists of a single value at 298.15 K published in 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was $\pm$ 10 percent. This is a reasonable observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions was assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1-bromo-2-chlorobenzene in water is tentative:

T/K	$10^4 mol(1)/dm^3$	$10g(1)/kg$	$10^5 x(1)$
298.15	6.46	1.24	1.17

REFERENCES

1. Yalkowsky, S.H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Bromo-2-chlorobenzene; C_6H_4BrCl; [694-80-4] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	1.237	6.46	1.167

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1-brom-2-chlorobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.	C_6H_4BrCl: Aldrich commercial grade, used as received. H_2O: Deionized.

	ESTIMATED ERROR:
	   Solubility: ±10%.
	
	   Temperature: ±1°K.

	REFERENCES:

COMPONENTS:	EVALUATOR:
(1)　1-Bromo-3-chlorobenzene; 　　　C_6H_4BrCl; [108-37-2] (2)　Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published in 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The sautrated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1-bromo-3-chlorobenzene in water is tentative:

T/K	$10^4 mol(1)/dm^3$	$10g(1)/kg$	$10^5 x(1)$
298.15	6.14	1.18	1.11

REFERENCES

1.　Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2.　Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Bromo-3-chlorobenzene; C_6H_4BrCl; [108-37-2] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	1.181	6.17	1.115

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1-bromo-3-chlorobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.	C_6H_4BrCl: Aldrich commercial grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS: -	EVALUATOR:
(1) 1-Bromo-4-chlorobenzene; C_6H_4BrCl; [106-39-8]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku
(2) Water; H_2O; [7732-18-5]	November 1979

CRITICAL EVALUATION:

A single solubility measurement of 1-bromo-4-chlorobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. All measurements were done at room temperature (25 $\pm$ 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of $\pm$ 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1-bromo-4-chlorobenzene in water is reported here as a tentative value:

T/K	10^4mol(1)/dm^3	10^2g(1)/kg	$10^6 x(1)$
298.15	2.3	4.42	4.16

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, 18(4), 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Bromo-4-chlorobenzene; C_6H_4BrCl; [106-39-8] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Ore, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	4.40	2.3	4.16

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was diluted and assayed spectrophotometrically. At least two independent determinations were carried out.	C_6H_4BrCl: Commercial product (Eastman or Aldrich), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Bromo-4-iodobenzene; C_6H_4BrI; [589-87-7]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku
(2) Water; H_2O; [7732-18-5]	November 1979

CRITICAL EVALUATION:

A single solubility measurement of 1-bromo-4-iodobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. All measurements were done at room temperature (25 $\pm$ 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of $\pm$ 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so that total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1-bromo-4-iodobenzene in water is reported here as a tentative value:

T/K	$10^5 \mathrm{mol(1)/dm^3}$	$10^3 \mathrm{g(1)/kg}$	$10^7 x(1)$
298.15	2.8	7.94	5.06

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Bromo-4-iodobenzene; C_6H_4BrI; [589-87-7] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	7.92	2.8	5.06

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was diluted and assayed spectrophotometrically. At least two independent determinations were carried out.	C_6H_4BrI: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2-Dibromobenzene; $C_6H_4Br_2$; [583-53-9]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published in 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1,2-dibromobenzene in water is tentative:

T/K	$10^4 mol(1)/dm^3$	$10^2 g(1)/kg$	$10^6 x(1)$
298.15	3.16	7.48	5.71

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, 18(4), 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dibromobenzene; $C_6H_4Br_2$; [583-53-9] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.

VARIABLES:
  One temperature
	PREPARED BY:
	  A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	7.455	3.16	5.710

a.   Calculated by compiler.
b.   Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1,2-dibromobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.	$C_6H_4Br_2$: Aldrich commercial grade, used as received. H_2O: Deionized.

	ESTIMATED ERROR:
	  Solubility: ±10%.
	  Temperature: ±1 K.

	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,3-Dibromobenzene; $C_6H_4Br_2$; [108-36-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water, H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION:

   The solubility of 1,3-dibromobenzene in water was reported by Hine et al. (1) at 308.15 K and by Yalkowsky et al. (2) at 298.15 K. Considering the small temperature difference of 10 degrees between the two measurements, one can judge that the data show a significant discrepancy.

   The reported experimental errors ± 5.6% (1) and ± 10% (2) are probably greater than the authors anticipated. A creful study of the experimental procedures described in both articles reveals no obvious shortcomings. Despite the long time allowed for equilibrium by Hine et al., their measurements resulted in a lower solubility value than that obtained by Yalkowsky et al. The most likely explanation for the discrepancy could be attributed to the analytical determinations used.

   It is well known that the solubility curve for halogenated benzenes in water has a positive slope above room temperature. However, the two measured points reported are against this trend, that is, the values decrease with rising temperature. In order to choose between the two solubility data values, use was made of the theoretical relationship between the molar solubilities and the molar volumes of the solutes at 298.15 K as described in the Introduction. The following solubility value for 1,3-dibromobenzene in water is tentative:

T/K	10^4mol(1)/dm^3	10^2g(1)/kg	$10^6 x(1)$
298.15	2.70	6.40	4.89

REFERENCES

1.   Hine, J.; Haworth, H. W.; Ramsay, O. B.   *J. Am. Chem. Soc.* 1963, *85(10)*, 1473-6.

2.   Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C.   *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dibromobenzene; $C_6H_4Br_2$; [108-36-1] (2) Water; H_2O; [7732-18-5]	Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* <u>1963</u>, *85(10)*, 1473-6.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [c]
30.0	6.747	2.86	5.184

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,3-dibromobenzene was added to a 4 ml of water in an ampoule which was then sealed. The sealed ampoule was rotated in a constant temperature water bath for a week to establish saturation. The 1,3-dibromobenzene solubility was determined by ultraviolet spectrophotometric measurements using a Beckman DU spectrophotometer.	$C_6H_4Br_2$: Eastman Kodak Co.; redistilled before use. H_2O: Not specified.
	ESTIMATED ERROR: Solubility: ±5.6% S.D. Temperature: ±0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dibromobenzene; $C_6H_4Br_2$; [108-36-1] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	9.838	4.17	7.536

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1,3-dibromobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.	$C_6H_4Br_2$: Aldrich commercial grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku. January 1979

CRITICAL EVALUATION:

There are only a few reported measurements dealing with the solubility of 1,4-dibromobenzene in water. In the published papers on the subject, the determination of solubility is not the primary purpose of the work, a fact that may affect the precision of the reported results. Of the values reported, only that of Andrews and Keefer (1) refers to 298.2 K. The measured data reported by Hine, Haworth, and Ramsay (2) at 308.2 K lend some support to the value assigned at 298.2 K.

The experimental procedure employed by Andrews and Keefer is adequate for the determination in question. However, the time of equilibrium (about 20 hours as given in (3)) seems quite short in the absence of tests for solution equilibrium. It is reasonable to attribute most of the uncertainty in the reported solubility of 8.5 x 10^{-5} mol(1)/dm^3 (7.0 x 10^{-5} molar at an ionic strength of 1.0 molar, a figure incorrectly cited for solubility in pure water in some papers). Support for the reliability of the value at 298.2 K is provided by the value of 1.12 x 10^{-4} mol(1)/kg(2) given by Hine et al. for 308.2 K. This value was obtained by employing a long equilibration (at least a week) and a direct spectrophotometric measurement. In fact, it seems reasonable that the latter measurements should be more reliable than those of Andrews and Keefer although the agreement between the two measurements is quite satisfactory. The increase in the solubility is about 30% for a temperature rise of 10 degrees from 298.2 K. This increase is about the same magnitude as that for 1,4-dichlorobenzene in water in the same range of temperature as measured by Wauchope and Getzen (4).

The following is the tentative solubility of 1,4-dibromobenzene in water at 298.15 K:

T/K	10^5mol(1)/dm^3	10^2g(1)/kg	$10^6 x(1)$
298.15	8.5	2.0	1.5

REFERENCES

1.   Andrews, L. M.; Keefer, R. M.   *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.

2.   Hine, J.; Haworth, H. W.; Ramsay, O. B.   *J. Am. Chem. Soc.* 1963, *85(10)*, 1473-6.

3.   Andrews, L. M.; Keefer, R. M.   *J. Am. Chem. Soc.* 1949, *71(11)*, 3644-7.

4.   Wauchope, R. D.; Getzen, F. W.   *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^6 x(1)$ [b]
25.0	2.0	8.48	1.53

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation process was done in sealed Erlenmeyer flasks. The time used for the equilibration was 20 hours. Measured volumes of the saturated solutions were then extracted using measured volumes of hexane to remove the aromatic matter from the aqueous layer. The solute concentration was measured spectrophotometrically using a Beckman DU spectrophotometer (1).	$C_6H_4Br_2$: Commercial product (Eastman Kodak Co.), used as received. H_2O: Source and purity not specified.

ESTIMATED ERROR:

Solubility: >10% (evaluator).

Temperature: ±0.2 K (evaluator).

REFERENCES:
1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71(11)*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dibromobenzene; $C_6H_4Br_2$; [106-37-6] (2) Water; H_2O; [7732-18-5]	Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* 1963, *85(10)*, 1473-6.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
35.0	2.642	1.12	2.030

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of the aromatic compound was combined with 4.0 ml of water in a 5.0 ml ampoule which was then sealed. The sealed ampoule was rotated in a constant temperature water bath for at least a week to establish saturation. The undissolved solid was removed by filtration and the concentration of the solute in the saturated filtrate solution was determined by ultraviolet spectrophotometric measurements using a Beckman DU spectrophotometer. Several measurements were taken at intervals of at least a day in order to be sure that an equilibrium had been established.	$C_6H_4Br_2$: Source not specified; presumably commercial material, recrystallized to constant melting point in agreement with literature values. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±7% (standard deviation reported by authors). Temperature: ±0.1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4-Dibromophenol; $C_6H_4Br_2O$; [615-58-7]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979

CRITICAL EVALUATION:

Only a rather old value, that of Werner (1), has been found in the literature for the solubility of 2,4-dibromophenol in water. Considering the incomplete information on the purity of the reagents used and the equilibration method itself coupled with the fact that the instrumentation used was relatively simple, one must regard the reported value as doubtful.

It must be noted that the solubility of this compound, like any protolytic solute, is considerably dependent upon the acidity of the solution. Here it is assumed that the pH value is that for the saturated solution without the addition of other protolytic solutes. Thus, the solubility value reported is for such a saturated solution.

Based upon an assumed density of 1.0 g/cm^3 for the solution (an estimate which has no effect on the accuracy of the reported value), the doubtful solubility of 2,4-dibromophenol in water at 298 K is as follows:

T/K	$10^3 mol(1)/dm^3$	g(1)/kg	$10^4 x(1)$
298	8.	2.	1.4

REFERENCES

1.   Werner, E. *Ann. Chim. Phys. Ser. 6* 1884, 571-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dibromophenol; $C_6H_4Br_2O$; [615-58-7] (2) Water; H_2O; [7732-18-5]	Werner, E. *Ann. Chim. Phys. Ser. 6* <u>1884</u>, *Vol. 3*, 571-2.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^4 x(1)$ [b]
15	1.94	7.701	1.391

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation procedure was not specified. The analysis of the saturated solution was done by titration with a standardized bromine solution.	$C_6H_4Br_2O$: Synthesized product, melting point 40°C, boiling point 154°C at 17 mmHg. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Chloro-2-iodobenzene; C_6H_4ClI; [615-41-8]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published by 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1-chloro-2-iodobenzene in water is tentative:

T/K	$10^4 mol(1)/dm^3$	$10^2 g(1)/kg$	$10^6 x(1)$
298.15	2.88	6.89	5.21

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, <u>1979</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Chloro-2-iodobenzene; C_6H_4ClI; [615-41-8] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H., Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	6.868	2.88	5.204

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1-chloro-2-iodobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometrically. Two independent determinations were carried out.	C_6H_4ClI: Aldrich commerical grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Chloro-3-iodobenzene; C_6H_4ClI; [625-99-0]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water, H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published in 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1-chloro-3-iodobenzene in water is tentative:

T/K	10^4 mol(1)/dm	10^2 g(1)/kg	$10^6 x(1)$
298.15	2.82	6.74	5.09

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, 18(4), 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Chloro-3-iodobenzene; C_6H_4ClI; [625-99-0] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	6.725	2.82	5.096

a. Calculated by compiler.
b. Reported.

<div align="center">AUXILIARY INFORMATION</div>

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1-chloro-3-iodobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The saturated filtrate solution was diluted and assayed spectrophotometri-cally. Two independent determinations were carried out.	C_6H_4ClI: Aldrich commercial grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Chloro-4-iodobenzene; C_6H_4ClI; [637-87-6]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979

CRITICAL EVALUATION:

A single solubility measurement of 1-chloro-4-iodobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurement is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1-chloro-4-iodobenzene in water is reported here as a tentative value:

T/K	$10^4 \text{mol}(1)/\text{dm}^3$	$10^2 \text{g}(1)/\text{kg}$	$10^6 x(1)$
298.15	1.3	3.11	2.35

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Chloro-4-iodobenzene; C_6H_4ClI; [637-87-6] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	3.10	1.3	2.35

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was diluted and assayed spectrophotometrically. At least two independent determinations were carried out.	C_6H_4ClI: Commercial reagent (Eastman or Aldrich), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION:

   Data for the solubility of 1,2-dichlorobenzene in water have been reported in several papers. The approximate solubility at 298.15 K was reported by Booth and Everson (1) while, somewhat earlier, Klemenc and Low (2) produced measurements between 293 and 333 K. More recent data have been published only between 276 and 307 K (8-11).

   The approximate value provided by Booth and Everson is not given further consideration here. The remaining available data from (2, 8-11) have been correlated relative to absolute temperature using a normal polynomial equation:

$$S_1 (g(1)/kg) = 19.2314 - 1.81140 \times 10^{-1}T$$
$$+ 5.6509 \times 10^{-4}T^2 - 5.77683 \times 10^{-7}T^3 \qquad [1]$$

   The significance of this equation is that the curve representing the solubility data passes through a minimum at 283.7 K. This behavior is consistent with the theory discussed by Gill et al. (12) for the solubility of aromatic compounds in water.

   Recommended solubility values between 273 and 333 K have been calculated from equation [1] and presented in Table 1. The solubility behavior described by equation [1] is shown also in Figure 1 which contains the reported experimental values for the solubility of 1,2-dichlorobenzene in water.

   The solubility of water in 1,2-dichlorobenzene has also been investigated and reported by a number of workers (3-7) in the 298 to 318 K temperature range. In general, these solubility values show some irregularity. While the agreement between the measurements of Jones and Monk (5) and those of Wing and Johnston (7) is reasonable, the deviation is considerable in relation to the measurements of Goldman (4) and of Kirchnerova and Cave (6) at 298.15 K. Identical measured values at 298.15 K were reported from the same department of McGill University by Goldman and by Kirchnerova and Cave.

   From the description of the experimental measurements and the reliability if the results reported, it is not reasonable to exclude any of the data points except that quoted by Dreisbach (3) from further analysis. Therefore, all the water in 1,2-dichlorobenzene solubility data except that from Dreisbach were combined and incorporated in a regression equation. However, because of the long equilibration times allowed in Goldman and in Kirchnerova and Cave, their data points were given a weight twice as large as those values provided in Jones and Monk and in Wing and Johnston. The correlation equation is given by:

$$\log_{10} x(2) = 2.23134 - 1448.67/T \qquad [2]$$

In this equation, $x(2)$ is the mole fraction solubility of water in the 1,2-dichlorobenzene-water system and T is the Absolute temperature. The calculated solubility values in the 273 and 333 K range are shown in Figure 2 along with the reported values.

   The calculated mole fraction values for the solubility of water in 1,2-dichlorobenzene from equation [2] are given in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 293 and 328 K.

COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION: (Continued)

Table 1. Solubility of 1,2-Dichlorobenzene in Water.

T/K	10^4 mol(1)/dm^3	$10g(1)$/kg	$10^5 x(1)$
273.15	9.64	1.42	1.74
278.15	9.20	1.35	1.66
283.15	9.04	1.33	1.63
288.15	9.13	1.34	1.65
293.15	9.44	1.39	1.70
298.15	9.94	1.47	1.80
303.15	10.6	1.57	1.92
308.15	11.4	1.69	2.07
313.15	12.3	1.82	2.23
318.15	13.2	1.97	2.41
323.15	14.2	2.12	2.60
328.15	15.3	2.28	2.79
333.15	16.2	2.43	2.98

Table 2. Solubility of Water in 1,2-Dichlorobenzene.

T/K	10^2 mol(2)/dm^3	$10g(2)$/kg	$10x(2)$
293.15	1.73	2.39	1.95
298.15	2.09	2.90	2.36
303.15	2.50	3.48	2.84
308.15	2.98	4.17	3.39
313.15	3.53	4.96	4.03
318.15	4.16	5.86	4.76
323.15	4.87	6.90	5.60
328.15	5.68	8.08	6.56

COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION: (Continued)

REFERENCES

1.   Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* <u>1948</u>, *40(8)*, 1491-3.

2.   Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* <u>1930</u>, *49(4)*, 629-40.

3.   Dreisbach, R. R. "Physical Properties of Chemical Compounds," Advances in Chemistry Series No. 15; American Chemical Society: Washington, D.C., <u>1955</u>; p. 135.

4.   Goldman, S., Ph.D. Dissertation, McGill University, Montreal, <u>1969</u>, p 84.

5.   Jones, J. R.; Monk, C. B. *J. Chem. Soc.* <u>1963</u>, *Part III*, 2633-5.

6.   Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* <u>1976</u>, *54(24)*, 3909-16.

7.   Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* <u>1957</u>, *79(4)*, 864-5.

8.   Chiou, C. T.; Freed, V. H. "Chemodynamic Studies on Bench Mark Industrial Chemicals"; National Technical Information Service: Springfield, Virginia, <u>1977</u>; PB-274263.

9.   Schwarz, F. P.; Miller, J. *Anal. Chem.* <u>1980</u>, *52(13)*, 2162-4.

10. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* <u>1980</u>, *14(10)*, 1227-9.

11. Chiou, C. T.; Schmedding, D. W.; Manes, M. *Environ. Sci. Technol.* <u>1982</u>, *16(1)*, 4-10.

12. Gill, S. J.; Nichols, N. F.; Wadso, I. *J. Chem. Thermodyn.* <u>1976</u>, *8(5)*, 445-52.

COMPONENTS:	EVALUATOR:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of 1,2-dichlorobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

X Goldman data (4).
□ Jones and Monk data (5).
△ Kirchnerova and Cave data (6).
● Wing and Johnston data (7).

Figure 2.   Logarithm of water mole fraction versus the reciprocal of Absolute temperature for water in 1,2-dichlorobenzene.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas.* 1930, *49(4)*, 629-40.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
20	1.34	0.9114	1.642
25	1.45	0.9862	1.777
30	1.71	1.163	2.096
35	1.83	1.245	2.243
40	1.94	1.319	2.377
45	2.03	1.381	2.488
55	2.23	1.517	2.733
60	2.32	1.578	2.843

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The determination of the solubility was based upon volumetric principles applied to the measurement of excess solute in a cali-brated apparatus as described by Rex (1).	$C_6H_4Cl_2$: Kahlbaum reagent, used as received. H_2O: Distilled.

ESTIMATED ERROR:
Solubility: ±10% (compiler).

Temperature: ±1 K (compiler).

REFERENCES:

1. Rex, A. Z. *Phys. Chem.* 1906, *55*, 355-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Booth, H. S.; Everson, H. E., *Ind. Eng. Chem.* 1948, *40*, 1491-3.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1} ml(1)/dm^3(2)$ [a]	$10 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	< 2	< 1.7	< 3.2

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made with samples contained in a stoppered Goetz tube placed in a constant temperature water bath. Equilibrium was assured through repeated shaking and centrifuging the mixture in the stoppered tube while it was temporarily removed from the water bath. The amount of solute dissolved was determined as the difference between total amount added and amount remaining in excess upon saturation. The determination of the excess amount of solute added has been described by Hanslick (1).	$C_6H_4Cl_2$: Commercial reagent, C. P. grade, used as received. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: <100%. Temperature: ±1 K (compiler).
	REFERENCES: 1. Hanslick, R. S., Dissertation, Columbia University, 1935.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p 135.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/kg(2)$ [a]	$mol(1)/kg$ [b]	$10x(1)$ [c]
25	2.1	1.14	1.46

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experimental methods were not described.	H_2O: Distilled. $C_6H_4Cl_2$: Dow Chemical Co., 99.85% pure, purified by distillation before use.
	ESTIMATED ERROR: Solubility: <100% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.
VARIABLES: One temperature	**PREPARED BY:** A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10ml(1)/dm^3$ [a]	$10^2mol(1)/dm^3$ [b]	$10^3x(1)$ [c]
25.0	3.09	1.710	1.930

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was equilibrated with 20 ml 1,2-dichlorobenzene by stirring in a flask in a constant temperature water bath for two hours. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. The tritium activities in the tritiated water samples were determined by the acetylene method (1,2). At least four independent experiments were done. The article was based upon work reported in a Ph.D. dissertation (2).	H_2O: Tracerlab Inc., tritiated water, used as received. $C_6H_4Cl_2$: Source not specified, chemical grade, redistilled before use.

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

REFERENCES:
1. Wing, J.; Johnston, W. H. *Science* 1955, *121*, 674-5. 2. Wing, J., Ph. D. Dissertation, Purdue University, Lafayette, 1956.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Jones, J. R.; Monk, C. B. *J. Chem. Soc.* <u>1963</u>, *Part III*, 2633-5.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10 ml(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	3.2	1.77	2.00
30	3.75	2.072	2.348
35	4.25	2.344	2.667

a.   Reported.
b.   Calculated by F. W. Getzen.
c.   Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was shaken with 1,2-dichlorobenzene in 1:10 volume ratios for 4 hours in a flask in a water thermostat bath. The water content was determined by tritium assay. The count rates were determined using a typical liquid scintillator solution technique.	H_2O: Tritiated. $C_6H_4Cl_2$: Source not known, laboratory grade, dried over $CaCl_2$ and fractionally distilled before use.

ESTIMATED ERROR:

Solubility: ±5%.

Temperature: ±0.5 K (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Goldman, S., Ph.D. Dissertation, McGill University, Montreal, 1969, p. 84.
VARIABLES: Temperature	**PREPARED BY:** A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	4.342	2.41	2.719
35.1	5.783	3.21	3.650
45.06	7.909	4.39	5.028

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium experiments were carried out in a constant temperature water bath using a stirrer. An equilibration period of at least 5 days was allowed. The total water content in the organic phase was determined by a Karl Fischer titration. Each reported water solubility was obtained as an average of at least two independent determinations.	H_2O: Distilled. $C_6H_4Cl_2$: Reagent grade, washed with conc. H_2SO_4 and with 1 M $NaHCO_3$ and then fractionally distilled over silica gel.
	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* *1976, 54(24)*, 3909-16.
(2) 1,2,-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	4.324	2.40	2.707

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 50 ml 1,2-dichlorobenzene and 6 ml water in a bottle was submerged in a water thermostat bath for 2 days. The concentration of the water in the organic phase was determined by a conventional Karl Fischer dead stop back titration. Determinations were done in triplicate. A detailed description of the complete experimental procedure has been included in a Ph.D. dissertation (1).	H_2O: Distilled and deionized. $C_6H_4Cl_2$: Fisher - B255, washed with cc. H_2SO_4 and K_2SO_3 solution and distilled water. Dried over silica gel and fractionally distilled, purity 99.8%.

ESTIMATED ERROR:

Solubility: ±1%.

Temperature: ±0.1 K.

REFERENCES:
1. Kirchnerova, J., Ph.D. Dissertation, McGill University, Montreal, Quebec, 1974.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Freed, V. H. "Chemodynamic Studies on Bench Mark Industrial Chemicals"; National Technical Information Service: Springfield, Virginia, 1977; PB-274263.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10 g(1)/dm^3(2)$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
3	1.33	0.9046	1.630
20	1.48	1.007	1.817
34	1.62	1.102	1.997

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2-dichlorobenzene, 5-10 g, was equilibrated with 100 ml distilled water in a bottle for 24 hours at constant temperature. The saturated aqueous phase was removed from the container and analyzed by gas chromatography using a chromatograph equipped with a Ni^{63} EC detector. The GLC column was packed with porous polymer Chromosorb 101. Further details on the determinations and evaluations of experimental procedures have been included in (1).	$C_6H_4Cl_2$: Commercial reagent, used as received. H_2O: Distilled.
	ESTIMATED ERROR:
	Solubility: ±10% (compiler). Temperature: ±0.5 K.
	REFERENCES:
	1. Chiou, C. T.; Schmedding, D. W. Test. Protoc. Environ. Fate Mov. Toxicants, Proc. Symp., 1980 (Publ. 1981), pp 28-42.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P.; Miller, J. *Anal. Chem.* <u>1980</u>, *52(13)*, 2162-4.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

Experimentally determined values:

$10g(1)/kg$

t/°C	Elution Chromatography	UV Absorption
10.0	1.69 ± 0.03	1.56 ± 0.17
20.0	1.28 ± 0.06	1.24 ± 0.04

Values derived from average measured solubilities:

t/°C	$10g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
10.0	1.62 ± 0.07	1.102 ± 0.048	1.986 ± 0.086
20.0	1.26 ± 0.02	0.8571± 0.0136	1.544 ± 0.025

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Both elution chromatography and UV absorption methods were used to determine the aqueous solubilities. The agreement was within an experimental error of 4% between the two methods. The average deviations were determined from several measurements made on different samples. The analytical procedures for determining organic liquid solubilities in water based on liquid phase elution chromatography has been described in (1).	$C_6H_4Cl_2$: Commercial, 98 wt. %. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.5 K.
	REFERENCES: 1. Schwarz, F. P. *Anal. Chem.* <u>1980</u>, *52(1)*, 10-15.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-dichlorobenzene; $C_6H_4Cl_2$: [95-50-1] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environm. Sci. Techn.* 1980, *14(10)*, 1227-9.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [c]
25	1.5583	1.060	1.9156

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2-dichlorobenzene was added to water in a stainless steel centrifuge tube which was then sealed. The equilibrium was established by allowing the sample to stand, with intermittent shaking, for a week at constant temperature. The mixture was then centrifuged and aliquots of the solution were removed either by a pipet or syringe for analysis. Liquid scintillation counting with ^{14}C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.	$C_6H_4Cl_2$: New England Nuclear, used as received. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±0.9% S.D. Temperature: ±0.3 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Schmedding, D. W.; Manes, M. *Environ. Sci. Technol.* <u>1982</u>, *16(1)*, 4-10.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25	1.5392	1.047	1.8921

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,2-dichlorobenzene was equilibrated with water in screwcapped bottles in a reciprocal shaker for 24 hours. After two days settling, samples were taken from the solution for analysis by gas chromatography. The chromatograph was equipped with a Ni[63] EC detector. Analyses were continued until a constant concentration was observed.	$C_6H_4Cl_2$: Not specified. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±5% (compiler). Temperature: ±0.5 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION:

Seven experimental determinations have been published on the solubility of 1,3-dichloro-benzene in water in various temperature intervals (1-7), see Figure 1. Some rather serious discrepancies between the various solubility measurements are evident in the figure. The discrepancy between the two determinations (3) and (6) is about 47 percent at ambient temperature. The solubility data of Klemenc and Low (1) cover the temperature range between 293 and 333 K, while the measurements of Vesala (2,3) fall in the temperature range between 283 and 308 K. The remaining measurements reported (4-7) fall in the room temperature range.

The solubility measurements of Vesala (2,3) have been taken as most reliable and, therefore, these values were heavily weighed in the correlation of solubility versus Absolute temperature by means of a normal, three degree polynomial equation:

$$S_1(g(1)/kg) = 27.6827 - 2.61597 \times 10^{-1} T +$$
$$8.19706 \times 10^{-4} T^2 - 8.4698 \times 10^{-7} T^3 \qquad [1]$$

The significance of this equation representing the solubility data is that the curve passes through a minimum at 298.2 K. This observation is consistent with the theory discussed by Gill et al. (8) for the solubility of aromatic compounds in water.

The errors in the recommended solubility values given below could be as large as ± 10 percent, particularly at the higher temperatures. Recommended solubility values calculated from equation [1] together with corresponding molarity and mole fraction values are listed in Table 1. Also, the solubility values calculated from equation [1] are shown in Figure 1 as a solid line along with the measured values.

Table 1. Solubility of 1,3-Dichlorobenzene in Water.

T/K	$10^4 mol(1)/dm^3$	$10 g(1)/kg$	$10^5 x(1)$
283.15	7.01	1.03	1.26
288.15	6.79	0.999	1.22
293.15	6.86	1.01	1.24
298.15	7.19	1.06	1.30
303.15	7.73	1.14	1.40
308.15	8.43	1.25	1.53
313.15	9.24	1.37	1.68
318.15	10.14	1.51	1.84
323.15	11.07	1.65	2.02
328.15	11.98	1.79	2.19
333.15	12.84	1.92	2.35

The recommended molar concentrations and mole fractions have been calculated from the g(1)/kg and the densities of the two components at the equilibrium temperatures indicated.

COMPONENTS:	EVALUATOR:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

REFERENCES

1. Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* <u>1930</u>, *49(4)*, 629-40.

2. Vesala, A. *Acta Chem. Scand.* <u>1974</u>, *28A(8)*, 839-45.

3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, <u>1973</u>.

4. Chiou, C. T.; Schmedding, D. W.; Maines, M. *Environ. Sci. Technol.* <u>1982</u>, *16(1)*, 4-10.

5. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* <u>1980</u>, *14(10)*, 1227-9.

6. Schwarz, F. P.   *Anal. Chem.* <u>1980</u>, *52(1)*, 10-15.

7. Schwarz, F. P., Miller, J.   *Anal. Chem.* <u>1980</u>, *52(13)*, 2162-4.

8. Gill, S. J.; Nichols, N. F.; Wadso, I. *J. Chem. Thermodyn.* <u>1976</u>, *8(5)*, 445-52.

COMPONENTS:	EVALUATOR:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of 1,3-dichlorobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Klemenc, A.; Löw, M. *Rec. trav. chim. Pays-Bas* <u>1930</u>, *49(4)*, 629-40.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10 g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
20	1.11	0.7550	1.360
25	1.23	0.8366	1.507
30	1.40	0.9522	1.716
35	1.50	1.020	1.838
40	1.67	1.136	2.047
45	1.77	1.204	2.169
55	1.96	1.333	2.402
60	2.01	1.367	2.463

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The determination of the solubility was based upon volumetric principles applied to the measurement of excess solute in a calibrated apparatus as described by Rex (1).	$C_6H_4Cl_2$: Kahlbaum reagent, purified by the method of Friedel and Crafts before use. H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±10% (compiler).

Temperature: ±1 K (compiler).

REFERENCES:

1. Rex, A. Z. *Phys. Chem.* <u>1906</u>, *55(A)*, 355-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^4 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
10.0	0.97632	6.642 ± 0.088	1.1966
15.2	0.97764	6.651 ± 0.091	1.1982
19.6	0.98323	6.689 ± 0.096	1.2051
25.1	1.0126	6.889 ± 0.079	1.2411
30.0	1.1274	7.670 ± 0.061	1.3818
35.0	1.2113	8.241 ± 0.159	1.4847

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The 1,3-dichlorobenzene was mixed with water in a sealed flask (1) with the aid of a magnetic stirrer for 48 hours in a water bath at constant temperature. After the solution was filtered through a glass-wool plug, the solute was extracted with 2,2,4-trimethylpentene. The optical density of each sample was determined spectrophoto-metrically (2). Mean and standard deviations were calculated from three measurements.	$C_6H_4Cl_2$: Fluka AG, puriss, >99% GLC, used as received. H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±1.93%.

Temperature: ±0.05 K.

REFERENCES:
1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* 1963, *Part III*, 2716-23.

2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^4 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
25	1.029	7.00	1.261

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established between the water and the 1,3-dichlorobenzene in a sealed flask (1) with the aid of a magnetic stirrer during 48 hours under isothermal conditions. After the sample was filtered through a glass-wool plug, the 1,3-dichlorobenzene was extracted with 2,2,4-trimethylpentene. Sample optical densities were determined spectrophotometrically (2). Five parallel determinations were done. The reported work was based upon a Ph.D. dissertation (3).	$C_6H_4Cl_2$: Commercial reagent of analytical grade distilled through a column resulting in a more than 99% pure sample. H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±1.0%.   Temperature: ±0.05 K.

REFERENCES:
1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* 1963, *Part III*, 2716-23.
2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.
3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P. *Anal. Chem.* 1980, *52(1)*, 10-15.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
23.5	1.49 ± 0.11	1.014	1.826
23.5	1.44 ± 0.03	0.9796	1.765

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were determined by using an elution chromatography analytical technique. The procedure involved the use of an inert solid packing coated with a known amount of solute in a transparent tube. Water was forced through the packed tube to remove amounts of solute. The solubility was calculated from the length of the solute depleted zone (as observed from the color difference between the depleted packing and that in the remaining portion of the tube) and the volume of water passed through the tube. Chemisorb P was used as the inert solid packing.	$C_6H_4Cl_2$: Commercial, 98 wt %. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±7% S.D. Temperature: ±1.5 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P.; Miller, J. *Anal. Chem.* <u>1980</u>, *52(13)*, 2162-4.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

Experimentally determined values:

$10g(1)/kg$

t/°C	Elution Chromatography	UV Absorption
10.0	1.16 ± 0.06	1.20 ± 0.06
20.0	0.89 ± 0.04	1.13 ± 0.05
30.0	1.39 ± 0.07	1.32 ± 0.05

Values derived from average measured solubilities:

t/°C	$10g(1)/kg$ [a]	$10^4 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
10.0	1.18 ± 0.02	8.027 ± 0.136	1.446 ± 0.025
20.0	1.01 ± 0.12	6.870 ± 0.816	1.238 ± 0.180
30.0	1.35 ± 0.03	9.183 ± 0.204	1.655 ± 0.037

a.   Reported.
b.   Calculated by F. W. Getzen.
c.   Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Both elution chromatography and UV absorption methods were used to determine the aqueous solubilities. The agreement was within an experimental error of 4% between the two methods. The average deviations were determined from several measurements made on different samples. The analytical procedures for determining organic liquid solubilities in water based on liquid phase elution chromatography has been described in (1).	$C_6H_4Cl_2$: Commercial, 98 wt. %. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.5 K.
	REFERENCES: 1. Schwarz, F. P. *Anal. Chem.* <u>1980</u>, *52(1)*, 10-15.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environm. Sci. Techn.* <u>1980</u>, *14(10)*, 1227-9.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	1.335	9.08	1.641

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

An excess of 1,3-dichlorobenzene was added to water in a stainless steel centrifuge tube which was then sealed. The equilibrium was established by allowing the sample to stand, with intermittent shaking, for a week at constant temperature. The mixture was then centrifuged and aliquots of the solution were removed either by a pipet or syringe for analysis. Liquid scintillation counting with ^{14}C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: New England Nuclear, used as received.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±1.1% S.D.

Temperature: ±0.3 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1] (2) Water; H_2O; [7732-18-5]	Chiou, C. T.; Schmedding, D. W.; Manes, M. *Environ. Sci. Technol.* <u>1982</u>, *16(1)*, 4-10.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25	1.341	9.12	1.648

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,3-dichlorobenzene was equilibrated with water in screwcapped bottles in a reciprocal shaker for 24 hours. After two days settling, samples were taken from the solution for analysis by gas chromatography. The chromatograph was equipped with a Ni[63] EC detector. Analyses were continued until a constant concentration was observed.	$C_6H_4Cl_2$: Not specified. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±5% (compiler). Temperature: ±0.5 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979.

CRITICAL EVALUATION:

Two sets of experimental data have been reported in the literature for the solubility of liquid 1,4-dichlorobenzene in water (1,2). Klemenc and Low (1) reported measurements in the temperature range between 328 and 333 K while Wauchope and Getzen (2) reported data in the narrow temperature interval between 332 and 346 K, see Figure 1. There is, however, a considerable discrepancy between the two results. For example, at 333 K, the difference is about 25 percent between the reported solubility values.

While the early solubility measurements of Klemenc and Low (1) in 1930 used the volumetric determination of the excess solute, the more recent determination of Wauchope and Getzen (2) in 1972 employed the extraction method followed by spectrophotometric analysis. The reagents used in the latter investigation were of higher purity.

Klemenc and Low (1) did not state the accuracy or the reliability of their method; neither duplicate nor triplicate samples were taken. Their temperature control during the equilibration periods of their measurements was about ± 1 K. Therefore, a conservative estimate of the possible errors in their solubility determinations is about ± 10 percent. The investigation of Wauchope and Getzen (2) was done under much more controlled conditions. The time required for completion of the equilibrium was assured in the experiment and replicate samples were always withdrawn and analyzed. The shorter equilibration times in the measurements of Klemenc and Low (1) may well account for the low solubility values at 328 and 333 K.

The solubility data of Wauchope and Getzen (2) have been assigned a higher weight in the establishment of recommended solubility values. The data have been correlated against Absolute temperature using the following second degree polynomial equation:

$$S_1(g(1)/kg) = 13.974 - 8.5829 \times 10^{-2} T +$$
$$1.3365 \times 10^{-4} T^2 \qquad\qquad [1]$$

Recommended solubility values calculated from equation [1] together with corresponding molarity and mole fraction values are listed in Table 1. Also, the solubility values calculated from equation [1] are shown in Figure 1 as a solid line along with the measured values.

Table 1. Solubility of 1,4-Dichlorobenzene in Water.

T/K	$10^3 mol(1)/dm^3$	$10g(1)/kg$	$10^5 x(1)$
328.15	1.35	2.01	2.46
333.15	1.43	2.14	2.62
338.15	1.56	2.33	2.86
343.15	1.72	2.59	3.18
348.15	1.94	2.92	3.58

The recommended molar concentrations and mole fractions have been calculated from the g(1)/kg and the densities of the two components at the equilibrium temperatures indicated.

REFERENCES

1.   Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* 1930, *49(4)*, 629-40.

2.   Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

NOTE:

The critical evaluation for *solid* 1,4-dichlorobenzene with water appears on page 103.

COMPONENTS:	EVALUATOR:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of 1,4-dichlorobenzene in water versus Absolute temperature, reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Klemenc, A.; Löw, M. *Rec. trav. chim. Pays-Bas* <u>1930</u>, *49(4)*, 629-40.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
55	1.56	1.061	1.912
60	1.63	1.109	1.998

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The determination of the solubility was based upon volumetric principles applied to the measurement of excess solute in a calibrated apparatus as described by Rex (1).	$C_6H_4Cl_2$: Prepared by chlorination of benzene using iodine as catalyst. The preparate was recrystallized several times in ethanol before use, m.p. = 52.7°C. H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±10% (compiler).

Temperature: ±1 K (compiler).

REFERENCES:
1. Rex, A. *Z. Phys. Chem.* <u>1906</u>, *55(A)*, 355-70.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
59.2	2.10	1.429	2.574
60.7	2.18	1.483	2.672
65.1	2.30	1.565	2.819
65.2	2.37	1.612	2.905
73.4	2.81	1.911	3.445

a. Reported (ppm(1) in original work).
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,4-dichlorobenzene, 20 g, in water was shaken gently for one week in a water bath at constant temperature. Replicate samples were filtered through a glass-wool plug. Then, the aqueous solution was extracted with cyclohexane which was then analyzed spectrophotometrically for organic solute using a Cary 14 spectrometer. The article was based upon a Ph.D. dissertation (1).	$C_6H_4Cl_2$: Recrystallized three times and vacuum-sublimed twice of Matheson, Coleman, and Bell reagent. H_2O: Distilled and deionized.
	ESTIMATED ERROR: Solubility: ±3%. Temperature: ±0.5 K.
	REFERENCES: 1. Wauchope, R. D., Ph.D. Dissertation, North Carolina State Univ., Raleigh, 1970.

COMPONENTS:	EVALUATOR:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

CRITICAL EVALUATION:

There have been eight published sets of data on the solubility of 1,4-dichlorobenzene in water at ordinary temperatures. Accordingly, the evaluation of the solubility data for this system lies on a firmer base than in the cases of the other solid halogenated benzenes in water.

The oldest data involving this system, determined by Klemenc and Low (1) in 1930, appear to be low and are imprecise because of the method used for saturation of water. There is, however, some evidence that the method allows the separation of the solubilities of the two crystallographic forms of 1,4-dichlorobenzene although the experimental values give no distinct temperature for the conversion from the α-form to the β-form. The solubility measured by Gross and Saylor (2) at 308.2 K is probably too low because of the short time periods involved in the equilibrations. For the same reason, the value determined by Andrews and Keefer (3) must be rejected as doubtful. Booth and Everson (4) have applied a residue-volume method of Vaughn and Nutting (5) and found the solubility of 1,4-dichlorobenzene in water to be less than 0.5 g(1)/dm^3(2). Their method is rapid but insensitive giving only rough values for substances having low solubilities.

More reliable data have been produced by Wauchope and Getzen (6) who reported errors to be in the range of 2 percent. These data are supported by the solubility values obtained by Vesala (7) as part of a study of the transfer free energies of certain nonelectrolytes from H_2O to D_2O. The recent data of Aquan-Yuen et al. (8) of the solubilities of 1,4-dichlorobenzene in aqueous electrolyte solutions produce a value for the solubility in water that agrees well with the above values. Banerjee et al. (9) report a solubility that is somewhat different from the former ones. The reason for the differences may be attributed to the radiochemical method of analysis used. For instance, the radiochemical purity of the substrate and the quenching of the samples in the scintillation analysis remain open to question. Their value can thus be regarded only as a slight support to the other data - even in cases of a full agreement.

The recommended solubility values are calculated on the basis of the data given by Wauchope and Getzen (6). However, instead of their smoothed equation, the calculations are done using an equation of simpler form. This, in turn, suggests that the magnitude of the reported errors is too optimistic. (In the work of Wauchope and Getzen, the meaning of the term "av.% dev.obsd. smoothed solubility" is somewhat unclear.) The values calculated from the simpler equation and the experimental data allow a fairly good estimate of precision. A standard deviation for a single value established in this fashion is of the order of 4.0 mg(1)/kg(2) or 0.027 mmol(1)/kg(2). The existence of the two crystallographic forms of the solute in the range of temperatures where the solubilities were measured is probably one reason for the deviations. However, this brings about no greater effect in the lower temperature range which suggests that the value for 298.2 K, for instance, is quite reliable. The simplified equation for concentration, g(1)/kg(2), in terms of Absolute temperature, T, is as follows:

$$\log_{10}(S_1(g(1))/kg(2)) = 2.86294 - 1176/T \qquad [1]$$

The observed values from the seven relevant data are shown in Figure 1 together with the calculated behavior (shown as a solid line) from the simpler equation discussed above. The densities of pure water and the saturated solutions were assumed to be equal for the determination of the reported molarity values from the calculated g(1)/kg(2) values.

The recommended g(1)/kg solubility values for solid 1,4-dichlorobenzene in water calculated from values obtained from equation [1] together with corresponding molarity and mole fraction values are listed in Table 1.

COMPONENTS:	EVALUATOR:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of solid 1,4-dichlorobenzene in water versus
Absolute temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku. September 1982.

CRITICAL EVALUATION: (Continued)

Table 1. Solubility of 1,4-Dichlorobenzene in Water.

T/K	10^4mol(1)/dm^3	10^2g(1)/kg	$10^5 x(1)$
283.15	3.48	5.12	0.628
288.15	4.11	6.05	0.741
293.15	4.82	7.10	0.870
298.15	5.62	8.29	1.016
303.15	6.52	9.63	1.18
308.15	7.53	11.13	1.36
313.15	8.65	12.8	1.57
318.15	9.88	14.7	1.80
323.15	11.25	16.7	2.05
328.15	12.4	19.0	2.33

a.   Std. dev. 0.027 mmol(1)/kg

b.   Std. dev. 4.0 mg(1)/kg

The recommended molar concentrations, g(2)/kg concentrations, and mole fractions have been determined from calculated g(1)/kg(2) values and the densities of the two components at the equilibrium temperatures indicated.

REFERENCES

1.   Klemenc, A.; Löw, M. *Rec. Trav. Chim. Pays-Bas* <u>1930</u>, *49(4)*, 629-40.

2.   Gross, P. M.; Saylor, J. H.   *J. Am. Chem. Soc.* <u>1931</u>, *53(5)*, 1744-51.

3.   Andrews, L. J.; Keefer, R. M.   *J. Am. Chem. Soc.* <u>1950</u>, *72(7)*, 3113-6.

4.   Booth, H. S.; Everson, H. E.   *Ind. Eng. Chem.* <u>1948</u>, *40(8)*, 1491-3.

5.   Vaughn, T. H.; Nutting, E. G.   *Ind. Eng. Chem. Anal. Ed.* <u>1942</u>, *14(6)*, 454-6.

6.   Wauchope, R. D.; Getzen, F. W.   *J. Chem. Eng. Data* <u>1972</u>, *17(1)*, 38-41.

7.   Vesala, A.   *Acta Chem. Scand.* <u>1974</u>, *28A(8)*, 839-45.

8.   Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y.   *J. Chem. Eng. Data* <u>1979</u>, *24(1)*, 30-4.

9.   Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C.   *Environ. Sci. Technol.* <u>1980</u>, *14(10)*, 1227-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1950</u>, *72(7)*, 3113-6.
VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^4mol(1)/dm^3$ [b]	$10^6x(1)$ [b]
25.0	7.6	5.17	9.34

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated with 1,4-dichlorobenzene in a sealed Erlenmeyer flask by rotating the flask in a constant temperature bath for 20 hours. Measured volumes of the saturated solution were extracted with measured volumes of n-hexane for analysis. The optical density of the extract was measured against a n-hexane standard at 234 nm using a Beckman spectrophotometer (1).	$C_6H_4Cl_2$: Commercial product (Eastman Kodak Co.), used as received. H_2O: Distilled.

ESTIMATED ERROR:
Solubility: >10% (compiler). Temperature: ±0.2 K (compiler).

REFERENCES:
1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1949</u>, *71(11)*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Klemenc, A.; Low, M. *Recl. Trav. Chim. Pays-Bas* 1930, *49(4)*, 629-40.

VARIABLES:	PREPARED BY:
Temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/kg(2)$ [a]		$10^4 mol(1)/kg$ [b]		$10^6 x(1)$ [b]	
20	6.89		4.687		8.444	
25	7.91		5.380		9.694	
30	9.33		6.346		11.04	
35[c]	10.4	8.30	7.074	5.646	12.75	10.17
40		10.1		6.870		12.38
45		12.2		8.298		14.95

a. Reported (mean values from at least two measurements).
b. Calculated by F. W. Getzen.
c. The system reported not stable at this temperature.

Measurements are shown graphically in Figure 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrations were done over periods from 2 to 17 days (average 7-10 days). Gravimetric analysis was the basis for the concentration determinations. The solute was placed in a spiral tube and weighed. Then, a known amount of water was passed through the tube and it was re-weighed. The weight loss and the mass of the water passed through the tube gave the solubility value directly.	$C_6H_4Cl_2$: Synthesized from benzene and chlorine, recrystallized from abs. ethanol, m.p. 53°C. The purity of the product was checked by elemental analysis. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: >10% (evaluated on the basis of deviations from the averages).
Temperature: ±0.5 K.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]	Klemenc, A.; Löw, M. *Recl. Trav. Chim.*
(2) Water; H_2O; [7732-18-5]	*Pays-Bas* <u>1930</u>, *49(4)*, 629-40.

EXPERIMENTAL VALUES: Continued ...

Figure 1.   Solubility of solid 1,4-dichlorobenzene in water versus
            Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.
VARIABLES: Temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg(2)$ [a]	$10^4 mol(1)/kg$ [b]	$10^5 x(1)$ [b]
22.2	0.778	5.292	0.9535
24.6	0.834	5.673	1.022
25.5	0.869	5.911	1.065
30.0	0.926	6.298	1.135
34.5	1.02	6.938	1.250
38.4	1.21	8.230	1.483
47.5	1.59	10.81	1.949
50.1	1.73	11.77	2.120

a. Reported.
b. Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium was established by allowing the mixtures to stand in glass stoppered flasks, with occasional shaking, for 1-3 week periods at constant temperature. Samples of the saturated aqueous solutions were withdrawn with pipettes through glass-wool plugs and transferred to separatory funnels for weighing. An extraction with cyclohexane was then performed after which the extracts were analyzed spectrophotometrically at 273 nm. The concentrations were established from previously obtained absorbance values of standard reference solutions (which were observed to obey Beer's law).

SOURCE AND PURITY OF MATERIALS:

$C_6H_4Cl_2$: Commercial product (Matheson, Coleman and Bell), recrystallized three times from abs. ethanol, vacuum sublimed twice, UV-spectrum and melting point were determined and were identical to published data.

H_2O: Distilled and deionized water.

ESTIMATED ERROR:

Solubility: ±2.3% (authors).

Temperature: ±0.5 K (authors).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* <u>1972</u>, *17(1)*, 38-41.

EXPERIMENTAL VALUES: Continued ...

Figure 1.   Solubility of solid 1,4-dichlorobenzene in water versus Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
VARIABLES: One temperature	PREPARED BY: H. Lonnberg

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/kg(2)$ [a]	$10^4 mol(1)/kg$ [b]	$10^5 x(1)$ [b]
25.0	8.55	5.816	1.048

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturation of the 1,4-dichlorobenzene in water was established by shaking the mixture in a sealed tube suspended in a thermostat water bath for 1-2 weeks. The sealed tube was allowed to stand for two to three days without shaking before analysis. Samples from the saturated solution were extracted with 2,2,4-trimethylpentene. Then, the optical densities of the liquid extracts were determined spectrophotometrically. The concentration was established from optical density using a previously prepared standard calibration curve.	$C_6H_4Cl_2$: Commercial product (E. Merck AG), recrystallized twice from abs. ethanol. H_2O: Distilled, deionized and degassed.
	ESTIMATED ERROR: Solubility: ±1.5% (author). Temperature: ±0.05 K (author).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* <u>1931</u>, *53(5)*, 1744-51.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/kg(2)$ [a]	$10^4 mol(1)/kg$ [b]	$10^6 x(1)$ [b]
30	7.7	5.24	9.44

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution was prepared by shaking the substances in a thermostat bath for at least 12 hours. An interferometric method was used for the analysis of the saturated solution (1). Samples were withdrawn from several saturation flasks and read against a pure water sample in an interferometer. The concentration was established from a calibration obtained from previous measurements made with a reference solution.	$C_6H_4Cl_2$: Commercial product (Eastman Kodak Co.), recrystallized twice from ethanol, m.p. 52.84°C. H_2O: Distilled water "of good quality".
	ESTIMATED ERROR: Solubility: ±5% (authors). Temperature: ±0.01 K (authors).
	REFERENCES: 1. Gross, P. M. *J. Am. Chem. Soc.* <u>1929</u>, *51(8)*, 2362-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1979, 24(1), 30-4.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [b]
25	8.715	5.9283	1.0713

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions were prepared by adding an excess of solute to water in a closed flask with standing for 24 hours. Then, the sample was allowed to settle at 25°C in a thermostat bath for at least 48 hours before analysis. The solubility was determined by solvent extraction followed by gas chromatographic analysis using a Hewlett Packard Model 5750 apparatus (equipped with a flame ionization detector and a 10 ft stainless steel column packed with 10% SE 30 ultraphase on high performance Chromosorb P, 60/80 mesh).	$C_6H_4Cl_2$: Commercial product (BDH), evidently used as received. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: ±3% (authors, the value is based on the std. error of the least squares fit on the solubility of 1,4-dichlorobenzene in water and aqueous electrolyte solutions.
Temperature: ±0.2 K (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Booth, H. S.; Everson, H. E. *Ind. Eng. Chem.* <u>1948</u>, *40(8)*, 1491-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [b]
25.4	<5	<3.4	<6.1

a. Reported.
b. Calculated by F. W. Getzen.

, AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The composition analysis was based upon a volumetric method described in (1). In this method, further addition of solute to a volume of solution yielded, upon saturation, proportional amounts of undissolved solute residue which could be measured volumetrically. A plot of added solute mass versus volume of residue gave a straight line the intercept of which gave the solubility. Stoppered tubes with capillaries graduated in steps of 0.05 ml were used for the measurements. A known volume of solvent (50 ml) was added to the tube in a constant temperature bath and weighted quantities of the solid solute were added to the liquid. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes, and centrifuged for 5 minutes. Then, the volume of residue was read. The procedures were repeated to ensure that the equilibrium had been reached.	$C_6H_4Cl_2$: Commercial reagents of highest grade, probably used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: Within 0.1 g as reported in Ref. (1). Temperature: ±0.2 K (compiler).
	REFERENCES: 1. Vaughn, T.H.; Nutting, E. G. *Ind. Eng. Chem., Anal. Ed.* <u>1942</u>, *14(6)*, 454-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environm. Sci. Techn.* 1980, *14(10)*, 1227-9.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	7.380	5.02	9.071

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium was performed in sealed stainless steel centrifugre tubes with constant or intermittent shaking. The equilibrium was generally complete within 1 week. The mixture was then centrifugred for 60 minutes after which aliquots of the solution were removed either by pipet or syringe for analysis. Liquid scintillation counting with ^{14}C-labelled solute was employed in the solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.	$C_6H_4Cl_2$: Commercial reagent. the ^{14}C-labeled compound was purchaed by NEN, the nonlabeled one by Aldrich. H_2O: Distilled.

	ESTIMATED ERROR: Solubility: ±6.0% (std. deviation estimated by authors). Temperature: ±0.2 K (equilibration), ±0.3 K (centrifugation).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4-Dichlorophenol; $C_6H_4Cl_2O$; [120-83-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The solubility of 2,4-dichlorophenol in water was determined many decades ago by Mosso (1). While the measurements may be subject to question because of their age and obscurity, the reported melting point strongly indicates that the "m-dichlorophenol" does refer to 1,2-dichlorophenol. Undoubtedly, the experimental procedure was based upon a classical gravimetric analysis. Because of the lack of other data, the value recommended here must be classified as doubtful.

The following solubility value for 2,4-dichlorophenol in water is based solely upon the work reported by Mosso.

T/K	$10^2 mol(1)/dm^3$	$g(1)/kg$	$10^4 x(1)$
293.15	2.7	4.5	4.9

REFERENCES

1. Mosso, U. *Jahresber. Fortschr. Chem.* <u>1887</u>, 1800.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dichlorophenol; $C_6H_4Cl_2O$; [120-83-2] (2) Water; H_2O; [7732-18-5]	Mosso, U. *Jahresber. Fortschr. Chem.* <u>1887</u>, 1800.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/kg(2)$ [a]	$10^2 mol(1)/kg$ [b]	$10^4 x(1)$ [b]
20	4.47–4.66	2.730–2.845	4.938–5.148

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experimental methods were not described.	$C_6H_4Cl_2O$: Synthesized from dry chlorine and phenol, distilled and re-crystallized from benzene, re-ported melting point 43 – 44°C. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2-Difluorobenzene; $C_6H_4F_2$; [367-11-3]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979.

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published in 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was $\pm$ 10 percent. This is a reasonble observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1,2-difluorobenzene in water is tentative:

T/K	10^2mol(1)/dm^3	g(1)/kg	$10^4 x(1)$
298.15	1.0	1.14	1.81

REFERENCES

1. Yalkowsky, S.H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4),* 351-3.

2. Yalkowsky, S.H., Personal Communication, <u>1979</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Difluorobenzene; $C_6H_4F_2$; [367-11-3] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^4 x(1)$ [c]
25	1.141	1.00	1.809

   a. Calculated by F. W. Getzen.
   b. Reported.
   c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1,2-difluorobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. The determination was done in duplicate.	$C_6H_4F_2$: Aldrich commercial grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,3-Difluorobenzene; $C_6H_4F_2$; [372-18-9] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION:

The experimental results consist of a single value at 298.15 K published in 1979 by Yalkowsky et al. (1) of the Upjohn Company, Kalamazoo, Michigan. According to the authors (2), the accuracy of the experimental determinations was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure.

The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1,3-difluorobenzene in water is tentative:

T/K	$10^2\,mol(1)/dm^3$	g(1)/kg	$10^4 x(1)$
298.15	1.0	1.14	1.81

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4),* 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Difluorobenzene; $C_6H_4F_2$; [372-18-9] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^4 x(1)$ [c]
25	1.141	1.00	1.809

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1,3-difluorobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. The determination was done in duplicate.	$C_6H_4F_2$: Aldrich commercial grade, used as received. H_2O: Deionized.

	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,4-Difluorobenzene; $C_6H_4F_2$; [540-36-3]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979.

CRITICAL EVALUATION:

Two experimental measurements have been reported on the solubility of 1,4-difluorobenzene in water (1,2). Jockers (1) has determined the solubility at high temperatures between 533 K and 553 K and high pressures only in connection with studies of the parameters that influence phase separation. The single solubility measurement reported by Yalkowsky et al. (2) cannot be easily compared with the results of Jockers. Both results are included in the table below.

According to the authors (3), the accuracy of the experimental determinations reported by Yalkowsky et al. was ± 10 percent. This is a reasonable observation considering the details available on the experimental procedure. The manufacturer's reagent (Aldrich and Eastman) was neither further purified nor degassed before use. The time required for equilibration was indicated as between 4 and 48 hours. The saturated solutions were assayed spectrophotometrically.

The solubility value was the average of at least two independent determinations according to the investigators. The experimental result was expressed in Briggsian logarithms only with three significant figures.

The objective of the solubility measurements was to extend the correlation technique of aqueous solubilities to a broader group of planar nonelectrolytes by involving the melting points and total molecular surface areas as dependent variables. Using such methods, the authors also showed that branched and cyclic compounds have greater solubilities in water than corresponding linear compounds.

To compare, relate, and correlate the solubility data for liquid halogenated benzenes in water, use was made of the theoretical relationship between the molar solubility and solute molar volumes at 298.15 K as discussed in the Introduction. A data comparison with previously selected solubilities shows that new measurements are urgently required in order to resolve the anomalous trend in the correlated experimental data reported by Yalkowsky et al.

The uncertainty in the single reported solubility value may be as large as 10 percent or even larger. The following solubility value for 1,4-difluorobenzene in water is tentative:

$$P/P_\theta = 1.0$$

T/K	10^2mol(1)/dm^3	g(1)/kg	$10^4x(1)$
298.15	1.07	1.22	1.94

$$P/P_\theta = 80 - 100 \times 10^5$$

T/K	mol(1)/dm^3	10^{-2}g(1)/kg	$10^2x(1)$
533.15-553.15	3.47	3.50	7.84

REFERENCES

1.   Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, 1976.

2.   Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C.   *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

3.   Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Difluorobenzene; $C_6H_4F_2$; [540-36-3] (2) Water; H_2O; [7732-18-5]	Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, 1976, pp 94-5.
VARIABLES: Temperature and pressure	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	P/bar	$10^{-2} g(1)/kg$ [a]	$mol(1)/kg$ [b]	$10^2 x(1)$ [c]
260.0	80	3.501	3.069	7.84
270.0	92	3.501	3.069	7.84
280.0	100	3.501	3.069	7.84

a.   Calculated by compiler.
b.   Calculated by F. W. Getzen.
c.   Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made using a high temperature, high pressure optical cell made from stainless steel with an internal stirrer. Predetermined mixtures of 1,4-difluorobenzene in water were introduced into the cell and homogenized at various temperatures and pressures. The phase transitions were observed through a sapphire window at the appropriate temperatures and pressures. Further details have been included in (1,2).	$C_6H_4F_2$: Fluka AG., Buchs, Schweiz, 99.5% pure, redistilled before use. H_2O: Boiled with $KMnO_4$ and redistilled before use.

ESTIMATED ERROR:

Solubility: ±1%.
Temperature: ±0.5 K.
Pressure: ±2 bar.

REFERENCES:
1.   Götze, G.; Jockers, R.; Schneider, G. M. 4th Inter. Conf. Chem. Thermodyn. IUPAC, Montpellier, Aug. 26-30, 1975, Part IV/9, pp 57-64.

2.   Jockers, R.; Schneider, G. M. *Ber. Bunsenges. Phys. Chem.* 1978, *83*, 576-62.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Difluorobenzene; $C_6H_4F_2$; [540-36-3] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^4 x(1)$ [c]
25	1.221	1.07	1.935

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of 1,4-difluorobenzene in water was agitated at room temperature for a period of about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. The determination was done in duplicate.	$C_6H_4F_2$: Aldrich commercial grade, used as received. H_2O: Deionized.

	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,2-Diiodobenzene; $C_6H_4I_2$; [615-42-9]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,2-diiodobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,2-diiodobenzene in water is reported here as a tentative value:

T/K	10^5mol(1)/dm^3	10^2g(1)/kg	$10^6 x$(1)
298.15	5.8	1.92	1.05

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C.   *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2-Diiodobenzene; $C_6H_4I_2$; [615-42-9] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	1.91	5.8	1.05

a.   Calculated by F. W. Getzen.
b.   Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted, diluted with solvent, and assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_4I_2$: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,3-Diiodobenzene; $C_6H_4I_2$; [626-00-6] (2) Water; H_2O; [7732-18-5]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku. November 1979.

CRITICAL EVALUATION:

A single solubility measurement of 1,3-diiodobenzene in water has been reported by Yalkowsky, Orr, and Valvani (1). The principal motivation for their study was to obtain certain correlations for solubilities of halogenated benzenes in water.

In these measurements, a conventional experimental procedure was employed. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (2), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The solubility of 1,3-diiodobenzene in water is reported here as a tentative value:

T/K	$10^5 mol(1)/dm^3$	$10^3 g(1)/kg$	$10^7 x(1)$
298.15	2.7	8.93	4.87

REFERENCES

1. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

2. Yalkowsky, S. H., Personal Communication, 1979.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Diiodobenzene; $C_6H_4I_2$; [626-00-6] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	8.91	2.7	4.88

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4-48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was extracted, diluted with solvent, and assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_4I_2$: Commercial reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not specified.
	ESTIMATED ERROR: Solubility: ±10% (authors). Temperature: ±1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,4-Diiodobenzene; $C_6H_4I_2$; [624-38-4]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1979.

CRITICAL EVALUATION:

Two experimental values have been reported for the solubility of 1,4-diiodobenzene in water, that determined by Andrews and Keefer (1) and a recent one measured by Yalkowsky, Orr, and Valvani (2). The former study deals with the argentation of substituted benzenes and the latter work presents some useful correlations for the solubilities of halogenated benzenes in water.

The analytical procedure used by Andrews and Keefer is, in principle, quite adequate for the purpose; however, the time for saturation equilibration seems to have been too short and no tests for reaching saturation equilibria were presented (3). Furthermore, the melting point of 360-361 K reported for 1,4-diiodobenzene deviates considerably from reported literature values of 402-403 K (4a,4b). Whether this difference resulted from impurities or from some other cause is difficult t.. establish.

The saturation equilibrium periods for the measurements of Yalkowsky et al. also seem rather short. The time for sample equilibration varied from 4 to 48 hours. The exact time was not reported in single cases. A conventional experimental procedure was employed in their measurements. Commercial reagents were used without further purification. All measurements were done at room temperature (25 ± 1°C). The saturated sample analyses were carried out spectrophotometrically either after dilution or after concentration by extraction with methylene chloride. At least two independent determinations were made. However, the separate measurements were not reported and the precision of the measurements is difficult to estimate. According to the authors in a private communication (5), the error in their solubility measurement may be as great as 10 percent. The estimate seems reasonable for the following reasons. First, the variation of temperature was considerable. Second, the sample equilibration time was sufficiently long to assure an accuracy of ± 5 percent but hardly better. The filtering and extraction procedures may well have produced further errors, so the total 10 percent error seems reasonable. The possible systematic errors should have no effect on the correlations obtained. Therefore, solubilities of comparable accuracy for many purposes may be calculated from the reported solubility correlations.

The value reported by Yalkowsky et al. appears to be more reliable than that of Andrews and Keefer. Therefore, the value of Yalkowsky et al. is reported here as a tentative solubility of 1,4-diiodobenzene in water:

T/K	10^6mol(1)/dm^3	10^3g(1)/kg	$10^7x(1)$
298.15	5.6	1.85	1.01

REFERENCES

1.   Andrews, L. J.; Keefer, R. M.   *J. Am. Chem. Soc.* <u>1950</u>, *72(7)*, 3113-6.

2.   Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C.   *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.

3.   Andrews, L. J.; Keefer, R. M.   *J. Am. Chem. Soc.* <u>1949</u>, *71(11)*, 3644-7.

4.   a.   Paulsen, O.   *Monatsh. Chem.* <u>1939</u>, *72*, 254.

     b.   "Handbook of Tables for Organic Compound Identification", 3rd ed.; Rappoport, Z., Compiler; CRC Press: Cleveland, Ohio, <u>1967</u>; p. 76.

5.   Yalkowsky, S. H., Personal Communication, <u>1979</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Diiodobenzene; $C_6H_4I_2$; [624-38-4] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	1.85	5.6	1.01

a.   Calculated by F. W. Getzen.
b.   Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of solute in water was agitated for a period of 4 - 48 hours (the exact time for equilibration was not reported in single cases) and then filtered. The saturated solution was diluted and assayed spectrophotometrically. At least two independent determinations were carried out.	$C_6H_4I_2$: Commerical reagent (Aldrich or Eastman), used as received. H_2O: Source and purity not reported.

ESTIMATED ERROR:
Solubility: ±10% (authors).

Temperature: ±1 K (authors).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Diiodobenzene; $C_6H_4I_2$; [624-38-4] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^6 mol(1)/dm^3$ [b]	$10^8 x(1)$ [b]
25.0	1.4	4.24	7.67

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation process was done in sealed Erlenmeyer flasks. The time used for the equilibration was 20 hours. Measured volumes of the saturated solution were then extracted using measured volumes of hexane to remove the aromatic compound from the aqueous layer. The solute concentration was measured spectrophotometrically (1).	$C_6H_4I_2$: Commercial product (Eastman Kodak Co.), recrystallized twice from ethanol, reporting melting point 360-361 K. H_2O: Source and purity not specified.

	ESTIMATED ERROR:
	Solubility: >10% (compiler). Temperature: ± 0.2 K.

	REFERENCES:
	1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71(11)*, 3644-7.

COMPONENTS:	EVALUATOR:
(1) Bromobenzene; C_6H_5Br; [108-86-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION:

The solubility of bromobenzene in water has been reported in eight published sets of data (1-6,14,15). The solubility behavior as a function of temperature is illustrated in Figure 1. Some rather serious discrepancies between the various solubility measurements are evident in the figure.

The solubility of water in bromobenzene has been measured by several investigators between 1932 and 1963 and reported in five published sets of data (7-10,14). As shown in Figure 2, which gives the solubility behavior relative to Absolute temperature, the agreement among experimental values is reasonable.

Of the more recent works, that of Nelson and Smit (4) reported the solubility data for temperatures in the range between 278 and 318 K. However, despite the equilibration period of 24 hours (which might not have been long enough), the solubility values obtained are substantially lower than those found by the earlier investigators. It is not possible to establish any shortcomings of their experimental procedure from the very brief description. No information was provided on the source and purity of materials used. Also, it was not indicated whether or not a water stripper had been employed for the analysis of the very dilute aqueous solutions by gas chromatography, or whether or not an internal standard had been used for the calibration of the gas chromatograph which employed a flame ionization detector. However, the authors agreed to re-examine their raw data in order to verify the reported values (13). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.

The reported solubility value of Yalkowsky et al. is too low. This could be due to an insufficient time allowed for saturation equilibrium. According to the authors, the accuracy of the experimental determination was ± 10 percent (11). The remaining reported data, that of Andrews and Keefer (1), Gross and Saylor (2), Hine et al. (3), and Vesala (5,15), have been correlated against Absolute temperature using a normal polynomial equation of second degree. In the regression, twice as much weight was assigned to the data of Vesala as was assigned to the remaining data. The equation below represents the solubility of bromobenzene in water between 283 and 308 K:

$$S_1 (g(1)/kg) = 1.8293 - 1.35675 \times 10^{-2} T$$
$$+ 2.99322 \times 10^{-5} T^2 \qquad [1]$$

The values calculated from equation [1] for the saturation of bromobenzene in water in the range of temperatures between 283 and 313 K together with corresponding molarities and mole fractions are given in Table 1. Also, the solubility values calculated from equation [1] are shown in Figure 1 as a solid line along with the measured values.

The solubility of water in bromobenzene has been reported in the temperature range between 288 and 308 K in five investigations. The original report from Columbia University by Hutchinson and Lyon (8) has been lost, and all details reported here on that work have been taken from a secondary source (12). The single value from Hutchinson and Lyon is too high in relation to other reported determinations at the same temperature so it was not included in the correlation of the data against temperature. On the other hand, the solubility reported by Donahue and Bartell (14) appears too low and this value also was not used in the correlation. The reported values of Bell (7), Jones and Monk (9), and Wing and Johnston (10) are represented by the equation:

$$\log_{10}x(2) = 2.43149 - 1514.54/T \qquad [2]$$

In this equation, $x(2)$ is the mole fraction solubility of water in the water-bromobenzene system and T is the Absolute temperature. The calculated solubility values in the 283 to 308 K range are shown in Figure 2 as a solid line along with the reported values.

The calculated mole fraction values for the solubility of water in bromobenzene from equation [2] are included in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 283 and 313 K.

COMPONENTS:	EVALUATOR:
(1) Bromobenzene; C_6H_5Br; [108-86-1]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION: (Continued)

Table 1. Solubility of Bromobenzene in Water.

T/K	10^3mol(1)/dm^3	10g(1)/kg	$10^5 x(1)$
283.15	2.47	3.87	4.45
288.15	2.58	4.05	4.65
293.15	2.70	4.24	4.87
298.15	2.83	4.45	5.11
303.15	2.96	4.67	5.36
308.15	3.11	4.91	5.63
313.15	3.26	5.16	5.92

Table 2. Solubility of Water in Bromobenzene.

T/K	10^2mol(2)/dm^3	10g(2)/kg	$10^3 x(2)$
283.15	1.16	1.39	1.21
288.15	1.43	1.72	1.50
293.15	1.76	2.12	1.84
298.15	2.13	2.58	2.25
303.15	2.58	3.14	2.73
308.15	3.09	3.78	3.29
313.15	3.69	4.53	3.94

REFERENCES

1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.

2. Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53(5)*, 1744-51.

3. Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* 1963,*85(10)*, 1473-6.

4. Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.

5. Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.

6. Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* 1979, *18(4)*, 351-3.

7. Bell, R. P. *J. Chem. Soc.* 1932, *Part II*, 2905-11.

8. Hutchinson, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, 1943.

9. Jones, J. R.; Monk, C. B. *J. Chem. Soc.* 1963, *Part III*, 2633-5.

10. Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.

11. Yalkowsky, S. H., Personal Communication, 1979.

12. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M.; Urey, H. C.; Kirshenbaum, I., Eds.; McGraw-Hill: New York, 1955; Part II, Chapter 7, pp 129-44.

COMPONENTS:	EVALUATOR:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

13. Nelson, H. D., Personal Communication, 1979.

14. Donahue, D. J.; Bartell, F. E. *J. Phys. Chem.* 1952, *56(4)*, 480-4.

15. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

COMPONENTS:	EVALUATOR:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION: (Continued)
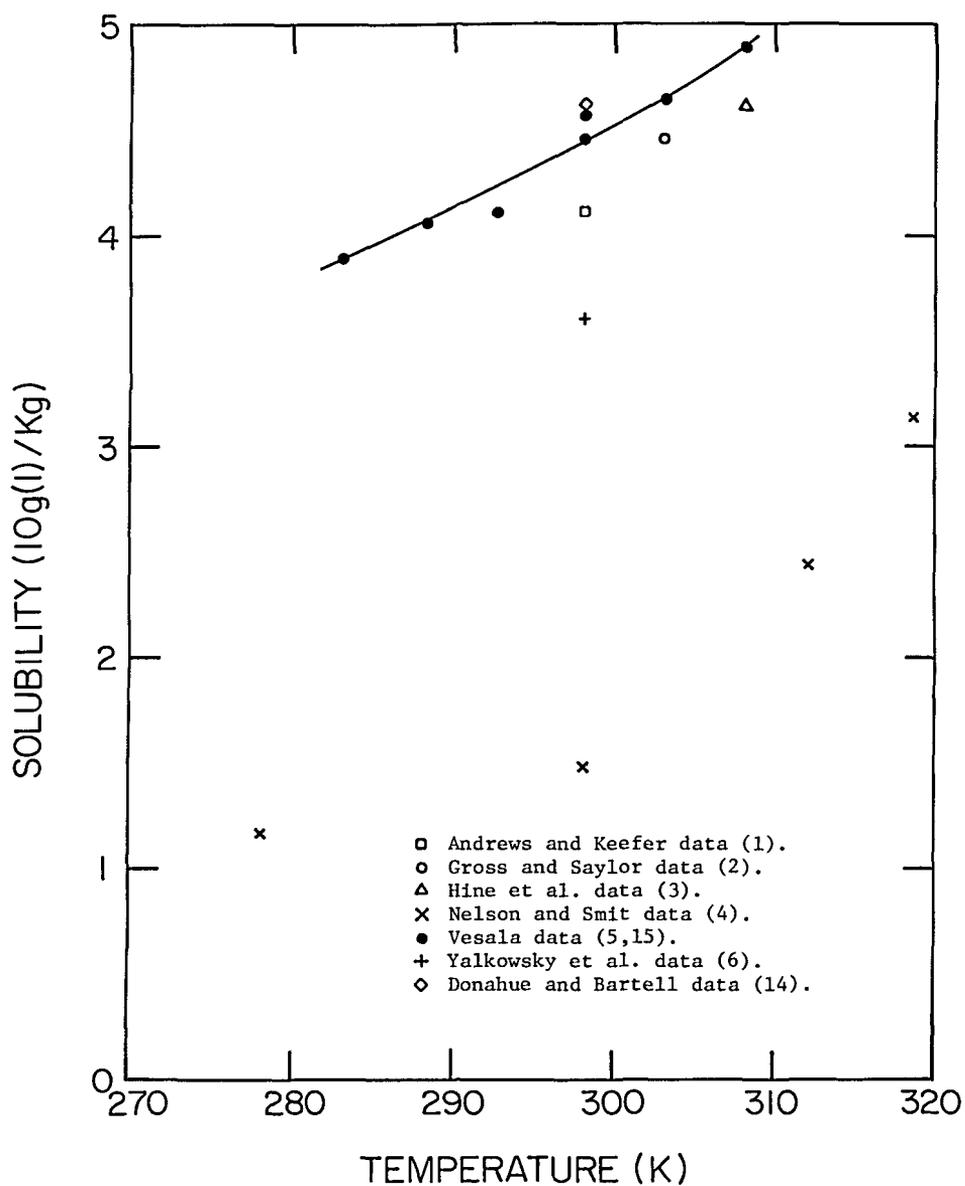
Figure 1.   Solubility of bromobenzene in water versus Absolute
temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Bromobenzene; C_6H_5Br; [108-86-1]	May 1979.

CRITICAL EVALUATION: (Continued)

Figure 2.   Logarithm of mole fraction solubility of water in
            bromobenzene versus reciprocal of Absolute temperature,
            reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* <u>1931</u>, *53(5)*, 1744-51.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
30	4.46	2.839	5.117

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of bromobenzene in 500 g water was shaken for 12 hrs. in a thermostat bath. Samples were then withdrawn and read against water in an interferometer made by Zeiss (1). A detailed description of the complete procedure is given in a Ph.D. dissertation (2).	C_6H_5Br: Eastman Kodak Co., was purified by fractional distillation before use. H_2O: Distilled.

	ESTIMATED ERROR: Solubility: ± 2%. Temperature: ± 0.02 K.

REFERENCES:

1. Gross, P. M. *J. Am. Chem. Soc.* <u>1929</u>, *51(8)*, 2362-6.

2. Saylor, J. H., Ph.D. Dissertation, Duke University, Durham, <u>1930</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Bromobenzene; C_6H_5Br; [108-86-1]	Bell, R. P. *J. Chem. Soc.* <u>1932</u>, Part II, 2905-11.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t°C	$10g(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
15	2.49	1.382	1.443
20	3.06	1.698	1.781
25	3.74	2.075	2.186

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 1 to 5 ratio solute/solvent mixtures were rotated in a thermostat bath for 12 hrs. After equilibrium was established, samples were taken and filtered through cottonwool. The determination of the water content was based on the reaction with α-naphthoxydichlorophosphine. The evolved HCl was absorbed in water and titrated with NaOH solution (1). Successive (2-4) determinations were carried out with the solvent.	H_2O: Distilled (compiler). C_6H_5Br: Merck reagent, analytical grade, redistilled before use.

ESTIMATED ERROR:
Solubility: ±2.6%. Temperature: ±0.02 K.

REFERENCES:
1. Bell, R. P. *J. Chem. Soc.* <u>1932</u>, Part II, 2903-5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Bromobenzene; C_6H_5Br; [108-86-1]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, <u>1943</u>.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [c]
25	3.009	1.67	2.616

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 1 to 15 volume ratio of solute to solvent was placed in an equilibration flask and then lowered into a thermostat water bath. The assembly was shaken mechanically for about 90 min. at constant temperature. The amount of water in the organic phase was determined by a modified Karl Fisher titration. The determination was done in triplicate. The description of the procedure was taken from a secondary source (1). The original report is no longer available.	H_2O: Distilled. C_6H_5Br: Source is not known, purified and dried before use.
	ESTIMATED ERROR: Solubility: ± 1%. Temperature: ± 0.05 K.
	REFERENCES: 1. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M.; Urey, H. C.; Kirshenbaum, I., Eds.; McGraw-Hill: New York, <u>1955</u>; Part II, Chapter 7, pp 129-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [c]
25.0	4.1	2.61	4.72

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a constant temperature bath, water was mixed with bromobenzene through rotation in a glass-stoppered Erlenmeyer flask for 30 hrs. The saturated solution was extracted with n-hexane. The optical density of the extract was measured against a n-hexane blank using a Beckman spectrophotometer (1).	C_6H_5Br: Eastman Kodak Co., commercial reagent, b.p. 156.3°C, fractionated before use. H_2O: Not specified.

ESTIMATED ERROR:

Solubility: ± 10% (compiler).

Temperature: ± 0.1 K (compiler).

REFERENCES:

1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* 1949, *71*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Donahue, D. J.; Bartell, F. E. *J. Phys. Chem.* <u>1952</u>, *56(4)*, 480-4.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)$/kg [a]	$10^3mol(1)$/kg [b]	$10^5x(1)$ [c]
25	4.62	2.94	5.3

t/°C	$10g(2)$/kg [a]	$10^2mol(2)$/kg [b]	$10^3x(2)$ [c]
25	3.34	1.85	2.9

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of water and bromobenzene was placed in a glass stoppered flask and shaken intermittently for at least three days in a constant temperature water bath. The water content of the organic phase was established by the Karl Fisher method and the organic content of the aqueous phase was established interferometrically.	C_6H_5Br: Reagent grade, purified by fractional distillation. H_2O: Purified by distillation.

	ESTIMATED ERROR: Solubility: ± 5% (compiler). Temperature: ± 0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Bromobenzene; C_6H_5Br; [108-86-1]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* <u>1957</u>, *79(4)*, 864-5.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10ml(1)/dm^3$ [a]	$10^2mol(1)/dm^3$ [b]	$10^3x(1)$ [c]
25.0	4.24	2.347	2.470

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was equilibrated with 20 ml bromobenzene by stirring in a flask in a constant temperature water bath for two hrs. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. The tritium activities for the tritiated water samples were determined by the acetylene method (1,2). At least four independent experiments were done. The article describes work reported in a Ph.D. dissertation (2).	H_2O: Tracerlab, Inc., tritiated water, used as received. C_6H_5Br: Source not specified, chemical grade, redistilled before use.

ESTIMATED ERROR:

Solubility: ± 2.3%.

Temperature: ± 0.02 K.

REFERENCES:

1. Wing, J.; Johnston, W. H. *Science* <u>1955</u>, *121*, 674-5.
2. Wing, J., Ph.D. Dissertation, Purdue University, Lafayette, IN, <u>1956</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Hine, J.; Haworth, H. W.; Ramsay, O. B. *J. Am. Chem. Soc.* <u>1963</u>, *85(10)*, 1473-6.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
35.0	4.585	2.92	5.294

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of bromobenzene was combined with 4 ml of water in an ampoule and sealed. The sealed ampoule was then rotated in a water bath for a week. The bromobenzene solubility was determined by ultraviolet spectrophotometric measurements using a Beckman DU spectrophotometer.	C_6H_5Br: Eastman Kodak Co., redistilled before use. H_2O: Not specified.
	ESTIMATED ERROR: Solubility: ±2% S.D. Temperature: ±0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Bromobenzene; C_6H_5Br; [108-86-1]	Jones, J. R.; Monk, C. B. *J. Chem. Soc.* <u>1963</u>, Part III, 2633-5.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^4 dm^3(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	4.1	2.27	2.39
30	4.7	2.60	2.75
35	5.3	2.92	3.10

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was shaken with bromobenzene in 1:10 volume ratios for 4 hours in a flask in a water thermostat bath. The water content was determined by tritium assay. The count rates were determined using a typical liquid scintillator solution technique.	H_2O: Tritiated. C_6H_5Br: Source not known, laboratory grade, dried over $CaCl_2$ and fractionally distilled before use.
	ESTIMATED ERROR: Solubility: ±5%. Temperature: ±0.5 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
10.0	3.8957	2.482 ± 0.008	4.4714
15.2	4.0605	2.587 ± 0.020	4.6605
19.6	4.1107	2.619 ± 0.020	4.7182
25.0	4.5719	2.913 ± 0.033	5.2478
30.0	4.6456	2.960 ± 0.040	5.3325
35.0	4.8919	3.117 ± 0.040	5.6153

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The bromobenzene was mixed with water in a sealed flask (1) with the aid of a magnetic stirrer for 48 hours in a water bath at constant temperature. After the solution was filtered through a glass-wool plug, the solute was extracted with 2,2,4-trimethyl-pentene. The optical density of each sample was determined spectrophotometrically (2). Mean and standard deviations were calculated from three measurements.	C_6H_5Br: Merck AG., >99% GLC, used as received. H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±1.35%. Temperature: ±0.05 K.

REFERENCES:
1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* 1963, Part III, 2716-23. 2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Vesala, A. *Acta Chem. Scand.* <u>1974</u>, *28A(8)*, 839-45.
VARIABLES: One temperature	**PREPARED BY:** A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^3 mol(1)/kg(2)$ [a]	$10 g(1)/kg$ [b]	$10^5 x(1)$ [c]
25	2.84	4.457	5.116

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established between the water and the bromobenzene in a sealed flask (1) with the aid of a magnetic stirrer during 48 hours under isothermal conditions. After the sample was filtered through a glass-wool plug, the bromobenzene was extracted with 2,2,4-trimethylpentene. Sample optical densities were determined spectrophotometrically (2). Five parallel determinations were done. The reported work was based upon a Ph.D. dissertation (3).	C_6H_5Br: Commercial reagent of analytical grade distilled through a column resulting in a more than 99% pure sample. H_2O: Distilled, deionized, and degassed.

	ESTIMATED ERROR: Solubility: ±1.1%. Temperature: ±0.05 K.
	REFERENCES: 1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* <u>1963</u>, Part III, 2716-23. 2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* <u>1972</u>, *17(1)*, 38-41. 3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, <u>1973</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^4 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
5	1.168	7.438	1.34
25	1.48	9.44	1.7
39	2.44	15.5	2.8
45.5	3.14	20.0	3.6

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated through the vapor phase with bromobenzene in a special flask (1) using a shaker in a thermostat bath for 24 hours. A gas chromatographic analysis of the samples was done by injection into a 5% Apiezon M stainless steel column with Celite as the supporter. The column length was 1.5 m and the temp. was 120°C. The chromatograph was equipped with a flame ionization detector. Three samples were analyzed from each flask.	C_6H_5Br: Not specified. H_2O: Not specified.

	ESTIMATED ERROR:
	Solubility: ±14.9% (compiler). Temperature: ±0.1 K (compiler).

	REFERENCES:
	1. Nelson, H. D.; de Ligny, C. L. *Rec. Trav. Chim.* 1968, *87*, 528-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Bromobenzene; C_6H_5Br; [108-86-1] (2) Water; H_2O; [7732-18-5]	Yalkowsky, S. H.; Orr, R. J.; Valvani, S. C. *Ind. Eng. Chem. Fundam.* <u>1979</u>, *18(4)*, 351-3.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [a]
25	3.596	2.29	4.139

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Samples of excess bromobenzene in water were agitated at room temperature for about 24 hours and then filtered. The filtrate was diluted and assayed spectrophotometrically. Determinations were carried out in duplicate.	C_6H_5Br: Aldrich commercial grade, used as received. H_2O: Deionized.
	ESTIMATED ERROR: Solubility: ±10%. Temperature: ±1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water-d_2; D_2O; [7789-20-0] (2) Bromobenzene; C_6H_5Br; [108-86-1]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, <u>1943</u>.
VARIABLES: One temperature	PREPARED BY: G. Jancso

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [a]
25.0	2.8261	1.411	2.2113

a. Calculated by F. W. Getzen.
b. Reported (average of two experimental values).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Between 25 and 100 ml bromobenzene and 1 to 2 ml D_2O were placed in a flask and shaken for about 90 min. The thermostat water bath temperature was maintained within ±0.05°C. Then, a sample was removed and the amount of D_2O dissolved was determined by a modified Karl Fischer titration (1). The original report was unavailable; however, the method and the results were described in sufficient detail in (1). The solubility of H_2O in bromobenzene was also determined and found to be 0.0167 mol(1)/kg. The average deviation for two experiments was ±0.0001 mol(1)/kg.	C_6H_5Br: Carefully purified and dried before use. Source and method not given. 100% D_2O: Source not specified.

	ESTIMATED ERROR:
	Solubility: ±1 x 10^{-6} mol (std. dev.) D_2O/100 g solution. Temperature: ±0.05 K.

REFERENCES:
1. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M.; Urey, H. C.; Kirshenbaum, I., Eds.; McGraw-Hill: New York, <u>1955</u>; Part II, Chapter 7, pp 129-44.

COMPONENTS:	EVALUATOR:
(1) 4-Bromophenol; C_6H_5BrO; [106-41-2]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The only two available reported measurements of the solubility of 4-bromophenol in water were published many years apart and the information concerning the methods of analysis provided in the earlier of these works is incomplete. The older one by Werner (1) appeared in 1884 and the other more recent work was published in 1971. Therefore, certain difficulties have been encountered in the evaluation of these combined data. The solubility measurements reported by Parsons, Rochester, and Wood (2) for 4-bromophenol in water appear quite reliable when the saturation equilibrium, the method of analysis, and the reported standard deviation have been considered. On the basis of these criteria, the value reported by Werner should be rejected. However, if one can accept a satisfactory state of purity for the synthesized material, the value of Werner, which refers to a temperature of 288 K, can be regarded as fairly good. Considering the difference in the temperatures of the reported solubility values, the agreement between the two values is quite satisfactory in spite of the long time interval between their determinations. However, the solubility value reported by Parsons et al. must be considered as only a tentative value.

It should be noted that the solubility of 4-bromophenol in water is considerably dependent upon the acidity of the solution. Here, it is assumed that the solubility established refers to that of a solution having a pH value prevailing for saturated 4-bromophenol in water. An entire series of measurements of solubilities at various pH values is required to complete the picture of the solubility behavior for protolyzing compounds such as 4-bromophenol in water.

The solubility of 4-bromophenol in water is reported here as a tentative value:

T/K	$10\,\text{mol}(1)/\text{dm}^3$	$10^{-1}g(1)/\text{kg}$	$10^3 x(1)$
298.15	1.07	1.86	1.97

REFERENCES

1.   Werner, E. *Ann. Chim. Phys. Series 6(III)* 1884, 567-74.

2.   Parsons, G. H.; Rochester, C. H.; Wood, C.E.C. *J. Chem. Soc. B* 1971, 533-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Bromophenol; C_6H_5BrO; [106-41-2] (2) Water; H_2O; [7732-18-5]	Werner, E. *Ann. Chim. Phys. Series 6(III)* <u>1884</u>, 567-74.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [b]
15	1.42	8.207	1.499

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Information about the saturation process was incomplete. The analysis of the saturated solution was done using titrimetry with bromine.	C_6H_5BrO: Synthesized product, melting point 64°C, boiling point 137°C at 28 mm Hg pressure. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Bromophenol; C_6H_5BrO; [106-41-2] (2) Water; H_2O; [7732-18-5]	Parsons, G. H.; Rochester, C. H.; Wood, C. E. C. *J. Chem. Soc. B* <u>1971</u>, 533-6.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/kg$ [a]	$10mol(1)/kg(2)$ [b]	$10^3x(1)$ [a]
25	1.8261	1.075	1.9330

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experimental procedure was probably similar to that reported in (1). Excess solid was shaken with water at 25 ± 0.1°C for 24 hours. The saturated solution was then filtered at thermostat temperature and, with appropriate dilution, analyzed spectrophotometrically. Linear calibration graphs of absorbance at a wave length of maximum absorbance of the neutral phenols against concentration confirmed the applicability of the Beer-Lambert law for the analyses.	C_6H_5BrO: Commercial product (manufacturer not reported), recrystallized to a constant melting point. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: ±2% (standard deviation of the average value from five determinations as reported by the authors).

REFERENCES:
1. Parsons, G. H.; Rochester, C. H.; Rostron, A.; Sykes, P. C. *J. Chem. Soc. Perkin Trans. II(1)* <u>1972</u>, 136-8.

COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION:

Thirteen experimental determinations of the solubility of chlorobenzene in water between 278 and 363 K have been reported in the literature (1-10,23-25), see Figure 1. The solubility at higher temperatures, between 513 and 533 K, have been reported also by Vorozhtsov and Kobelev (11) in graphical form only without further details concerning the source of the original measurements.

The solubility of water in chlorobenzene has been reported in eleven published works (5,9,12-20) in the temperature range between 288 and 322 K, see Figure 2.

Some of the more recent data for the solubility of chlorobenzene in water is that of Nelson and Smit (8) in the temperature range between 278 and 318 K. However, despite equilibrium periods of 24 hours (which might not have been long enough), the measured solubilities are substantially lower than those found by earlier investigators. It is not possible to establish any shortcomings of the experimental procedures from the very brief description. No information was provided on the source and purity of materials used. Also, it was not indicated whether or not a water stripper had been employed for the analysis of the very dilute aqueous solutions by gas chromatography, or whether or not an internal standard had been used for the calibration of the gas chromatograph which employed a flame ionization detector. However, the authors agreed to re-examine their raw data in order to verify the reported values (21). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.

The reported solubilities of Othmer et al. (9) and those of Newman et al (23) are too high in relation to the other reported solubility data. Consequently, these values have not been included in the correlation procedure. The approximate value given by Booth and Everson (3) has been excluded also from further consideration. The solubility data at high temperatures by Vorozhtsov and Kobelev (11) could not be correlated with the other data given. These remaining data given in (1,2,4-7,10,24,25) were correlated with Absolute temperature using polynomial equations of various degrees. The equation given below represents the solubility of chlorobenzene in water between 283 and 363 K within an estimated 10 percent. Equal weight was given to each of the data points in the regression procedure for the following equation:

$$S_1(g(1)/kg) = 11.3351 - 3.0290 \times 10^{-2} T$$
$$- 1.8716 \times 10^{-4} T^2 + 0.559466 \times 10^{-6} T^3 \quad [1]$$

The significance of this equation is that the curve representing the solubility data passes through a minimum at 286.1 K. This behavior is consistent with the theory discussed by Gill et al. (27) for the solubility of aromatic compounds in water.

Recommended solubility values between 283 and 363 K have been calculated from equation [1] and presented in Table 1. The solubility behavior described by equation [1] is shown also in Figure 1 which contains the reported experimental values for the solubility of chlorobenzene in water.

The solubility of water in chlorobenzene has also been investigated and reported by a number of workers (9,13,17,18,19,20,26) in the 298 to 318 K temperature range. In general, these solubility values show some irregularity, but those showing reasonable agreement can be correlated with respect to Absolute temperature. The reported solubilities of Zielinski (20) and of Othmer et al. (9) are too high while those of Jones and Monk (17) are too low. Consequently, these data are not considered further. Also, the solubility expressed as a distribution coefficient by an equation only (26) cannot be included in the correlation. The good agreement of the values at 298.15 K reported in (13,18,19) are heavily weighed in the correlation. The remaining data were all assigned equal weight to produce the following equation:

$$\log_{10} x(2) = 2.99105 - 1668.56/T \quad [2]$$

In this equation, $x(2)$ is the mole fraction solubility of water in the chlorobenzene-water system and T is the Absolute temperature. The calculated solubility values in the 273 to 333 K range are shown in Figure 2 along with the reported values.

COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)

The calculated mole fraction values for the solubility of water in chlorobenzene from equation [2] are given in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 283 and 333 K.

The azeotrope temperature (363.35 K) and composition (284 g(2)/kg) at 1.0133×10^5 Pa pressure were also reported (22).

Table 1. Solubility of Chlorobenzene in Water.

T/K	10^3mol(1)/dm^3	10g(1)/kg	$10^5 x(1)$
283.15	4.03	4.54	7.27
288.15	4.02	4.52	7.24
293.15	4.13	4.66	7.46
298.15	4.38	4.95	7.92
303.15	4.77	5.39	8.63
308.15	5.30	6.00	9.60
313.15	5.97	6.77	10.84
318.15	6.78	7.71	12.34
323.15	7.74	8.82	14.13
328.15	8.85	10.11	16.20
333.15	10.12	11.58	18.56
338.15	11.53	13.24	21.22
343.15	13.11	15.09	24.18
348.15	14.84	17.13	27.46
353.15	16.73	19.37	31.06
363.15	20.98	24.47	39.24

Table 2. Solubility of Water in Chlorobenzene;

T/K	10^2mol(2)/dm^3	10g(2)/kg	$10^3 x(2)$
283.15	1.24	2.01	1.25
288.15	1.57	2.54	1.59
293.15	1.96	3.19	1.99
298.15	2.43	3.98	2.48
303.15	2.99	4.92	3.07
308.15	3.66	6.05	3.77
313.15	4.44	7.39	4.60
318.15	5.36	8.97	5.58
323.15	6.43	10.82	6.72
328.15	7.67	12.99	8.06
333.15	9.10	15.50	9.61

COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983.

CRITICAL EVALUATION: (Continued)

REFERENCES

1.   Andrews, L. J.; Keefer, R. M.   *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.

2.   Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y.   *J. Chem. Eng. Data* 1979, *24(1)*, 30-4.

3.   Booth, H. S.; Everson, H. E.   *Ind. Eng. Chem.* 1948, *40(8)*, 1491-3.

4.   Chey, W.; Calder, G. V.   *J. Chem. Eng. Data* 1972, *17(2)*, 199-200.

5.   Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p 134.

6.   Gross, P. M.; Saylor, J. H.   *J. Am. Chem. Soc.* 1931, *53(5)*, 1744-51.

7.   Kisarov, V. M.   *Zh. Prikl. Khim.* 1962, *35(10)*, 2347-9.

8.   Nelson, H. D.; Smith, J. H.   *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.

9.   Othmer, D. F.; White, R. C.; Truegar, E.   *Ind. Eng. Chem.* 1941, *33(12)*, 1513.

10. Vesala, A.   *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.

11. Vorozhtsov, N. N.; Kobelev, V. A.   *Zh. Obs. Khim.* 1938, *8(12)*, 1106-19.

12. Bell, R. P.   *J. Chem. Soc.* 1932, *Part II*, 2905-11.

13. Filippov, T. S.; Furman, A. A.   *Zh. Prikl. Khim.* 1952, *25*, 895-7.

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16. Hutchinson, C. A.; Lyon, A. M.   Columbia University Report A-745, July 1, 1943.

17. Jones, J. R.; Monk, C. B.   *J. Chem. Soc.* 1963, *Part III*, 2633-5.

18. Kirchnerova, J.; Cave, G.C.B.   *Can. J. Chem.* 1976, *54(24)*, 3909-16.

19. Wing, J.; Johnston, W. H.   *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.

20. Zielinski, A. Z.   *Chem. Stosowana* 1959, *3*, 377-84.

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23. Newman, M.; Hayworth, C. B.; Treybal, R. E.   *Ind. Eng. Chem.* 1949, *41(9)*, 2039-43.

24. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

25. Schwarz, F. P.; Miller, J.   *Anal. Chem.* 1980, *52(13)*, 2162-4.

26. Prosyanov, N. N.; Shalygin, V. A.; Zel'venskii, Ya. D. *Tr. Mosk. Khim. Tekhnol. Inst.* 1974, *81*, 55-6.

27. Gill, S. J.; Nichols, N. F.; Wadso, I.   *J. Chem. Thermodyn.* 1976, *8(5)*, 445-52.

COMPONENTS:	EVALUATOR:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. January 1983.

CRITICAL EVALUATION: (Continued)
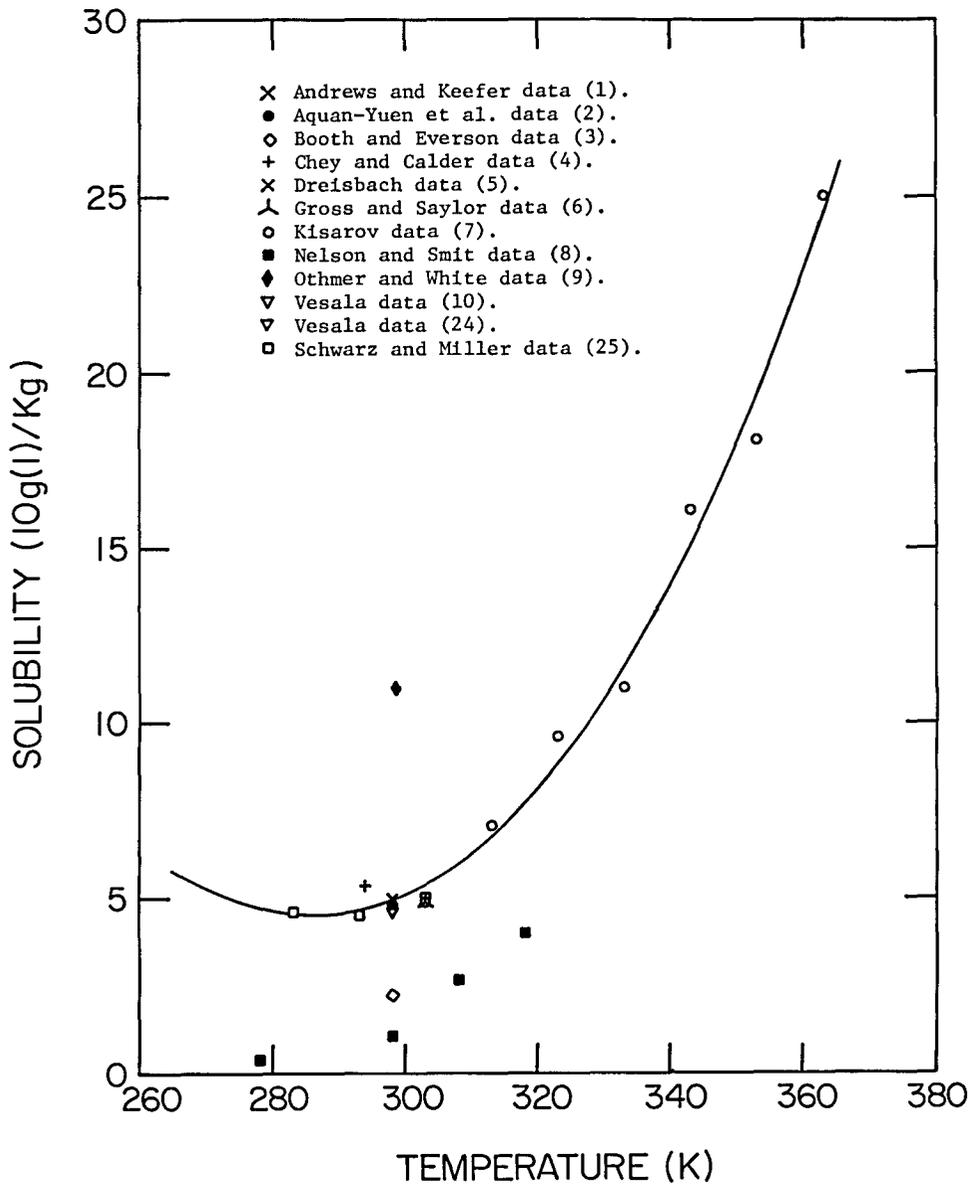
Figure 1.   Solubility of chlorobenzene in water versus Absolute
temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION: (Continued)
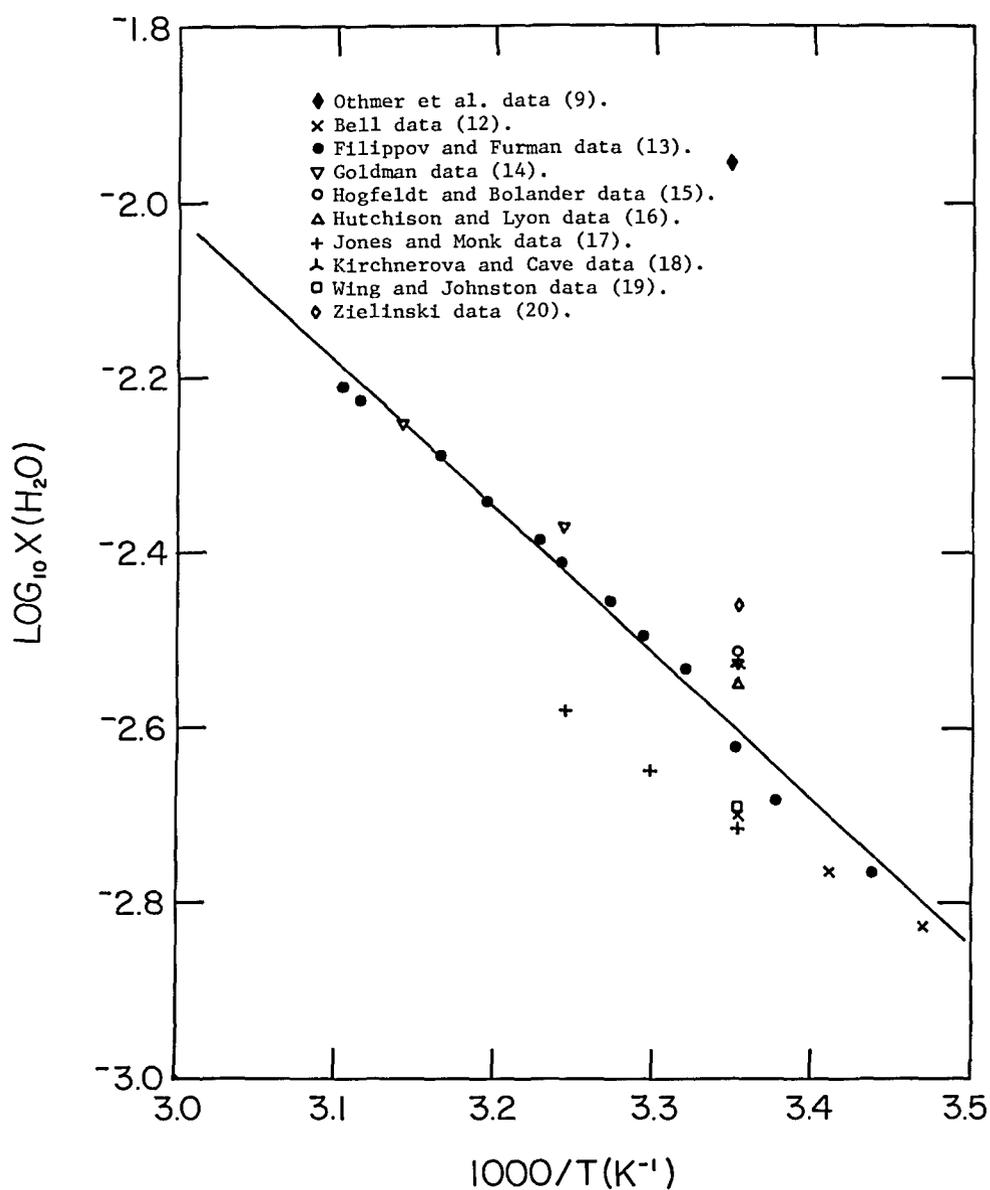
Figure 2.   Logarithm of mole fraction solubility of water in chlorobenzene versus reciprocal of Absolute temperature, reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* <u>1931</u>, *53(10)*, 1744-51.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
30	4.88	4.333	7.810

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of chlorobenzene in 500 g water was shaken for 12 hours in a thermostat bath. Samples were then withdrawn and read against water as a reference using an interferometer made by Zeiss (1). A detailed description of the complete procedure has been described in a Ph.D. dissertation (2).	C_6H_5Cl: Eastman Kodak Co., was purified by fractional distillation before use. H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±1.0%.

Temperature: ±0.02 K.

REFERENCES:

1. Gross, P. M. *J. Am. Chem. Soc.* <u>1929</u>, *51(8)*. 2362-6.

2. Saylor, J. H., Ph.D. Thesis, Duke University, Durham, <u>1930</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Bell, R. P. *J. Chem. Soc.* <u>1932</u>, Part II, 2905-11.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
15	2.64	1.471	1.488
20	3.05	1.691	1.719
25	3.54	1.953	1.995

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixtures of solute and solvent in about 1 to 5 ratios were rotated in a thermostat bath for 12 hours. After equilibrium was attained, samples were withdrawn and filtered through cotton-wool. The determination of the water content was based upon the reaction of water with α-naphthoxy-dichlorophosphine. The evolved HCl was absorbed in water and titrated with standard NaOH solution (1). From 2-4 successive determinations were made with the solvent.	H_2O: Distilled (compiler). C_6H_5Cl: Merck reagent, analytical grade, redistilled before use.
	ESTIMATED ERROR: Solubility: ±1.6%. Temperature: ±0.02 K.
	REFERENCES: 1. Bell, R. P. *J. Chem. Soc.* <u>1932</u>, Part II, 2903-5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Vorozhtsov, N. N.; Kobelev, V. A. *Zh. Obs. Khim.* <u>1938</u>, *8(12)*, 1106-19.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/kg$ [a]	$10 mol(1)/kg$ [b]	$10^3 x(1)$ [c]
240	5.8	5.15	9.76
250	6.2	5.51	10.5
260	6.8	6.04	11.5

a. Values obtained from graph plot (Fig. 4).
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Not specified.	Not specified.

ESTIMATED ERROR:
Solubility: ±10% (compiler).
Temperature: ±1 K (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Othmer, D. F.; White, R. E.; Trueger, E. *Ind. Eng. Chem.* <u>1941</u>, *33(12)*, 1513.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	g(1)/kg	10^3mol(1)/kg	$10^4x(1)$
25.5	1.1	9.77	1.76

t/°C	g(2)/kg	10^2mol(2)/kg	$10^2x(2)$
25.5	1.8	9.99	1.11

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measurements were made using about 15 ml water in a 125 ml Erlenmeyer flask (1). The solute was added to the water from a buret and the flask was agitated until the solution became turbid. The amounts of reagent added were converted from volume to mass using the known densities of the pure components.	C_6H_5Cl: Source not specified. Purified until it distilled within 1 or 2°C range. H_2O: Distilled.

	ESTIMATED ERROR:
	  Solubility: ±10% (compiler).
	
	  Temperature: ±0.5 K.

	REFERENCES:
	  1. Othmer, D. F.; White, R. E.; Trueger, E.
	     Ind. Eng. Chem. <u>1941</u>, *33(10)*, 1240-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene: C_6H_5Cl; [108-90-7]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, <u>1943</u>.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [c]
25	4.504	2.50	2.807

    a. Calculated by F. W. Getzen.
    b. Reported.
    c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixtures of 1 to 15 volume ratios of solute to solvent were introduced into an equili-bration flask and placed in a water ther-mostat bath. The assembly was shaken mechanically for about 90 minutes at con-stant temperature. The amount of water in the organic phase was determined by a modi-fied Karl Fischer titration. The determi-nations were done in triplicate. The ex-perimental procedure was taken from a secondary source (1). The original re-port is no longer available.	H_2O: Distilled. C_6H_5Cl: Source is not known, purified and dried before use.

SOURCE AND PURITY OF MATERIALS:

H_2O: Distilled.

C_6H_5Cl: Source is not known, purified
          and dried before use.

ESTIMATED ERROR:
  Solubility: ±1%.

  Temperature: ±0.05 K.

REFERENCES:
1. Eidinoff, M. L. In "Production of Heavy
    Water", National Nuclear Energy Series
    Division III-Vol. 4F, Murphy, G. M.,
    Urey, H. C., Kirshenbaum, I., Eds.;
    McGraw-Hill: New York, <u>1955</u>; Part II,
    Chapter 7, pp 129-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Booth, H. S.; Everson, H. E. *Ind. Eng.* *Chem.* <u>1948</u>, *40(8)*, 1491-3.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10ml(1)/dm^3(2)$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [c]
25.0	< 2	< 2.0	< 3.6

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made with samples contained in a stoppered Goetz tube placed in a constant temperature water bath. E-quilibrium was assured through repeated shaking and centrifuging the mixture in the stoppered tube while it was temporarily removed from the water bath. The amount of solute dissolved was determined as the difference between total amount added and amount remaining in excess upon saturation. The determination of the excess amount of solute added has been described by Hanslick (1).	C_6H_5Cl: Commercial reagent, C.P. grade, used as received. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: <100%. Temperature: ±1 K (compiler).
	REFERENCES: 1. Hanslick, R. S., Ph.D. Dissertation, Columbia University, New York, <u>1935</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Newman, M.; Hayworth, C. B.; Treybal, R. E. *Ind. Eng. Chem.* <u>1949</u>, *41(9)*, 2039-43.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^4 x(1)$ [c]
25	4.0	3.55	6.42

$t/°C$	$10g(1)/kg$ [d]	$10^3 mol(1)/kg$ [d]	$10^5 x(1)$ [d]
25	4.0	3.55	6.40

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.
d. Calculated for 0.1x reported value by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium between the solute and solvent was established in a constant temperature bath with sufficient agitation. The composition analysis was by standard procedures (1) with specific gravity as the basis of analysis.	C_6H_5Cl: Not specified. H_2O: Not specified.

ESTIMATED ERROR:
Solubility: Too large by a factor of 10 (compiler).   Temperature: ±0.3 K (compiler).

REFERENCES:
1. Smith, J. C. *Ind. Eng. Chem.* <u>1942</u>, *34(2)*, 234-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1950</u>, *72(9)*, 3113-6.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25.0	5.0	4.44	8.03

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated with chlorobenzene in a glass stoppered Erlenmeyer flask by rotating the flask in a constant temperature bath for 20 hours. The saturated solution was extracted with n-hexane for analysis. The optical density of the extract was measured against a n-hexane standard using a Beckman spectrophotometer (1).	C_6H_5Cl: Eastman Kodak Co., commercial reagent, b.p. 131.9-132°C, fractionated before use. H_2O: Not specified.

	ESTIMATED ERROR:
	Solubility: ±10% (compiler). Temperature: ±0.1 K (compiler).

	REFERENCES:
	1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1949</u>, *71(11)*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Filippov, T. S.; Furman, A. A. *Zh. Prikl. Khim.* 1952, *25*, 895-7.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [c]
17.7	2.75	1.526	1.716
22.9	3.33	1.848	2.077
25.2	3.82	2.120	2.382
28.0	4.70	2.609	2.929
30.4	5.12	2.842	3.190
32.4	5.60	3.108	3.489
35.3	6.21	3.447	3.867
36.6	6.60	3.663	4.109
39.8	7.31	4.058	4.550
42.7	8.25	4.579	5.132
47.9	9.55	5.301	5.937
49.0	9.90	5.495	6.153

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measured amounts of water and chlorobenzene were introduced into a tared ampoule which was then sealed. The ampoule was constantly shaken in a thermostat at a series of regulated temperatures until it appeared cloudy. Variations in temperature for clouding and clearing conditions were not more than 0.2-0.3°C. This procedure for solubility measurements has been referred to as the cloud point method by Alexejew (1).	H_2O: Double distilled. C_6H_5Cl: Source not known, distilled three times over freshly calcined calcium oxide.

	ESTIMATED ERROR:
	Solubility: ±5% (compiler). Temperature: ±0.1 K (compiler).

	REFERENCES:
	1. Alexejew, Wladimir *Ann. d. Phys. u. Chem.* 1886, *28*, 305-38.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenezene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p 134.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^3mol(1)/kg$ [b]	$10^5x(1)$ [c]
25	5.0	4.44	8.00

$t/°C$	$10^{-1}g(2)/kg(1)$ [a]	$mol(2)/kg$ [b]	$10x(2)$ [c]
25	4.4	2.34	2.16

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No details are available.	C_6H_5Cl: Dow Chemical Co., 99.98% pure, purified by distillation before use. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: (1) in (2) ±10% (compiler). (2) in (1) <100% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene: C_6H_5Cl; [108-90-7]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* <u>1957</u>, *79(4)*, 864-5.

VARIABLES:
 	
  One temperature
	PREPARED BY:
	
	  A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10ml(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	3.60	1.992	2.035

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

Tritiated water was equilibrated with 20 ml chlorobenzene through stirring in a flask in a constant temperature water bath for two hours. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. For the tritiated water samples, the tritium activities were determined by the acetylene method (1,2). At least four independent determinations were made.
 	
The article was based upon work reported in a Ph.D. dissertation (2).
	H_2O: Tracerlab Inc., tritiated water,
	            used as received.
	
	C_6H_5Cl: Source not specified, chemical
	            grade, redistilled before use.

ESTIMATED ERROR:
Solubility: ±2.8%. Temperature: ±0.02 K.

REFERENCES:
1. Wing, J.; Johnston, W. H. *Science* <u>1955</u>, *121*, 674-6. 2. Wing, J., Ph.D. Dissertation, Purdue University, Lafayette, <u>1956</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Zieleinski, A. Z. *Chem. Stosowana* <u>1959</u>, *3*, 377-84.

VARIABLES:
  One temperature
	PREPARED BY:
	  A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [b]
25	6.1	3.39	3.45

a. Reported.
b. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:
 	
  Not specified.
	SOURCE AND PURITY OF MATERIALS:
	
	  Not specified.

	ESTIMATED ERROR:
	  Solubility: ±10% (compiler).
	
	  Temperature: ±1 K (compiler).

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Kisarov, V. M. *Zh. Prikl. Khim.* <u>1962</u>, *35(10)*, 2347-9.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3mol(1)/kg$ [b]	$10^4x(1)$ [c]
30	4.90	4.353	0.7846
40	7.05	6.263	1.129
50	9.60	8.529	1.538
60	11.00	9.7726	1.7623
70	16.05	14.259	2.5724
80	18.05	16.036	2.8934
90	25.00	22.210	4.0098

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

Temperatures were maintained using a thermostat bath with continuous stirring. Partial pressures of chlorobenzene were determined over 2 liter aqueous solutions in a flask. The equilibrium chlorobenzene content of the vapor was calculated from the gas laws. The amount of water vapor was obtained from the total weight increase of the absorber less the weight of the chlorobenzene absorbed. The chlorobenzene vapor pressure was directly proportional to its content in water. Duplicate measurements were made at each temperature.	C_6H_5Cl: Source not specified,
	          n_D^{20} = 1.5248
	          b.p. = 132°C
	
	H_2O: Redistilled before use.

	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Högfeldt, E.; Bolander, B. *Ark. Kemi* <u>1963</u>, *21(16)*, 161-86.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^2mol(1)/dm^3$ [b]	$10^3x(1)$ [c]
25	5.40	3.0	3.06

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

A mixture of 15 ml chlorobenzene with 10 ml distilled water was shaken in a glass-stoppered bottle overnight at room temperature. After centrifugation, duplicate samples were taken for the determination of the water content in the organic phase. Titration of the samples was carried out by a modified Karl Fischer method (1). A small correction was made for water in the vapor phase and adsorbed on the pipet.	H_2O: Distilled.
	
	C_6H_5Cl: Source not specified,
	             purity: 99.8%,
	             impurity: 0.11% benzene.

	ESTIMATED ERROR:
	Solubility: ±10%. Temperature: ±0.3 K.

	REFERENCES:
	1. Johansson, A. *Sven. Papperstidn.* <u>1947</u>, *50(11B)*, 124-33.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Jones, J. R.; Monk, C. B. *J. Chem. Soc.* 1963, Part III, 2633-5.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10ml(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	3.4	1.88	1.92
30	3.95	2.182	2.239
35	4.6	2.54	2.62

a.   Reported.
b.   Calculated by F. W. Getzen.
c.   Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was shaken with chlorobenzene in 1:10 volume ratios for 4 hours in flasks placed in a water thermostat bath. The water content was determined by tritium assay of samples taken from the flasks. The count rates were determined using a typical liquid scintillator solution technique.	H_2O: Tritiated. C_6H_5Cl: Source not known, laboratory grade, dried over $CaCl_2$ and fractionally distilled before use.

ESTIMATED ERROR:
Solubility: ±5%.

Temperature: ±0.5 K (compiler).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Goldman, S., Ph.D. Dissertation, McGill University, Montreal, 1969, p. 84.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^2mol(1)/dm^3$ [b]	$10^3x(1)$ [c]
25.0	5.225	2.90	2.959
35.1	7.405	4.11	4.234
45.06	9.639	5.35	5.567

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibration experiments were carried out in a constant temperature water bath using a stirrer. An equilibration period of at least 5 days was allowed. The total water content in the organic phase was determined by a Karl Fischer titration. Each reported water solubility was obtained as an average of at least two independent determinations.	H_2O: Distilled. C_6H_5Cl: Reagent grade, washed with conc. H_2SO_4 and with 1 M $NaHCO_3$ and then fractionally distilled over silica gel.

	ESTIMATED ERROR:
	Solubility: ±2%.
	Temperature: ±0.1 K.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Chey, W.; Calder, G. V. *J. Chem. Eng. Data* *1972*, *17(2)*, 199-200.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
21	5.34	4.742	8.546

a.   Reported.
b.   Calculated by F. W. Getzen.
c.   Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A 1 to 50 volume ratio solute/solvent mixture was stirred in a separatory funnel for 20 hr in a thermostat bath. Then, the solution was passed through a separation column of nonpolar resin. The solute was eluted with isopropyl ether. Traces of water were removed using molecular sieve pellets, and the sample was injected into a gas chromatograph fitted with a stainless steel column packed with Chromosorb having a liquid phase of Carbowax for analysis. The determination was done in duplicate.	C_6H_5Cl: Source not specified, Analytical Reagent grade. H_2O: Distilled.

	ESTIMATED ERROR:
	  Solubility: ±2%.
	
	  Temperature: ±1 K.

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
25.0	4.622	4.108 ± 0.062	7.4004

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solute was equilibrated with water by stirring in a sealed flask (1) with a magnetic stirrer for 48 hours at constant temperature. A sample was withdrawn and filtered through a glass-wool plug and the solute was extracted with 2,2,4-trimethylpentene. The optical densities were determined spectrophotometrically (2). The mean and standard deviation were obtained from eight independent measurements.	C_6H_5Cl: Merck AG., >99% GLC, used as received. H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±1.51%.

Temperature: ±0.05 K.

REFERENCES:

1. Franks, F.; Gent, M.; Johnson, H. H.
    J. Chem. Soc. 1963, Part III, 2716-23.

2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Vesala, A. *Acta Chem. Scand.* <u>1974</u>, *28A(8)*, 839-45.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
25.0	4.624	4.11	7.404

    a. Calculated by compiler.
    b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium between the water and chlorobenzene was established by stirring the sample in a sealed flask (1) with a magnetic stirrer for 48 hours. The sample was filtered through a glass-wool plug and the chlorobenzene was extracted with 2,2,4-trimethylpentene. The optical density was determined spectrophotometrically (2). Five parallel determinations were made. The reported work was based upon a Ph.D. dissertation (3).	C_6H_5Cl: Commercial reagent of analytical grade distilled through a column resulting in a more than 99% pure sample. H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±1.7%.

Temperature: ±0.05 K.

REFERENCES:
1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* <u>1963</u>, Part III, 2716-23.

2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* <u>1972</u>, *17(1)*, 38-41.

3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, <u>1973</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Prosyanov, N. N.; Shalygin, V. A; Zel'venskii, Ya. D. *Tr. Mosk. Khim.* *Tekhnol. Inst.* <u>1974</u>, *81*, 55-6.
VARIABLES: Temperature: 298-361 K	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$$\log_{10}\alpha = \frac{1222.37}{T(K)} - 1.3225$$

where α = distribution coefficient.

At the normal boiling point of C_6H_5Cl: $\alpha = 49.0$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The water concentration in the saturated solutions was determined radiometrically using tritium labelled water. The method of investigation has been described in greater detail in (1).	H_2O: Not specified. C_6H_5Cl: Not specified.

ESTIMATED ERROR:
  Solubility: ±10% (compiler).
 	
  Temperature: ±0.5 K (compiler).

REFERENCES:
 	
1. Prosyanov, N. N.; Shalygin, V. A.;
    Zel'venskii, Ya. D. *Tr. Mosk. Khim.*
    Tekhnol. Inst. <u>1973</u>, *75*, 100-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* <u>1976</u>, *54(24)*, 3909-16.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	5.225	2.90	2.959

a. Calculated by F. W. Getzen.
b. Reported.
c. Calculated by compiler.

<div align="center">AUXILIARY INFORMATION</div>

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of 50 ml chlorobenzene and 6 ml water in a bottle was submerged in a water thermostat bath for 2 days. The concentration of the water in the organic phase was determined by a conventional Karl Fischer dead stop back titration. Determinations were done in triplicate. A detailed description of the complete experimental procedure has been included in a Ph.D. dissertation (1).	H_2O: Distilled and deionized. C_6H_5Cl: Fischer - B255, washed with cc. H_2SO_4 and K_2CO_3 solutions and distilled water. Dried over silica gel and fractionally distilled, purity: 99.8%.

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

REFERENCES:
1. Kirchnerova, J., Ph.D. Dissertation, McGill University, Montreal, Quebec, <u>1974</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10 g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
5	0.400	0.355	0.64
25	1.068	0.9492	1.71
35	2.674	2.376	4.28
45	4.005	3.558	6.41

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated with chlorobenzene from the vapor phase in a special flask (1) placed in a thermostat bath using a shaker for a 24 hour equilibration period. A gas chromatographic analysis was done by sample injection into a 1.5 m stainless steel column having a 5% Apiezon M coating on Celite operated at 120°C. The chromatograph was fitted with a flame ionization detector. Three samples from each flask were analyzed.	C_6H_5Cl: Not specified. H_2O: Not specified.

ESTIMATED ERROR:

Solubility: ±2.9% (compiler).

Temperature: ±0.1 K (compiler).

REFERENCES:

1. Nelson, H. D.; de Ligny, C. L. *Rec. Trav. Chim.* 1968, *87*, 528-44.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Aquan-Yuen, M.; Mackay, D.; Shiu, W. Y. *J. Chem. Eng. Data* 1979, *24(1)*, 30-4.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25	4.717	4.1907	7.5753

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of solute was added to pure water in a flask which was then placed in a constant temperature bath for equilibration for at least 48 hours before analysis. The concentration of the chlorobenzene was determined by solvent extraction, followed by gas chromatographic analysis. The chromatograph was equipped with a flame ionization detector as described in (1).	C_6H_5Cl: Fisher Scientific Inc., certified grade, used as received. H_2O: Specified as "pure".

ESTIMATED ERROR:
Solubility: ±3.8%. Temperature: ±0.5 K (evaluator).

REFERENCES:
1. Mackay, D.; Shiu, W. Y. *Bull. Environ. Contam. Toxicol.* <u>1976</u>, *15*, 101-12.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Chlorobenzene; C_6H_5Cl; [108-90-7] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P.; Miller, J. *Anal. Chem.* *1980*, *52(13)*, 2162-4.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

Experimentally determined values:

$10g(1)/kg$

t/°C	Elution Chromatography	UV Absorption
10.0	4.4 ± 0.2	4.9 ± 0.3
20.0	4.2 ± 0.2	4.8 ± 0.4
30.0	4.9 ± 0.1	5.0 ± 0.2

Values derived from average measured solubilities:

t/°C	$10g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
10.0	4.6 ± 0.2	4.09 ± 0.18	7.37 ± 0.32
20.0	4.5 ± 0.4	4.00 ± 0.36	7.21 ± 0.64
30.0	5.0 ± 0.1	4.44 ± 0.09	8.01 ± 0.16

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Both elution chromatography and UV absorption methods were used to determine the aqueous solubilities. The agreement was within an experimental error of 4% between the two methods. The average deviations were determined from several measurements made on different samples. The analytical procedures for determining organic liquid solubilities in water based upon liquid phase elution chromatography has been described in (1).	C_6H_5Cl: Commercial, 98 wt %. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±4%. Temperature: ±0.5 K.
	REFERENCES: 1. Schwarz, F. P. *Anal. Chem.* *1980*, *52(1)*, 10-15.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water-d_2; D_2O; [7729-20-0] (2) Chlorobenzene; C_6H_5Cl; [108-90-7]	Hutchison, C. A.; Lyon, A. M. Columbia University Report A-745, July 1, <u>1943</u>.
VARIABLES: One temperature	PREPARED BY: G. Jancso

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg$ [a]	$10^2 mol(1)/kg$ [b]	$10^3 x(1)$ [a]
25.0	4.386	2.19	2.460

a. Calculated by F. W. Getzen.
b. Reported (average of two experimental measurements).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Between 25 and 100 ml of chlorobenzene and 1 to 2 ml of D_2O were introduced into a flask and shaken for about 90 min. The water bath temperature was maintained within ±0.05°C. Then, a sample was taken and the dissolved D_2O content was determined by a modified Karl Fischer titration as described in (1). The original report was unavailable, but the method and results have been described in sufficient detail in (1). The solubility of H_2O in chlorobenzene was also determined and found to be 0.00250 ± 0.00003 mol H_2O/ 100 g solution from three separate experiments.	Chlorobenzene was carefully purified and dried before use. Source and method not given. 100% D_2O: Source not specified.

ESTIMATED ERROR:
Solubility: av. dev. ±1 x 10^{-5} mol D_2O/100 g solution.   Temperature: ±0.05 K.

REFERENCES:
1. Eidinoff, M. L. In "Production of Heavy Water", National Nuclear Energy Series Division III-Vol. 4F, Murphy, G. M.; Urey, H. C.; Kirshenbaum, I.; Eds.; McGraw-Hill: New York, <u>1955</u>; Part II, Chapter 7, pp 129-44.

COMPONENTS:	EVALUATOR:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

CRITICAL EVALUATION:

The mutual solubility of 2-chlorophenol and water was investigated by Sidgwick and Turner (1) in 1922. While the measurements seem to be performed with care and the method, which involved classical synthetic procedures based upon gravimetry, gives relatively accurate results, there is some difficulty in resolving a solubility value at 298 K from the data. This circumstance arises because of the range of temperatures over which the measurements were made which makes the interpolation of the data inaccurate. Also, some of the data values scatter considerably in the low temperature range.

Kuroda (2) found the solubility of 2-chlorophenol in water to be in the order of 2 percent at room temperature (291 K). Better agreement is obtained when the data of Mulley and Metcalf (3) are compared with the values of Sidgwick and Turner. The 24.65 g(1)/dm^3 value of Mulley and Metcalf corresponds to a value of 25 g(1)/kg (assuming a density of 1.0 g/cm^3 for the solution).

The more recent work of Banerjee et al. (4) gives a value of 88.3 mmol(1)/dm^3 corresponding to approximately 11 g(1)/kg, a value that does not agree well with the earlier values. One possible reason for this lack of agreement may be associated with the use of a radiochemical method of analysis by Banerjee et al. For instance, a systematic error could have resulted from radiochemical impurities of the substrate. In any event, the lack of relevant information makes an evaluation here too speculative. The available experimental data are shown in Figure 1.

It should be mentioned that the pH of the solutions exerts a considerable influence on the solubility values of those solutes such as 2-chlorophenol capable of protolytic action. Here it is assumed that the reported solubilities refer to the pH values which prevail in the saturated solutions of 2-chlorophenol in water.

No more than a tentative value can be assigned to the solubility of 2-chlorophenol in water. The following value has been obtained from the data shown in Figure 1 by a graphical interpolation:

T/K	$10 mol(1)/dm^3$	$10^{-1}g(1)/kg$	$10^3 x(1)$
298.15	1.6	2.	2.9

REFERENCES

1. Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

2. Kuroda, T. cf. *Chem. Zentralbl.* 1926, *I*, 3610.

3. Mulley, R. A.; Metcalf, A. D. *Sci. Pharm.* 1966, *2*, 481-8.

4. Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environ. Sci. Technol.* 1980, *14(10)*, 1227-9.

COMPONENTS:	EVALUATOR:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	September 1982.

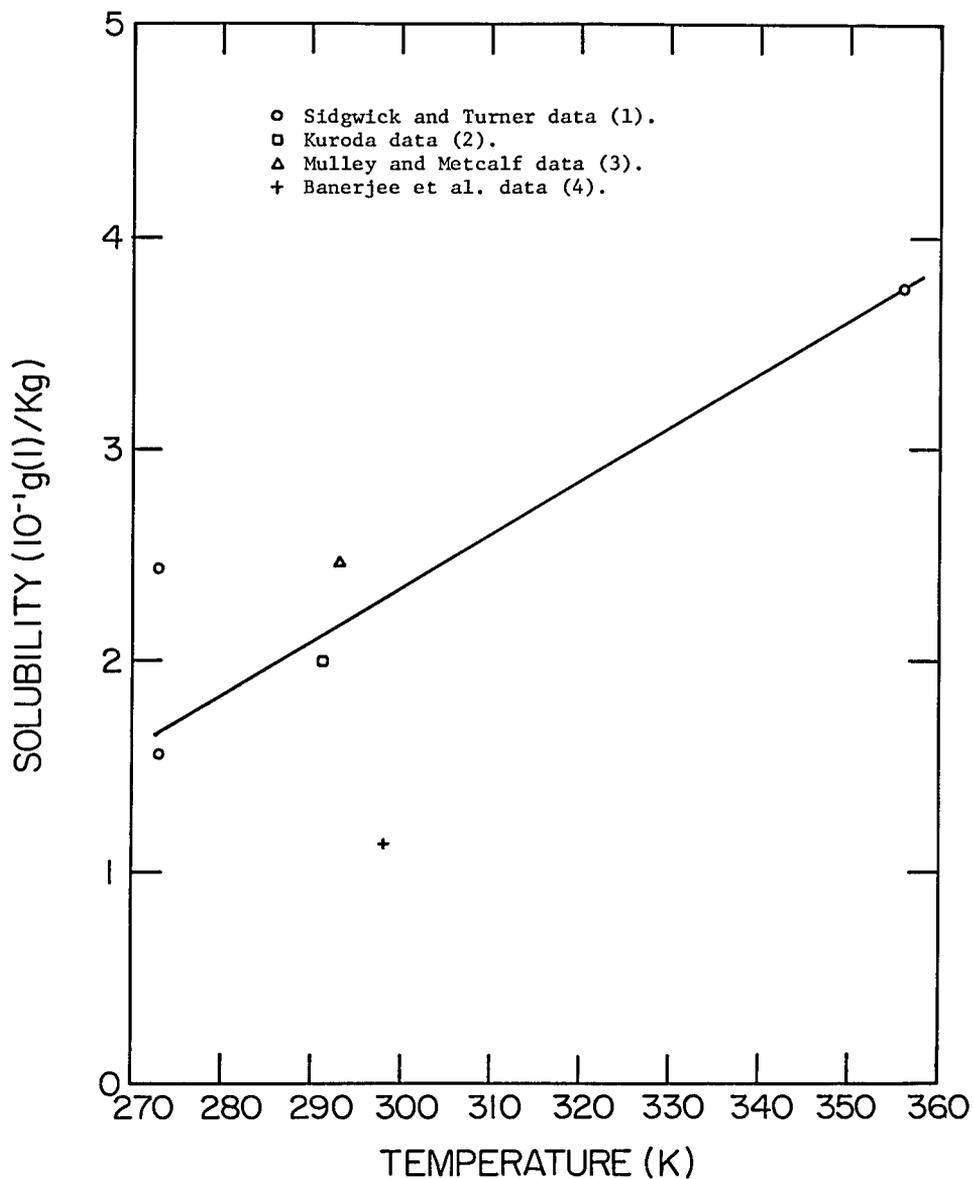CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of 2-chlorophenol in water versus Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* <u>1922</u>, *121*, Part II, 2256-63.
VARIABLES: Temperature: -8.2 - 173.0°C	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

t/°C	$10^{-2}g(1)/kg$ [a]	$mol(1)/kg$ [b]	$10x(1)$ [b]
-8.2	9.220	7.1719	6.2357
-8.0	9.087	7.0685	5.8243
-6.0	9.393	7.3065	6.8440
-5.0	8.962	6.9712	5.4750
-4.0	8.925	6.9424	5.3778
-2.0	8.773	6.8242	5.0050
-1.5	9.676	7.5266	8.0714
-0.30	0.244	0.1898	0.03493
-0.20	0.156	0.1213	0.02216
2.0	9.839	7.6534	8.9544
7.0	10.00	7.7787	10.0
82.9	0.376	0.2925	0.05445
91.5	8.590	6.6819	4.6056

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility versus temperature measurements were made by the so called synthetic method which involved the mixing of known masses of solute and solvent and the testing of miscibility with temperature. A bracketing procedure was applied. In this method, two adjustable thermostats, one above and the other below the solubility temperature, were used. The contents of sample tubes in the two thermostat baths were observed to maintain one homogeneous and the other heterogeneous as the temperature interval between the two thermostats were reduced by successive steps.	C_6H_5ClO: Synthesized by the chlorination of phenol in carbon tetrachloride, purified as described in Ref. 1, no criterions of the purity given. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES: 1. Wohlleben, W. J. *Ber. Dtsch. Chem. Ges.* <u>1909</u>, *42*, 4370.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* <u>1922</u>, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: continued ....

t/°C	10^{-2}g(1)/kg [a]	mol(1)/kg [b]	$10x(1)$ [b]
106.3	0.512	0.3983	0.07506
118.9	8.282	6.4423	4.0319
156.6	7.062	5.4933	2.5197
159.1	1.358	1.0563	0.21547
165.8	1.695	1.3185	0.27806
166.2	6.072	4.7232	1.7806
170.1	5.495	4.2744	1.4598
170.7	2.259	1.7572	0.39289
172.9	4.504	3.5035	1.0301
173.0	3.300	2.5670	0.64568

a.   Reported.
b.   Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem.* *Soc.* <u>1922</u>, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: Continued ....

Figure 1. 2-Chlorophenol, water solubility behavior versus Centrigrade
          temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8] (2) Water; H_2O; [7732-18-5]	Mulley, B. A.; Metcalf, A. D. *Sci. Pharm.* <u>1966</u>, *2*, 481-8.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/dm^3$ [a]	$10mol(1)/dm^3$ [b]	$10^3x(1)$ [b]
20	2.465	1.9174	3.5357

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The sample preparation and equilibration procedures were not specified. Saturated solutions were prepared and analyzed spectrophotometrically. Also, duplicate determinations were probably made by a synthetic method described in (1).	C_6H_5ClO: Commercial reagent, manufacturer not specified, suitably purified until physical constants corresponded with literature values. The reagent was dried in a desiccator for two days before use. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: <4% (estimated here on the basis of the deviations in the reported values).

REFERENCES:

1. Mulley, B. A.; Metcalf, A. D. *J. Pharm. Pharmacol.* <u>1956</u>, *8*, 774.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Chlorophenol; C_6H_5ClO; [95-57-8] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S. H.; Valvani, S. C. *Environm. Sci. Techn.* 1980, *14(10)*, 1227-9.
VARIABLES: One temperature	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [a]
25	1.135	8.83	1.611

a. Calculated by F. W. Getzen.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The equilibrations were performed in sealed stainless steel centrifuge tubes with constant or intermittent shaking. The equilibration was generally complete within 1 week. The mixture was then centrifuged for 60 minutes after which aliquots of the solution were removed for analysis either by a pipet or a syringe. Liquid scintillation counting with ^{14}C-labeled solute was employed in solubility determinations. The entire procedure was carried out at least twice and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

C_6H_5ClO: Commercial reagent, the ^{14}C-labeled compound was purchased by NEN, the nonlabeled one by Aldrich.

H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±0.5% (std. deviation estimated by authors).

Temperature: ±0.2 K (equilibration).
±0.3 K (centrifugation).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

The earliest and most thorough investigation of the mutual solubilities of 3-chlorophenol and water was done in 1922 by Sidgwick and Turner (1). Their measurements of solubilities were accomplished using the so called synthetic method, i.e., the determination of solubilities from weighed masses of 3-chlorophenol and water at the appropriate temperatures. They reported no directly measured values for the solubilities at 298 K, the nearest measured values were obtained at temperatures relatively far from room temperature (276 K and 359 K), which makes an accurate interpolation difficult.

The solubilities of three isomers of monochlorophenols in water have been determined by Kuroda (2) who reported the magnitude of this solubility to be 2 percent. More support for the work of Sidgwick and Turner is provided by the value measured by Mulley and Metcalf (3) at 293.15 K. Their result of 22.4 g(1)/dm^3 (which corresponds to 22.4 g(1)/kg assuming a density of 1.0 for the solution) agrees quite satisfactorily with the values of Sidgwick and Turner as shown in Figure 1. There are not, however, enough data to allow a more rigorous evaluation to be made; therefore, the solubility value reported here must be tentative.

It should be mentioned that the pH of the solutions exerts a considerable influence on the solubility values of those solutes such as 3-chlorophenol capable of protolytic action. Here it is assumed that the reported solubilities refer to the pH values which prevail in the saturated solutions of 3-chlorophenol in water.

No more than a tentative value can be assigned to the solubility of 3-chlorophenol in water 298.15 K as follows:

T/K	$10\,mol(1)/dm^3$	$10^{-1}g(1)/kg$	$10^3x(1)$
298.15	1.7	2.2	3.2

REFERENCES

1. Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

2. Kuroda, T. cf. *Chem. Zentralbl.* 1926, *I*, 3610.

3. Mulley; B. A.; Metcalf, A. D. *Sci. Pharm.* 1966, *2*, 481-8.

Figure 1. Solubility of 3-chlorophenol in water versus Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

VARIABLES:	PREPARED BY:
Temperature: -17.0 - 130.8°C	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-2} g(1)/kg$ [a]	$mol(1)/kg$ [b]	$10x(1)$ [b]
-17.0	9.223	7.1743	6.2455
-13.2	9.173	7.1354	6.0852
-8.2	9.011	7.0093	5.6080
-4.8	8.866	6.8966	5.2282
-0.9	8.487	6.6017	4.4012
-0.18	0.073	0.0568	0.0103
1.2	0.125	0.09723	0.01771
2.5	0.185	0.1439	0.02635
3.2	8.487	6.6017	4.4012
4.5	8.719	6.7822	4.8819
10.8	9.223	7.1742	6.2455
11.8	8.290	6.4485	4.0455
17.0	9.510	7.3975	7.3117

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility versus temperature measurements were made by the so called synthetic method which involved the mixing of known masses of solute and solvent and the testing of miscibility with temperature. A bracketing procedure was applied. In this method, two adjustable thermostats, one above and the other below the solubility temperature, were used. The contents of sample tubes in the two thermostat baths were observed to maintain one homogeneous and the other heterogeneous as the temperature interval between the two thermostats was reduced by successive steps.	C_6H_5ClO: Synthesized from 1-chloro-3-nitrobenzene by reduction and diazotisation. Melting point 32.5°C. H_2O: No specifications given.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: Continued ....

t/°C	10^{-2}g(1)/kg [a]	mol(1)/kg [b]	$10x(1)$ [b]
22.2	9.711	7.5538	8.2484
23.1	8.230	6.4018	3.9453
32.5	10.00	7.7787	10.0
85.25	0.512	0.3983	0.07506
109.8	7.123	5.5407	2.5759
118.0	1.113	0.86576	0.17248
123.0	1.356	1.0548	0.21511
127.5	1.784	1.3877	0.29531
129.1	5.565	4.3288	1.4955
130.5	4.612	3.5875	1.0711
130.7	3.889	3.0251	0.81882
130.8	3.202	2.4907	0.61922

a. Reported.
b. Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-0] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem.* *Soc.* <u>1922</u>, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: Continued ....
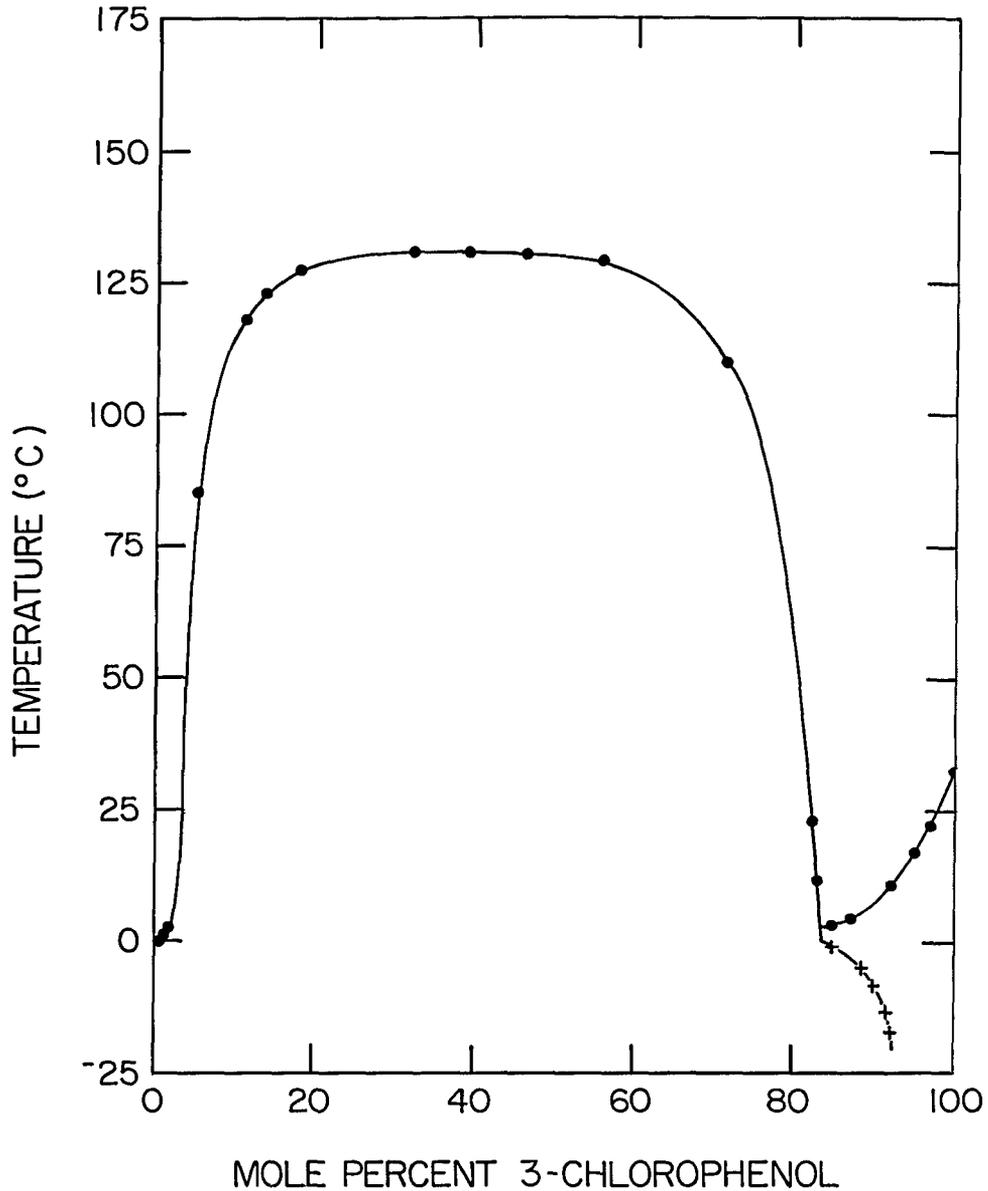
Figure 1. 3-Chlorophenol, water solubility behavior versus Centrigrade
temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Chlorophenol; C_6H_5ClO; [108-43-01]	Mulley, B. A.; Metcalf, A. D. *Sci. Pharm.* 1966, *2*, 481-8.
(2) Water; H_2O; [7732-18-5]	

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/dm^3$ [a]	$10mol(1)/dm^3$ [b]	$10^3x(1)$ [b]
20	2.242	1.7439	3.2095

a. Reported.
b. Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The sample preparation and equilibration procedures were not specified. Saturated solutions were prepared and analyzed spectrophotometrically. Also, duplicate determinations were probably made by a synthetic method described in (1).	C_6H_5ClO: Commercial reagent, suitably purified, until physical constants corresponded with literature values. The reagent was dried in a desiccator for two days before use. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: <4% (estimated here on the basis of the deviations in the values reported for the solubility of this phenol in cetomagrol solns).

REFERENCES:
1. Mulley, B. A.; Metcalf, A. D. *J. Pharm. Pharmacol.* 1956, *8*, 774.

COMPONENTS:	EVALUATOR:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION:

   The earliest of the published works on the solubility of 4-chlorophenol in water is that of Sidgwick and Turner (1). Even though this work has been available for more than 50 years, it still serves as a useful reference for comparison of later results. No solubility value at 298.15 K has been reported as a measured value; the nearest measurements reported have been relatively far from room temperature (274 K and 339 K by Sidgwick and Turner) making an interpolation difficult.

   Kuroda (2) reported an approximate solubility of the three isomeric monochlorophenols in water in the range of 2 percent. More support for the work of Sidgwick and Turner is given by the work of Blackman et al. (3) and that of Mulley and Metcalf (4). The data reported in these two works are in good agreement. For an assumed solution density of 1.0 g/cm^3, a value of 27 g(1)/kg results from the work of Blackman et al. and a value of 26 g(1)/kg results from the work of Mulley and Metcalf.

   In reviewing the work of Blackman et al. it should be stressed that the solubility was determined at a pH of 5.1, a condition being controlled by the addition of a phosphate buffer (a KH_2PO_4 solution). However, the effect of the buffer solution can be minimized since the pH of a saturated 4-chlorophenol solution can be assumed to be of the same magnitude as that of the buffer and the ionic effects can be assumed to be quite low (as reported by Robinson and Stokes (5), the pK for 4-chlorophenol in water is 9.4). Even so, one should remember that the pH does exert some influence on the solubility of protolytic solutes such as 4-chlorophenol and attention should be paid to agents in the solution which change its acidity.   The data are shown in Figure 1.

   The solubility of 4-chlorophenol in water at normal temperatures has a reliable value as deduced from the three references. However, the mutual solubility of 4-chlorophenol and water as reported by Sidgwick and Turner over its entire temperature range must be considered tentative because of the lack of other supporting data.

   The following solubility of 4-chlorophenol in water is tentative and based primarily on the reported value of Blackman et al.:

T/K	$10 mol(1)/dm$	$10^{-1} g(1)/kg$	$10^3 x(1)$
298.15	2.1	2.7	3.9

REFERENCES

1. Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

2. Kuroda, T. cf. *Chem. Zentralbl.* 1926, *I*, 3610.

3. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

4. Mulley, B. A.; Metcalf, A. D. *Sci. Pharm.* 1966, 2, 481-8.

5. Robinson, R. A.; Stokes, R. H. "Electrolyte Solutions"; Butterworths: London, 1970; p 533.

COMPONENTS:	EVALUATOR:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9]	A. Vesala, Department of Chemistry and Biochemistry, University of Turku.
(2) Water; H_2O; [7732-18-5]	November 1979.

CRITICAL EVALUATION: (Continued)

Figure 1.   Solubility of 4-chlorophenol in water versus Absolute temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* <u>1922</u>, *121*, Part II, 2256-63.
VARIABLES: Temperature: -0.2 - 128.7°C	PREPARED BY: A. Vesala

EXPERIMENTAL VALUES:

t/°C	10^{-2} g(1)/kg	mol(1)/kg	$10x(1)$
-0.2	0.207	0.1610	0.02953
0.5	8.892	6.9168	5.2934
5.5	8.619	6.7044	4.6656
6.2	9.248	7.1937	6.3282
11.0	9.448	7.3493	7.0576
14.2	9.570	7.4442	7.5722
17.0	8.542	6.6445	4.5086
18.0	9.682	7.5313	8.1013
19.5	9.729	7.5678	8.3419
35.5	8.402	6.5356	4.2424
41.0	10.00	7.7787	10.0
65.0	0.391	0.3041	0.05670
97.0	7.403	5.7585	2.8545

Continued ...

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility versus temperature measurements were made by the so called synthetic method which involved the mixing of known masses of solute and solvent and the testing of miscibility with temperature. A bracketing procedure was applied. In this method, two adjustable thermostats, one above and the other below the solubility temperature, were used. The contents of sample tubes in the two thermostat baths were observed to maintain one homogeneous and the other heterogeneous as the temperature interval between the two thermostats was reduced by successive steps.	C_6H_5ClO: Synthesized from 4-chloroaniline, melting point of the product 40.9°C. H_2O: Source and purity not specified.
	ESTIMATED ERROR:
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: Continued ....

t/°C	$10^{-2}g(1)/kg$	mol(1)/kg	$10x(1)$
107.7	6.936	5.3953	2.4083
113.8	1.066	0.82920	0.16446
115.5	6.505	5.0600	2.0687
122.4	5.962	4.6376	1.7144
125.0	2.050	1.5946	0.34876
125.8	5.349	4.1608	1.3880
128.2	2.916	2.2683	0.54540
128.7	4.257	3.3114	0.94104

a.   Reported.
b.   Calculated by F. W. Getzen.

Measurements are shown graphically in Figure 1.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9] (2) Water; H_2O; [7732-18-5]	Sidgwick, N. V.; Turner, S. L. *J. Chem. Soc.* 1922, *121*, Part II, 2256-63.

EXPERIMENTAL VALUES: Continued ....

Figure 1.   4-Chlorophenol, water solubility behavior versus Centrigrade
            temperature.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9] (2) Water; H_2O; [7732-18-5]	Mulley, B. A.; Metcalf, A. D. *Sci. Pharm.* *1966*, *2*, 481-8.

VARIABLES:	PREPARED BY:
One temperature	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/dm^3$ [a]	$10 mol(1)/dm^3$ [b]	$10^3 x(1)$ [b]
20	2.625	2.0418	3.7705

a.   Reported.
b.   Calculated by F. W. Getzen.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The sample preparation and equilibration procedures were not specified. Saturated solutions were prepared and analyzed spectrophotometrically. Also, duplicate determinations were probably made by a synthetic method described in (1).	C_6H_5ClO: Commercial reagent, manufacturer not specified, suitably purified until physical constants corresponded with literature values. The reagent was dried in a desiccator for two days before use. H_2O: Source and purity not specified.

ESTIMATED ERROR:
Solubility: <4% (estimated here on the basis of the deviations in the reported values).

REFERENCES:

1.   Mulley, B. A.; Metcalf, A. D. *J. Pharm. Pharmacol.* *1956*, *8*, 774.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chlorophenol; C_6H_5ClO; [106-48-9] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	A. Vesala

EXPERIMENTAL VALUES:

$t/°C$	$10^{-1}g(1)/dm^3$ [a]	$10\,mol(1)/dm^3$ [b]	$10^3 x(1)$ [a]
25	2.70	2.1	3.89

a. Calculated by F. W. Getzen.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The samples were equilibrated in a thermostat bath with temporary shaking over periods of 3-4 weeks. During the equilibration time, the pH values of the solutions were controlled by dropwise addition of phosphate buffer solution. The analysis of the solute concentration in the saturated samples was done spectrophotometrically either directly or by using proper colorizing agents.	C_6H_5ClO: Probably a commercial reagent, source and purity not specified. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two techniques of analysis).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Fluorobenzene; C_6H_5F; [462-06-6]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION:

Four experimental measurements of the solubility of fluorobenzene in water have been reported in the literature (1-4), see Figure 1. However, only one single measurement of the solubility of water in fluorobenzene has been reported (5).

Some of the more recent data for the solubility of fluorobenzene in water is that of Nelson and Smit (4) in the temperature range between 278 and 318 K. However, despite equilibrium periods of 24 hours (which might not have been long enough), the measured solubilities are substantially lower than those found by earlier investigators. It is not possible to establish any shortcomings of the experimental procedures from the very brief description. No information was provided on the source and purity of materials used. Also, it was not indicated whether or not a water stripper had been employed for the analysis of the very dilute aqueous solutions by gas chromatography, or whether or not an internal standard had been used for the calibration of the gas chromatograph which employed a flame ionization detector. However, the authors agreed to re-examine their raw data in order to verify the reported values (6). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.

Jockers (3) reported the solubility of fluorobenzene in water at high temperatures and high pressures only. The objective of these measurements was to establish the phase equilibria and thermodynamics for fluid mixtures in which fluorobenzene and water are miscible in all proportions. The critical curve was also determined (7,8). There are no other solubility measurements in the temperature range between 546 and 562 K and in the pressure range between 96×10^5 and 114×10^5 Pa for comparison.

The two experimental determinations by Andrews and Keefer (1) at 298.15 K and Gross et al. (2) at 303.15 K are in good agreement with respect to the errors estimated by the authors. The recommended solubility has been established as the arithmetic mean of the two solubilities and temperatures.

Only a single solubility measurement for the solubility of water in fluorobenzene has been reported in the literature (5). This experimental determination was done by Wing in 1956 (9) at Purdue University in partial fulfillment of the requirements for the Doctor of Philosophy degree. This measurement was made by an isotopic dilution technique using tritiated water as the tracer. There are no other reported values for comparison and selection.

Recommended solubility values are as follows (that for water in fluorobenzene is tentative):

T/K	$10^2 mol(1)/dm^3$	g(1)/kg	$10^4 x(1)$
300.65	1.59	1.54	2.89

T/K	$10^2 mol(2)/dm^3$	10g(2)/kg	$10^3 x(2)$
298.15	1.75	3.08	1.65

COMPONENTS:	EVALUATOR:
(1) Fluorobenzene; C_6H_5F; [462-06-6]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	May 1979

CRITICAL EVALUATION: (Continued)

REFERENCES

1.   Andrews, L. J.; Keefer, R. M.   *J. Am. Chem. Soc.* <u>1950</u>, *72(7)*, 3113-6.

2.   Gross, P. M.; Saylor, J. H.; Gorman, M. A.   *J. Am. Chem. Soc.* <u>1933</u>, *55(2)*, 650-2.

3.   Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, <u>1976</u>.

4.   Nelson, H. D.; Smit, J. H.   *S.-Afr. Tydskr. Chem.* <u>1978</u>, *31(2)*, 76.

5.   Wing, J.; Johnston, W.H.   *J. Am. Chem. Soc.* <u>1957</u>, *79(4)*, 864-5.

6.   Nelson, H. D.; Smit, J. H., Personal Communication, <u>1979</u>.

7.   Götze, G.; Jockers, R.; Schneider, G. M., 4th Internat. Conf. Chem. Thermodyn. IUPAC, Montpellier, Aug. 26-30, <u>1975</u>, Part IV/9, 57-64.

8.   Jockers, R.; Schneider, G. M. *Ber. Bunsenges, Phys. Chem.* <u>1978</u>, *83*, 576-82.

9.   Wing, J., Ph.D. Dissertation, Purdue University, Lafayette, <u>1956</u>.

COMPONENTS:	EVALUATOR:
(1) Fluorobenzene; C_6H_5F; [462-06-6] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION: (Continued)
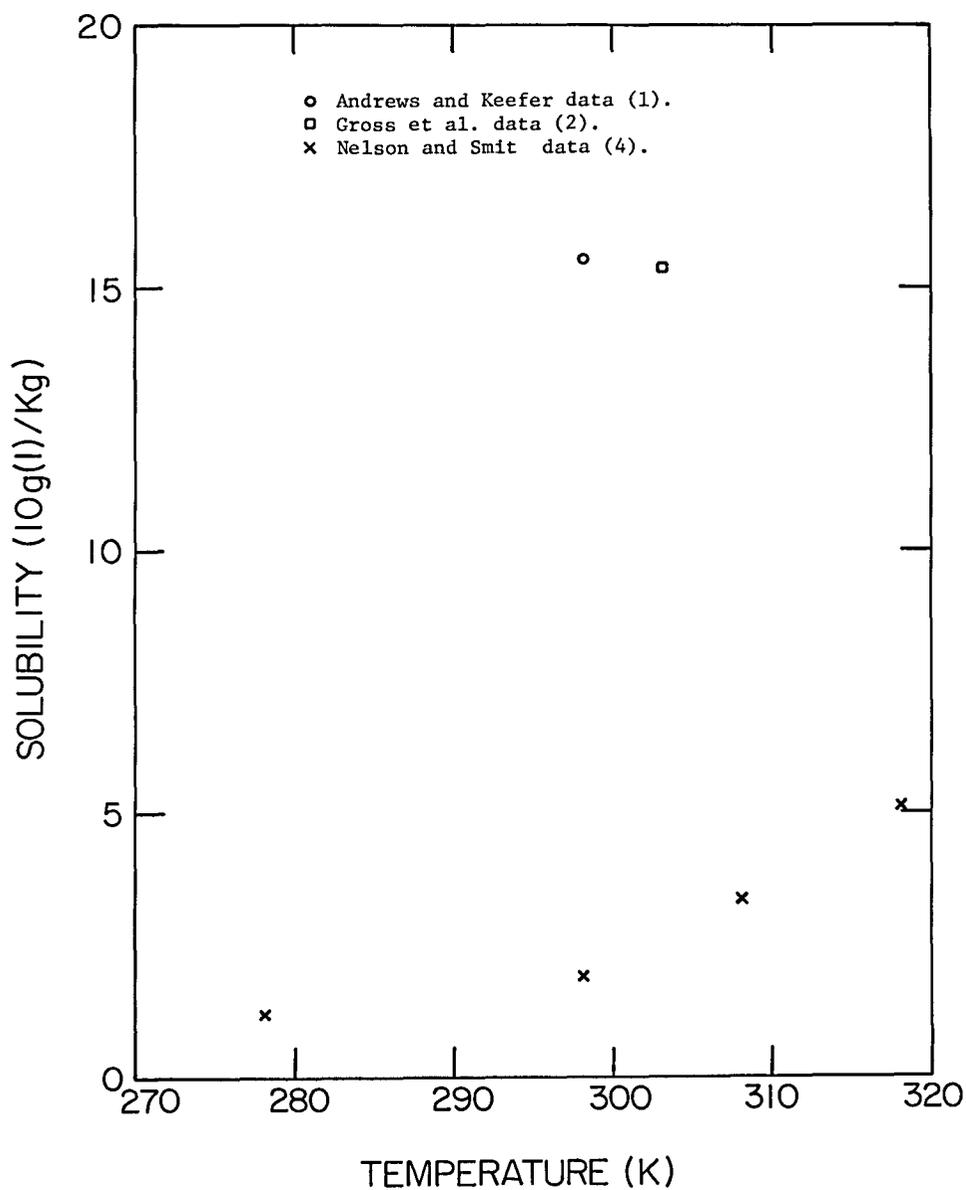
Figure 1.   Solubility of fluorobenzene in water versus Absolute temperature, reported values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorobenzene; C_6H_5F; [462-06-6] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H.; Gorman, M. A. *J. Am. Chem. Soc.* <u>1933</u>, *55(1)*, 650-2.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	g(1)/kg(2) [a]	10^2 mol(1)/kg [b]	$10^4 x(1)$ [c]
30	1.54	1.600	2.886

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solution was prepared in a flask placed in a water thermostat bath. The samples were analyzed by means of a Zeiss combination liquid and gas interferometer as described in (1). A detailed description of the complete procedure has been included in a M.A. dissertation (2).	C_6H_5F: Eastman Kodak Co., distilled fractionally before use, b.p. range 84.55° - 84.63°C. H_2O: Distilled.

ESTIMATED ERROR:

Solubility: ±1.5%.

Temperature: ±0.02 K.

REFERENCES:
1. Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* <u>1931</u>, *53(5)*, 1744-51.

2. Gorman, M. A., M.A. Thesis, Duke University, Durham, <u>1932</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorobenzene; C_6H_5F; [462-06-6] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1950</u>, *72(7)*, 3113-6.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	g(1)/dm^3 ^{a}	10^2mol(1)/dm^3 ^{b}	$10^4x(1)$ ^{c}
25.0	1.55	1.613	2.918

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The water was saturated with fluorobenzene in a glass-stoppered Erlenmeyer flask rotated in a constant temperature bath for 20 hours. The saturated solution was extracted with n-hexane. The optical density of the extract was measured against a standard n-hexane blank with a Beckman spectrophotometer (1).	C_6H_5F: Eastman Kodak Co., commercial reagent, b.p. 84.4°C, fractionated before use. H_2O: Not specified.
	ESTIMATED ERROR: Solubility: ±10% (compiler). Temperature: ±0.1 K (compiler).
	REFERENCES: 1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1949</u>, *71(11)*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Fluorobenzene; C_6H_5F; [462-06-6]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.

VARIABLES:	PREPARED BY:
One temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10 ml(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	3.16	1.749	1.651

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

Tritiated water was equilibrated with 20 ml fluorobenzene for two hours in a flask placed in a constant temperature bath. The sample was stirred throughout the equilibration period. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. The tritium activities in the tritiated water were determined by the acetylene method (1,2). At least four independent experiments were done.
 	
The article was based upon work reported in a Ph.D. dissertation (2).
	H_2O: Tracerlab Inc., tritiated water,
	         used as received.
	
	C_6H_5F: Source not specified, chemical
	         grade, redistilled before use.

ESTIMATED ERROR:
Solubility: ±2.8%. Temperature: ±0.02 K.

REFERENCES:

1. Wing, J.; Johnston, W. H. *Science*
    1955, *121*, 674-6.

2. Wing, J., Ph.D. Dissertation, Purdue
    University, Lafayette, 1956.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorobenzene; C_6H_5F; [462-06-6] (2) Water; H_2O; [7732-18-5]	Jockers, R., Ph.D. Dissertation, University of Bochum, Bochum, 1976, pp. 91-2.
VARIABLES: Temperature and pressure	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	P/bar	10^{-2}g(1)/kg [a]	mol(1)/kg [b]	$10x(1)$ [c]
284.0	100	4.9130	5.1123	1.533
289.5	114	5.6684	8.8985	1.970
279.0	103	5.6684	8.8985	1.970
273.5	96	5.6684	8.8985	1.970

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made using a high temperature, high pressure optical cell made from stainless steel with an internal stirrer. Predetermined mixtures of fluoro-benzene in water were introduced into the cell and homogenized at various tempera-tures and pressures. The phase transitions were observed through a sapphire window at the appropriate temperatures and pressures. Further details have been included in (1,2).	C_6H_5F: Fluka AG., Buchs, Schweiz, 99.5% pure, redistilled before use. H_2O: Boiled with $KMnO_4$ and redis-tilled before use.
	ESTIMATED ERROR: Solubility: ±1%. Temperature: ±0.5 K. Pressure: ±2 bar.
	REFERENCES: 1. Götze, G.; Jockers, R.; Schneider, G. M. 4th Inter. Conf. Chem. Thermodyn. IUPAC, Montpellier, Aug. 26-30, 1975, Part IV/9, pp 57-64. 2. Jockers, R.; Schneider, G. M. *Ber. Bunsenges. Phys. Chem.* 1978, *83*, 576-82.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluorobenzene; C_6H_5F; [462-06-6] (2) Water; H_2O; [7732-18-5]	Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* <u>1978</u>, *31(2)*, 76.
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

t/°C	$10g(1)/kg$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
5	1.184	1.232	2.22
25	1.893	1.970	3.55
35	3.36	3.50	6.3
45	5.12	5.33	9.6

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated through the vapor phase with fluorobenzene in a special flask (1) using a shaker in a thermostat bath for 24 hours. A gas chromatographic analysis of the samples was done by injection into a 5% Apiezon M stainless steel column with Celite as the supporter. The column length was 1.5 m and the temp. was 120°C. The chromatograph was equipped with a flame ionization detector. Three samples were analyzed from each flask.	C_6H_5F: Not specified. H_2O: Not specified.

ESTIMATED ERROR:
Solubility: ±1.9% (compiler).

Temperature: ±0.1 K (compiler).

REFERENCES:
1. Nelson, H. D.; de Ligny, C. L. *Rec. Trav. Chim.* <u>1968</u>, *87*, 528-44.

COMPONENTS:	EVALUATOR:
(1) Iodobenzene; C_6H_5I; [591-50-4]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION:

    Five experimental determinations have been published on the solubility of iodobenzene in water in the temperature interval between 278 and 318 K (1-4,8), see Figure 1. The serious discrepancies between the various solubility measurements for iodobenzene in water are evident in Figure 1. The solubility of water in iodobenzene between 298 and 308 K has been reported in two publications (5,6), see Figure 2.

    Some of the more recent data for the solubility of iodobenzene in water is that of Nelson and Smit (3) in the temperature range between 278 and 318 K. However, despite equilibrium periods of 24 hours (which might not have been long enough), the measured solubilities are substantially lower than those found by earlier investigators. It is not possible to establish any shortcomings of the experimental procedures from the very brief description. No information was provided on the source and purity of materials used. Also, it was not indicated whether or not a water stripper had been employed for the analysis of the very dilute aqueous solutions by gas chromatography, or whether or not an internal standard had been used for the calibration of the gas chromatograph which employed a flame ionization detector. However, the authors agreed to re-examine their raw data in order to verify the reported values (7). Consequently, for the present evaluation, their results have not been considered for inclusion in the selected solubility values.

    The solubility value for iodobenzene in water reported by Gross et al. (2) is too high in relation to other reported values (1,4). While the equilibration time was 20 hours for measurements made by Andrews and Keefer (1), the time was 48 hours for those of Vesala (4). This equilibration time difference may have affected the reported results. For this reason, the higher solubility value given by Vesala is recommended, see Table 1. The remaining available data have been correlated relative to Absolute temperature using a normal polynomial equation:

$$S_1(g)l)/kg) = 0.59293 - 4.8616 \times 10^{-3}T$$
$$+ 1.21754 \times 10^{-5}T^2 \qquad [1]$$

    The values calculated from equation [1] for the saturation of iodobenzene in water in the range of temperatures between 283 and 318 K together with corresponding molarities and mole fractions are given in Table 1. Also, the solubility values calculated from equation [1] are shown in Figure 1 as a solid line along with the measured values.

    For the solubility of water in iodobenzene, the agreement between the two solubilities reported by Jones and Monk (5) and by Wing and Johnston (6) at 298.15 K is quite good. At higher temperatures, measurements were made only by Jones and Monk (5); therefore, there are no other data for comparison. The data from both investigations (5,6) were correlated using the following equation:

$$\log_{10} x(2) = 0.792324 - 985.707/T \qquad [2]$$

In this equation, $x(2)$ is the mole fraction solubility of water in the water-iodobenzene system and T is the Absolute temperature. The calculated solubility values in the 283 to 308 K range are shown in Figure 2 along with the reported values.

    The calculated mole fraction values for the solubility of water in iodobenzene from equation [2] are included in Table 2 together with the corresponding molarities and g(2)/kg values in the temperature range between 293 and 313 K.

COMPONENTS:	EVALUATOR:
(1) Iodobenzene; C_6H_5I; [591-50-4]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England.
(2) Water; H_2O; [7732-18-5]	January 1983

CRITICAL EVALUATION: (Continued)

Table 1. Solubility of Iodobenzene in Water.

T/K	$10^4 mol(1)/dm^3$	$10 g(1)/kg$	$10^5 x(1)$
283.15	9.43	1.93	1.70
288.15	9.94	2.03	1.79
293.15	10.5	2.14	1.89
298.15	11.0	2.26	1.99
303.15	11.6	2.38	2.10
308.15	12.2	2.51	2.22
313.15	12.9	2.64	2.34
318.15	13.5	2.79	2.46

Table 2. Solubility of Water in Iodobenzene.

T/K	$10^2 mol(2)/dm^3$	$10 g(2)/kg$	$10^3 x(2)$
293.15	2.42	2.38	2.69
298.15	2.74	2.71	3.06
303.15	3.10	3.08	3.47
308.15	3.49	3.48	3.92
313.15	3.90	3.91	4.41

REFERENCES

1.   Andrews, L. J.; Keefer, R. J.   *J. Am. Chem. Soc.* 1950, *72(7)*, 3113-6.

2.   Gross, P. M.; Saylor, J. H.; Gorman, M. A.   *J. Am. Chem. Soc.* 1933, *55(2)*, 650-2.

3.   Nelson, H. D.; Smit, J. H.   *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.

4.   Vesala, A.   *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.

5.   Jones, J. R.; Monk, C. B.   *J. Chem. Soc.* 1963, *Part III*, 2633-5.

6.   Wing, J.; Johnston, W. H.   *J. Am. Chem. Soc.* 1957, *79(4)*, 864-5.

7.   Nelson, H. D., Personal Communication, 1979.

8.   Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

COMPONENTS:	EVALUATOR:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION: (Continued)

Figure 1. Solubility of iodobenzene in water versus Absolute
temperature, reported and calculated values.

COMPONENTS:	EVALUATOR:
(1) Water; H_2O; [7732-18-5] (2) Iodobenzene; C_6H_5I; [591-50-4]	A. L. Horvath, Imperial Chemical Industries Limited, Runcorn, England. May 1979.

CRITICAL EVALUATION: (Continued)

Figure 2. Logarithm of mole fraction solubility of water in
           iodobenzene versus reciprocal of Absolute temperature,
           reported and calculated values.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Gross, P. M.; Saylor, J. H.; Gorman, M. J. *J. Am. Chem. Soc.* 1933, *55(2)*, 650-2.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^5 x(1)$ [c]
30	3.4	1.67	3.00

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

The saturated solution was prepared in a thermostat water bath. The samples were analyzed by means of a Zeiss combination liquid and gas interferometer described in (1). A detailed description of the complete procedure has been included in a M.A. thesis (2).	C_6H_5I: Eastman Kodak Co., distilled
	              fractionally before use, b.p.
	              range 84.55° - 84.63°C.
	
	H_2O: Distilled.

ESTIMATED ERROR:
Solubility: ±4%.

Temperature: ±0.02 K.

REFERENCES:
1. Gross, P. M.; Saylor, J. H. *J. Am. Chem. Soc.* 1931, *53(5)*, 1744-51.

2. Gorman, M. A., M. A. thesis, Duke University, Durham, 1932.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1950</u>, *72(7)*, 3113-6.
VARIABLES: One temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^5 x(1)$ [c]
25.0	1.8	8.82	1.59

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated with iodobenzene in a glass-stoppered Erlenmeyer flask by rotating the flask in a constant temperature bath for 20 hours. The saturated solution was extracted with n-hexane for analysis. The optical density of the extract was measured against a n-hexane standard using a Beckman spectrophotometer (1).	C_6H_5I: Eastman Kodak Co., commercial reagent, b.p. 188.3°C, fractionated before use. H_2O: Not specified.

ESTIMATED ERROR:
Solubility: ±10% (compiler). Temperature: ±0.1 K (compiler).

REFERENCES:
1. Andrews, L. J.; Keefer, R. M. *J. Am. Chem. Soc.* <u>1949</u>, *71(11)*, 3644-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Iodobenzene; C_6H_5I; [591-50-4]	Wing, J.; Johnston, W. H. *J. Am. Chem. Soc.* <u>1957</u>, *79(4)*, 864-5.
VARIABLES: One temperature	**PREPARED BY:** A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10 ml(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25.0	5.03	2.784	3.107

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was equilibrated with 20 ml iodobenzene through stirring in a flask in a constant temperature water bath for two hours. The concentration of the tritiated water in the organic phase was determined by isotopic dilution. For the tritiated water samples, the tritium activities were determined by the acetylene method (1,2). At least four independent determinations were made. The article was based upon work reported in a Ph.D. dissertation (2).	H_2O: Tracerlab Inc., tritiated water, used as received. C_6H_5I: Source not specified, chemical grade, redistilled before use.

<table>
<tr><td colspan="2">ESTIMATED ERROR:
Solubility: ±1.6%.

Temperature: ±0.02 K.</td></tr>
<tr><td colspan="2">REFERENCES:
1. Wing, J.; Johnston, W. H. <i>Science</i>
    <u>1955</u>, <i>121</i>, 674-5.

2. Wing, J., Ph.D. Dissertation, Purdue
    University, Lafayette, <u>1956</u>.</td></tr>
</table>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) Iodobenzene; C_6H_5I; [591-50-4]	Jones, J. R.; Monk, G. B. *J. Chem. Soc.* **1963**, *Part III*, 2633-5.
VARIABLES: Temperature	**PREPARED BY:** A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10ml(1)/dm^3(2)$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [c]
25	4.9	2.71	3.03
30	5.6	3.09	3.47
35	6.35	3.502	3.940

a. Reported.
b. Calculated by F. W. Getzen.
c. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Tritiated water was shaken with iodobenzene in 1:10 volume ratios for 4 hours in flasks placed in a water thermostat bath. The water content was determined by tritium assay of samples taken from the flasks. The count rates were determined using a typical liquid scintillatior solution technique.	H_2O: Tritiated. C_6H_5I: Source not known, laboratory grade, dried over $CaCl_2$ and fractionally distilled before use.
	ESTIMATED ERROR: Solubility: ±5%. Temperature: ±0.5 K (compiler).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973,
VARIABLES: Temperature	PREPARED BY: A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
10.0	1.9529	0.9574 ± 0.0093	1.7248
15.2	1.9656	0.9636 ± 0.0084	1.7360
19.6	2.1642	1.061 ± 0.033	1.9115
25.1	2.2845	1.120 ± 0.032	2.0177
30.0	2.3620	1.158 ± 0.026	2.0862
35.0	2.5109	1.231 ± 0.007	2.2177

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:

The iodobenzene was mixed with water in a sealed flask (1) with the aid of a magnetic stirrer for 48 hours in a water bath at constant temperature. After the solution was filtered through a glass-wool plug, the solute was extracted with 2,2,4-trimethylpentene. The optical density of each sample was determined spectrophotometrically (2). Mean and standard deviations were calculated from three measurements.	C_6H_5I: Flika AG, puriss, >99% GLC,
	            used as received.
	
	H_2O: Distilled, deionized, and
	            degassed.

ESTIMATED ERROR:
Solubility: ±3.11%. Temperature: ±0.05 K.

REFERENCES:
1. Franks, F.; Gent, M.; Johnson, H. H.
      J. Chem. Soc. 1963, *Part III*, 2716-23.

2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Vesala, A. *Acta Chem. Scand.* 1974, *28A(8)*, 839-45.
VARIABLES: One temperature	**PREPARED BY:** A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^3 mol(1)/kg(2)$ [b]	$10^5 x(1)$ [a]
25.0	2.2845	1.120	2.0177

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The iodobenzene was mixed with water in a sealed flask (1) with the aid of a magnetic stirrer for 48 hours in a water bath at constant temperature. After the solution was filtered through a glass-wool plug, the solute was extracted with 2,2,4-trimethyl-pentene. The optical density of each sample was determined spectrophotometrically (2). Mean and standard deviations were established from five parallel determinations. The reported work was based upon a Ph.D. dissertation (3).	C_6H_5I: Commercial reagent of analytical grade distilled through a column resulting in a more than 99% pure sample. H_2O: Distilled, deionized, and degassed.

ESTIMATED ERROR:
Solubility: ±2.7%. Temperature: ±0.05 K.

REFERENCES:
1. Franks, F.; Gent, M.; Johnson, H. H. *J. Chem. Soc.* 1963, *Part III*, 2716-23.

2. Wauchope, R. D.; Getzen, F. W. *J. Chem. Eng. Data* 1972, *17(1)*, 38-41.

3. Vesala, A., Ph.D. Dissertation, University of Turku, Turku, 1973.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Iodobenzene; C_6H_5I; [591-50-4] (2) Water; H_2O; [7732-18-5]	Nelson, H. D.; Smit, J. H. *S.-Afr. Tydskr. Chem.* 1978, *31(2)*, 76.

VARIABLES:	PREPARED BY:
Temperature	A. L. Horvath

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg$ [a]	$10^4 mol(1)/kg$ [b]	$10^6 x(1)$ [c]
5	0.5492	2.692	4.85
25	0.9500	4.657	8.39
35	1.438	7.048	12.7
45.5	2.072	10.16	18.3

a. Calculated by compiler.
b. Calculated by F. W. Getzen.
c. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated through the vapor phase with iodobenzene in a special flask (1) using a shaker in a thermostat bath for 24 hours. A gas chromatographic analysis of the samples was done by injection into a 5% Apiezon M stainless steel column with Celite as the supporter. The column length was 1.5 m and the temp. was 120°C. The chromatograph was equipped with a flame ionization detector. Three samples were analyzed from each flask.	C_6H_5I: Not specified. H_2O: Not specified.

ESTIMATED ERROR:
Solubility: ±2% (compiler).
Temperature: ±0.1 K (compiler).

REFERENCES:
1. Nelson, H. D.; de Ligny, C. L. *Rec. Trav. Chim.* 1968, *87*, 528-44.

COMPONENTS:	EVALUATOR:
(1) 2,4,5,6-Tetrachloro-3-methylphenol; $C_7H_4Cl_4O$; [10460-33-0] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA July 1983.

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4,5,6-tetrachloro-3-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4,5,6-tetrachloro-3-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4,5,6-tetrachloro-3-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 2,4,5,6-tetrachloro-3-methylphenol in water is tentative:

t/°C	$10^3 g(1)/dm^3$	$10^5 mol(1)/dm^3$	$10^7 x(1)$
25	6.15	2.5	4.52

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,5,6-Tetrachloro-3-methylphenol; $C_7H_4Cl_4O$; [10460-33-0] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	6.15	2.5	4.52

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation.	$C_7H_4Cl_4O$: Probably a commercial reagent. H_2O: Distilled water.

METHOD (cont.)	ESTIMATED ERROR:
Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:

1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>.
2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2,4,6-Trichloro-3-methylphenol; $C_7H_5Cl_3O$; [551-76-8] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA July 1983.

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4,6-trichloro-3-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4,6-trichloro-3-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4,6-trichloro-3-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 2,4,6-trichloro-3-methylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^4 mol(1)/dm^3$	$10^6 x(1)$
25	1.12	5.3	9.58

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Trichloro-3-methylphenol; $C_7H_5Cl_3O$; [551-76-8]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
(2) Water; H_2O; [7732-18-5]	

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	1.12	5.3	9.58

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation.

Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution to to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.

SOURCE AND PURITY OF MATERIALS:

$C_7H_5Cl_3O$:   Probably a commerical reagent.

H_2O: Distilled water.

ESTIMATED ERROR:

Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936.
2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Water; H_2O; [7732-18-5] (2) 3,4-Dichlorotoluene; $C_7H_6Cl_2$; [95-75-0]	Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p. 140.
VARIABLES: One temperature	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/kg(2)$ [a]	$10^3 mol(1)/kg$ [b]	$10^4 x(1)$ [b]
30	2.6	1.44	2.32

a. Reported.
b. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No experimental details were available.	$C_7H_6Cl_2$: Dow Chemical Co., purified by distillation before use. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: <100% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,6-Dichloro-4-methylphenol; $C_7H_6Cl_2O$; [2432-12-4]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA
(2) Water; H_2O; [7732-18-5]	July 1983.

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,6-dichloro-4-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,6-dichloro-4-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,6-dichloro-4-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 2,6-dichloro-4-methylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^3 mol(1)/dm^3$	$10^5 x(1)$
25	6.73	3.8	6.87

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,6-Dichloro-4-methylphenol; $C_7H_6Cl_2O$; [2432-12-4] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10 g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	6.73	3.8	6.87

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in the glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_7H_6Cl_2O$: Probably a commercial reagent. H_2O: Distilled water.

ESTIMATED ERROR:

Solubility: <5% (evaluated on the basis of
             the reported results of the
             two analytical techniques).

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>.
2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2,4-Dichloro-6-methylphenol; $C_7H_6Cl_2O$; [1570-65-6] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4-dichloro-6-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4-dichloro-6-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4-dichloro-6-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 2,4-dichloro-6-methylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^3mol(1)/dm^3$	$10^5x(1)$
25	2.83	1.6	2.89

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G. *Arch, Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dichloro-6-methylphenol; $C_7H_6Cl_2O$: [1570-65-6] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	2.83	1.6	2.89

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_7H_6Cl_2O$: Probably a commercial reagent. H_2O: Distilled water.

SOURCE AND PURITY (continued) section above.

	ESTIMATED ERROR:
	Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936.
2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Bromotoluene; C_7H_7Br; [106-38-7] (2) Water; H_2O; [7732-18-5]	Dreisbach, R. R. "Physical Properties of Chemical Compounds", Advances in Chemistry Series No. 15; American Chemical Society: Washington, D. C., 1955; p. 153.
VARIABLES: One temperature	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/kg(2)$ [a]	$10^4 mol(1)/kg$ [b]	$10^5 x(1)$ [b]
25	1.1	6.43	1.16

a. Reported.
b. Calculated by compiler.

	AUXILIARY INFORMATION	

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No experimental details were available.	C_7H_7Br: Dow Chemical Co., purified by distillation before use. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: <100% (compiler). Temperature: ±1 K (compiler).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-2-methylphenol; C_7H_7ClO; [1570-64-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA
(2) Water; H_2O; [7732-18-5]	

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 4-chloro-2-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 4-chloro-2-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 4-chloro-2-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 4-chloro-2-methylphenol in water is tentative:

t/°C	g(1)/dm^3	10^2mol(1)/dm^3	10^4x(1)
25	6.84	4.8	8.73

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-2-methylphenol; C_7H_7ClO; [1570-64-5] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^4 x(1)$ [a]
25	6.84	4.8	8.73

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	C_7H_7ClO: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).
	REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>. 2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-3-methylphenol; C_7H_7ClO; [59-50-7] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 4-chloro-3-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 4-chloro-3-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 4-chloro-3-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 4-chloro-3-methylphenol in water is tentative:

$t/°C$	$g(1)/dm^3$	$10^2 mol(1)/dm^3$	$10^4 x(1)$
25	3.99	2.8	5.08

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-3-methylphenol; C_7H_7ClO; [59-50-7] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^4 x(1)$ [a]
25	3.99	2.8	5.08

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

<div align="center">AUXILIARY INFORMATION</div>

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	C_7H_7ClO: Probably a commercial reagent. H_2O: Distilled water.

ESTIMATED ERROR:
Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>.
2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2-Chloro-6-methylphenol; C_7H_7ClO; [87-64-9] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA July 1983.

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2-chloro-6-methylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2-chloro-6-methylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2-chloro-6-methylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 2-chloro-6-methylphenol in water is tentative:

$t/°C$	$g(1)/dm^3$	$10^2 mol(1)/dm^3$	$10^4 x(1)$
25	3.56	2.5	4.53

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G.   *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Chloro-6-methylphenol; C_7H_7ClO: [87-64-9] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^4 x(1)$ [a]
25	3.56	2.5	4.53

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	C_7H_7ClO: Probably a commercial reagent. H_2O: Distilled water.

ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936.
2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-bis(trifluoromethyl)benzene; $C_6H_4(CF_3)_2$; [402-31-3] (2) Water; H_2O; [7732-18-5]	Strachan, A. N.; Field, J. P.; Fleming, K. A. Int. Solvent Extr. Conf., (Proc.), Vol. 2, <u>1980</u>, page paper 80-2, 6 pp.
VARIABLES: One temperature	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	4.090	1.91	3.451

a. Calculated by compiler.
b. Reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An excess of 1,3-bis(trifluoromethyl)benzene was stirred with 100 ml water in a closed flask in a thermally regulated bath (±0.1°C) for 30 min. After phase separation and standing for several hours, two samples of known amounts were removed from the aqueous phase and extracted with hexane. The absorbances of the extracted samples were measured (265 nm) with a Pye Unicam SP 30 spectrophotometer. Hexane solutions of the solute in known concentrations were used to establish the extinction coefficient ($246\ dm^3mol^{-1}cm^{-1}$). The procedure was repeated to give a total of four concentration measurements.	$C_6H_4(CF_3)_2$: Fluorochem Limited 97-100%; redistilled and middle cut used. H_2O: Distilled.
	ESTIMATED ERROR: Solubility: ±3% (authors). Temperature: ±0.1 K (authors).
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4,6-Trichloro-3,5-dimethylphenol; $C_8H_7Cl_3O$; [6972-47-0] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4,6-trichloro-3,5-dimethylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4,6-trichloro-3,5-dimethylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4,6-trichloro-3,5-dimethylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 2,4,6-trichloro-3,5-dimethylphenol in water is tentative:

$t/^\circ C$	$10^3 g(1)/dm^3$	$10^5 mol(1)/dm^3$	$10^7 x(1)$
25	4.96	2.2	3.98

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4,6-Trichloro-3,5-dimethylphenol; $C_8H_7Cl_3O$; [6972-47-0] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	4.96	2.2	3.98

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_8H_7Cl_3O$: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR:
	Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).
	REFERENCES:
	1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936. 2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2,4-Dichloro-6-ethylphenol; $C_8H_8Cl_2O$; [24539-94-4]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA
(2) Water; H_2O; [7732-18-5]	

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4-dichloro-6-ethylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4-dichloro-6-ethylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4-dichloro-6-ethylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 2,4-dichloro-6-ethylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^3 mol(1)/dm^3$	$10^5 x(1)$
25	2.48	1.3	2.35

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dichloro-6-ethylphenol; $C_8H_8Cl_2O$; [24539-94-4] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^3mol(1)/dm^3$ [b]	$10^5x(1)$ [a]
25	2.48	1.3	2.35

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation.	$C_8H_8Cl_2O$: Probably a commerical reagent. H_2O: Distilled water.

METHOD/APPARATUS/PROCEDURE (cont.):	
Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques). REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>. 2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-2,5-dimethylphenol; C_8H_9ClO; [1124-06-7] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 4-chloro-2,5-dimethylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 4-chloro-2,5-dimethylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 4-chloro-2,5-dimethylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 4-chloro-2,5-dimethylphenol in water is tentative:

$t/°C$	$g(1)/dm^3$	$10^2 mol(1)/dm^3$	$10^3 x(1)$
25	8.93	5.7	1.04

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-2,5-dimethylphenol; C_8H_9ClO; [1124-06-7] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ [a]	$10^2 mol(1)/dm^3$ [b]	$10^3 x(1)$ [a]
25	8.93	5.7	1.04

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	C_8H_9ClO: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).
	REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>. 2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-2,6-dimethylphenol; C_8H_9ClO; [1123-63-3]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA
(2) Water; H_2O; [7732-18-5]	

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 4-chloro-2,6-dimethylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 4-chloro-2,6-dimethylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 4-chloro-2,6-dimethylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 4-chloro-2,6-dimethylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^3 mol(1)/dm^3$	$10^5 x(1)$
25	5.17	3.3	5.97

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-2,6-dimethylphenol; C_8H_9ClO; [1123-63-3] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55–71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

t/°C	$10g(1)/dm^3$ [a]	$10^3 mol(1)/dm^3$ [b]	$10^5 x(1)$ [a]
25	5.17	3.3	5.97

a. Calculated by compiler.
b. Reported value measured by pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	C_8H_9ClO: Probably a commercial reagent. H_2O: Distilled water.

ESTIMATED ERROR:
Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>.
2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-3,5-dimethylphenol; C_8H_9ClO; [88-04-0] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 4-chloro-3,5-dimethylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 4-chloro-3,5-dimethylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 4-chloro-3,5-dimethylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 4-chloro-3,5-dimethylphenol in water is tentative:

$t/°C$	$g(1)/cm^3$	$10^2 mol(1)/dm^3$	$10^4 x(1)$
25	3.45	2.2	3.99

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-3,5-dimethylphenol; C_8H_9ClO; [88-04-0] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

VARIABLES:	PREPARED BY:
One temperature One pH: 5.1	F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$g(1)/dm^3$ ^{a}	$10^2 mol(1)/dm^3$ ^{b}	$10^4 x(1)$ ^{a}
25	3.45	2.2	3.99

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	C_8H_9ClO: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).
	REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>. 2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2,4-Dichloro-6-propylphenol; $C_9H_{10}Cl_2O$; [91399-12-1] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4-dichloro-6-propylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4-dichloro-6-propylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4-dichloro-6-propylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as $\pm$ 5 percent. The following solubility value for 2,4-dichloro-6-propylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^4 mol(1)/dm^3$	$10^6 x(1)$
25	1.00	4.9	8.85

REFERENCES

1.   Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dichloro-6-propylphenol; $C_9H_{10}Cl_2O$; [91399-12-1] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	1.00	4.9	8.85

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_9H_{10}Cl_2O$: Probably a commercial reagent. H_2O: Distilled water. --- ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques). --- REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>. 2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239. 2. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-3-methyl-5-ethylphenol; $C_9H_{11}ClO$; [1125-66-2] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 4-chloro-3-methyl-5-ethylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished both by direct spectrophotometric techniques and, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. The agreement between the measurements of concentration using the two methods of analysis was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 4-chloro-3-methyl-5-ethylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 4-chloro-3-methyl-5-ethylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 4-chloro-3-methyl-5-ethylphenol in water is tentative:

$t/°C$	$10g(1)/dm^3$	$10^3mol(1)/dm^3$	$10^5x(1)$
25	3.58	2.1	3.80

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-3-methyl-5-ethylphenol; $C_9H_{11}ClO$; [1125-66-2] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$$10^3 mol(1)/dm^3 \text{ a}$$

t/°C	Spectrophotometry	Colorimetry
25	2.0	2.2

Values derived from average measured solubilities:[b]

t/°C	$10g(1)/dm^3$	$10^3 mol(1)/dm^3$	$10^5 x(1)$
25	3.58	2.1	3.80

a. Reported value measured at pH 5.1
b. Calculated by compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined both by direct spectrophotometric techniques and by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements. Agreement between the two methods was within an experimental error of 5%.	$C_9H_{11}ClO$: Probably a commercial reagent. H_2O: Distilled water. **ESTIMATED ERROR:** Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques). **REFERENCES:** 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936, 2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2,4-Dichloro-6-butylphenol; $C_{10}H_{12}Cl_2O$; [91399-13-2] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4-dichloro-6-butylphenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4-dichloro-6-butylphenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4-dichloro-6-butylphenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 2,4-dichloro-6-butylphenol in water is tentative:

$t/°C$	$10^2 g(1)/dm^3$	$10^4 mol(1)/dm^3$	$10^6 x(1)$
25	5.26	2.4	4.34

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dichloro-6-butylphenol; $C_{10}H_{12}Cl_2O$; [91399-13-2] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10^2 g(1)/dm^3$ [a]	$10^4 mol(1)/dm^3$ [b]	$10^6 x(1)$ [a]
25	5.26	2.4	4.34

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_{10}H_{12}Cl_2O$: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).
	REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936. 2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 2,4-Dichloro-6-(phenylmethyl)-phenol; $C_{13}H_{10}Cl_2O$; [19578-81-5] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the solubility of 2,4-dichloro-6-(phenylmethyl)-phenol in water. The determination was part of a study to provide some insight into the mode of biological action of substituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either by direct spectrophotometric techniques or, indirectly, by colorimetry using added colorizing reagents. The colorimetry method was based upon a standard procedure in which suitable colorizing agents were added either to the saturated phenol solution or to appropriately diluted solutions to yield an optical density proportional to the phenol concentration. A standardized curve obtained from measurements using known phenol concentrations was required for the determinations.

The concentration was obtained from three replicate measurements as an average value. Where both analytical procedures were used for the same solute, the agreement between the measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial product). The water was probably distilled. The ionic effects of the buffer upon the saturation value can be taken as minimal. However, it must be noted that pH does affect the solubility of protolytic solutes such as 2,4-dichloro-6-(phenylmethyl)-phenol. In this work, it can be assumed that the reported solubility refers, within experimental error, to the saturation value at the pH which exists for the saturated solution of 2,4-dichloro-6-(phenylmethyl)-phenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent. The following solubility value for 2,4-dichloro-6-(phenylmethyl)-phenol in water is tentative:

$t/°C$	$10^3 g(1)/dm^3$	$10^5 mol(1)/dm^3$	$10^7 x(1)$
25	5.82	2.3	4.16

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dichloro-6-(phenylmethyl)-phenol; $C_{13}H_{10}Cl_2O$; [19578-81-5] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* 1955, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

$t/°C$	$10^3 g(1)/dm^3$ [a]	$10^5 mol(1)/dm^3$ [b]	$10^7 x(1)$ [a]
25	5.82	2.3	4.16

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 51. in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_{13}H_{10}Cl_2O$: Probably a commercial reagent. H_2O: Distilled water.

| | ESTIMATED ERROR:
Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques). |

REFERENCES:
1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, 1936.
2. Folin, O.; Denis, W. *J. Biol. Chem.* 1912, *12*, 239.
3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* 1927, *73*, 627.

COMPONENTS:	EVALUATOR:
(1) 4-Chloro-3,5-dimethyl-2-(phenylmethyl)- phenol; $C_{13}H_{15}ClO$; [1867-85-2] (2) Water; H_2O; [7732-18-5]	F. W. Getzen, Chemistry Department, North Carolina State University, Raleigh, North Carolina, USA

CRITICAL EVALUATION:

Only one measurement, that of Blackman et al. (1), was found in the literature for the
solubility of 4-chloro-3,5-dimethyl-2-(phenylmethyl)-phenol in water. The determination
was part of a study to provide some insight into the mode of biological action of sub-
stituted phenols as related to differences in physical properties.

Saturation was established at 298.15 K over a 3-4 week period, a reasonably sufficient
time interval for saturation equilibrium. The system pH was adjusted to 5.1 by addition
of small amounts of KH_2PO_4 buffer. Concentration determinations were accomplished either
by direct spectrophotometric techniques or, indirectly, by colorimetry using added colori-
zing reagents. The colorimetry method was based upon a standard procedure in which suit-
able colorizing agents were added either to the saturated phenol solution or to appro-
priately diluted solutions to yield an optical density proportional to the phenol concen-
tration. A standardized curve obtained from measurements using known phenol concentra-
tions was required for the determinations.

The concentration was obtained from three replicate measurements as an average value.
Where both analytical procedures were used for the same solute, the agreement between the
measurements of concentration was within 5 percent.

No mention was made of further purification of the solute reagent (probably a commercial
product). The water was probably distilled. The ionic effects of the buffer upon the
saturation value can be taken as minimal. However, it must be noted that pH does affect
the solubility of protolytic solutes such as 4-chloro-3,5-dimethyl-2-(phenylmethyl)-phenol.
In this work, it can be assumed that the reported solubility refers, within experimental
error, to the saturation value at the pH which exists for the saturated solution of 4-
chloro-3,5-dimethyl-2-(phenylmethyl)-phenol alone, in water.

The uncertainty in the single reported value can be assumed to be as large as ± 5 percent.
The following solubility value for 4-chloro-3,5-dimethyl-2-(phenylmethyl)-phenol in water
is tentative:

t/°C	$10^2 g(1)/dm^3$	$10^5 mol(1)/dm^3$	$10^7 x(1)$
25	1.11	5.0	9.03

REFERENCES

1. Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Chloro-3,5-dimethyl-2-(phenylmethyl)-phenol; $C_{13}H_{15}ClO$; [1867-85-2] (2) Water; H_2O; [7732-18-5]	Blackman, G. E.; Parke, M. H.; Garton, G. *Arch. Biochem. Biophys.* <u>1955</u>, *54(1)*, 55-71.
VARIABLES: One temperature One pH: 5.1	PREPARED BY: F. W. Getzen

EXPERIMENTAL VALUES:

t/°C	$10^2 g(1)/dm^3$ a	$10^5 mol(1)/dm^3$ b	$10^7 x(1)$ a
25	1.11	5.0	9.03

a. Calculated by compiler.
b. Reported value measured at pH 5.1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibrium was established by mixing the solute with distilled water buffered with KH_2PO_4 at a pH of 5.1 in a glass-stoppered bottle suspended in a thermostat bath at 25°C. The sample was shaken periodically for 2 days with appropriate adjustment of pH to 5.1. After the pH became stabilized (usually about 1 week), the sample was equilibrated for an additional 2 weeks to assure saturation. Concentration was determined either directly by spectrophotometric techniques or by a colorimetric method based upon that given by (1) in which suitable colorizing agents (2,3) were added either to the saturated solution or to an appropriately diluted solution to yield an optical density proportional to the solute concentration. Concentration was obtained as the average of three replicate measurements.	$C_{13}H_{15}ClO$: Probably a commercial reagent. H_2O: Distilled water.
	ESTIMATED ERROR: Solubility: <5% (evaluated on the basis of the reported results of the two analytical techniques).
	REFERENCES: 1. Snell, F. D.; Snell, C. T. "Colorimetric Methods of Analysis", Vol. II; Chapman and Hall: London, England, <u>1936</u>, 2. Folin, O.; Denis, W. *J. Biol. Chem.* <u>1912</u>, *12*, 239. 3. Folin, O.; Ciocalteu, V. *J. Biol. Chem.* <u>1927</u>, *73*, 627.

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