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SOLUBILITY DATA SERIES

Volume 38

HYDROCARBONS WITH WATER AND SEAWATER

Part II: *Hydrocarbons C_8 to C_{36}*

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES

Editor-in-Chief
A.S. KERTES

Volume 38

HYDROCARBONS WITH WATER AND SEAWATER

Part II: *Hydrocarbons C_8 to C_{36}*

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CONTENTS

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.

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 presents solubility data for binary systems in which one component is a hydrocarbon containing 8 to 36 carbon atoms and the second component is water, heavy water or seawater. Other volumes in this series either presently available or in preparation present analogous data for other hydrocarbons. The interested reader should consult the Solubility Data Series list of volume titles on page 561. For this volume seawater has been defined as, "all natural waters, synthetic seawater and aqueous solutions in which sodium chloride predominates."

A variety of units for the expression of solubility has appeared in the primary literature. For the purpose of comparison the compilers of this volume have, so far as possible, expressed all original results in terms of mass percent and mole fraction as well as the units presented by the original investigators. Where such conversions have been made, they are clearly attributed to the compiler and the source of any data not provided by the original investigators (such as hydrocarbon or seawater density) is specified. Definitions of mass percent and mole fraction as well as their relationship to other common measures of solubility are given in the Introduction to this volume.

The expression of the solubility of a hydrocarbon in natural seawater on a mole fraction basis presents special difficulties since the composition of seawater is not fully known and somewhat variable. However, the uncertainty introduced by this factor is generally less than 3%, smaller than the measurement uncertainty associated with many of these data. Some of the data for hydrocarbon solubility in seawater have been presented in terms of the Setschenow (also transliterated Sechenov and Setchenoff) equation. A thorough discussion, "The Sechenov Salt Effect Parameter", is presented in Volume 10 of this series (pp. xxix-xliii).

By far the most common approach to the measurement of solubility in hydrocarbon/water systems has been to prepare a saturated solution and then to analytically determine the concentration of the less abundant component. In these systems of low solubility the careful preparation of saturated solutions is critically important. The presence of only a small amount of the minor component in the form of colloidal droplets can significantly influence the solubility results obtained. This can lead to major positive systematic errors. Unfortunately, lack of experimental detail in some published reports makes these errors extremely difficult to evaluate. Users of this volume are advised to be aware of this potential source of error, especially for systems where only one or a few measurements have been reported or when solubilities are very low.

Another approach to evaluating solubility data in these systems is to determine whether a particular result fits into a "reasonable" trend for a series of related compounds. While this approach undoubtedly has qualitative value, it must be used with caution. For instance, the solubilities of anthracene and phenanthrene differ by about a factor of 20; a fact that is supported by careful experimentation but not by "reasonable" inference.

Most measurements of hydrocarbon/water solubility have been made within the temperature range considered "room temperature" (275-300 K). In many reports system pressure is unspecified but can be assumed to be approximately 100 kPa (1 atm). Some measurements at elevated temperatures have been in sealed tubes. Generally the system pressure for these measurements is not known. For most purposes this lack of specification of system pressure is not important since hydrocarbon/water solubilities do not vary strongly with pressure.

This volume is the result of a careful search of the chemical literature. The goal of that search was to include all published data for the systems indicated in the title. Each evaluation includes a closing date for the literature search of that system, November 1981 or later. In spite of these efforts, some published measurements may have been missed. The editor will appreciate having his attention brought to any omitted source of solubility data for inclusion in future volumes.

The compilation and critical evaluation of solubility data presented here was a group effort. Each participant brought an individual style to the work. The editor's goal was to ensure that all text is simple, unambiguous English; not to attempt stylistic uniformity. Finally the editor wishes to acknowledge the dedicated efforts of the compilers, evaluators and reviewers whose efforts have resulted in this volume, and especially to thank Mauricette Nicpon, Sheila Chapin and Bronwyn Airey for final typing.

David Shaw

INTRODUCTION TO THE SOLUBILITY OF LIQUIDS IN LIQUIDS

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 is available. In those systems where data from different sources agree sufficiently, recommended values are proposed. In other cases, values may be described as "tentative", "doubtful" or "rejected".

This volume is primarily concerned with liquid-liquid systems, but related gas-liquid and solid-liquid systems are included when it is logical and convenient to do so. Solubilities at elevated and low temperatures and at elevated pressures may be included, as it is considered inappropriate to establish artificial limits on the data presented.

For some systems the two components are miscible in all proportions at certain temperatures or pressures, and data on miscibility gap regions and upper and lower critical solution temperatures are included where appropriate and if 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, with no distinction being made between solvent and solute.

The *solubility* of a substance 1 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 $x(1)$:

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

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 percent of component 1 is $100w_1$, and may be described as g(1)/100 g sln which makes it clear that it is mass percent of solute relative to solution and not solvent. The equivalent terms "weight fraction" and "weight percent" 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 1 in a solution of volume V,

$$c_1 = n_1/V$$

is expressed in units of mol dm^{-3}. The terms "molarity" and "molar" and the unit symbol M are not used.

Mass ratio is occasionally used in a two-component solution in the form g(1)/g(2), mg(1)/g(2), etc. The term "part per million" (ppm) is not used, but may be expressed as mg(1)/kg sln.

Molality of component 1 in component 2 is often used in solid-liquid systems, defined $m_1 = n_1/n_2 M_2$, with units mol kg^{-1}, but is not used in liquid-liquid systems where the distinction between "solute" 1 and "solvent" 2 is inappropriate. The term molality alone is inadequate, and the unit (mol kg^{-1}, mmol kg^{-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 (e.g. cycloalkene, diene, alkyne, cycloalkane, alkane), 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 of substitution, then

(vi) alphabetically by IUPAC name.

For example,

C_5H_8	cyclopentene 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
$C_{18}H_{12}$	benzanthracene chrysene naphthacene triphenylene

Deuterated 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 Foreword. Additional information on the individual sections of each sheet is now provided in the following.

"Components". Each component is listed by IUPAC name (ref 1), chemical formula according to the Hill system, and Chemical Abstracts Registry Number. Also included are trivial name or names if appropriate.

"Original Measurements". References are expressed in "Chemical Abstracts" style, journal names being abbreviated, and if necessary transliterated, in the forms given by the "Chemical Abstracts Service Source Index" (CASSI).

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

"Prepared by". The compiler is named here.

"Experimental Values". Components are described as (1) and (2), as defined in "Components". The experimental data are presented in the units used 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 authors'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 percent are included if the original data do not use these units. 1975 or 1977 atomic weights (ref 5) are used in such calculations. When appropriate, conversions from concentrations to mole fractions are included in the compilation sheets, 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" in parentheses.

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure.

"Method". 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) or (2), the following information (in this order and in abbreviated form) is provided if it is available in the original paper:

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" in parentheses) from the internal consistency, the type of apparatus, and other relevant information. Methods used by the compilers for reporting estimating errors are based on the papers by 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 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) *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 is *rejected*, the reference being included in the evaluation together with a reason for its rejection by the evaluator.

(d) *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.

(e) *Units.* The final recommended values are reported in SI units (ref 3).

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

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THE PHASE BEHAVIOR OF WATER AND HYDROCARBON SYSTEMS

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In order to understand solubility in hydrocarbon + water systems at high pressure it is desirable to be aware of the various types of fluid phase equilibria possible in binary mixtures. Fluid phase equilibria of binary mixtures are conveniently discussed in terms of the classification proposed by Scott and van Konynenburg[1-4]. They proposed that the phase behavior of binary mixtures could be classified into six broad groups. They found that five groups could be predicted using the van der Waals equation of state. The sixth class, which could not be predicted by the van der Waals equation, arises only in aqueous mixtures. The classification is most easily understood in terms of the pressure-temperature projection of the pressure-temperature-composition diagram. The six types of phase behavior are represented schematically in fig. 1. Only the "general" characteristics of the type of phase behavior can be understood from the diagrams given below. In practice solid phases often complicate the diagrams.

Type I. The phase diagram has a simple continuous gas-liquid critical locus with or without azeotropy.

Type II. The phase diagram is as for type I but with the addition of a three phase (liquid-liquid-gas) line ending at an upper critical end point, UCEP, and a (liquid-liquid) critical line starting from the UCEP and rapidly approaching high pressures. This type can occur with or without azeotropy.

Type III. This phase diagram has two distinct critical lines, one starts at the critical point of the pure component with the higher critical temperature but never approaches the critical point of the other component moving rapidly to high pressures. The other critical line starts at the critical point of the component with the lower critical temperature and meets a three phase (liquid-liquid-gas) line in an UCEP. The three phase line may be between the vapor pressure curves of the two components (as shown in fig. 1C) or may be above the vapor pressure curves of both components. There are several subgroups in type III behavior depending on whether there is a heteroazeotrope or not and on the shape of the critical line starting at the critical point with the higher temperature.

Type IV. This phase diagram has three distinct critical loci, one of which (the liquid-liquid critical line) starts at an UCEP on a three phase (liquid-liquid-gas) line and moves rapidly to higher pressures. The second line starts at the critical point of the component with the lower critical temperature and ends at an UCEP on a three phase line. The third line starts at the critical point of the other component and ends in a lower critical end point, LCEP, on the same three phase line as the second critical line.

Type V. This type is the same as type IV but without the liquid-liquid critical line and the three phase line at lower temperatures.

Type VI. This type of phase behavior is characterized by a continuous critical locus between the critical point of the two pure components. However, at lower temperatures there is a three phase line which is bounded above and below by critical end points. A liquid-liquid critical line joins these two critical end points. There are several known configurations of the line joining the ends of the three phase line. In the example illustrated (fig. 1F) the liquid-liquid critical line has two branches with a region of complete liquid miscibility between them.

Most hydrocarbon + water systems studied to date exhibit type III phase behavior. Typical pressure-temperature-composition diagrams for type III behavior are illustrated in fig. 2A and 2B. The most common type of phase behavior found in hydrocarbon water mixtures corresponds to fig. 2A. The behavior shown in fig. 2B has not yet been observed in hydrocarbon + water systems. From fig. 1 and 2 it can be seen that the three phase line on the pressure-temperature projection is derived from three lines on the pressure-temperature-composition diagram representing, the composition of gas, liquid 1 and liquid 2.

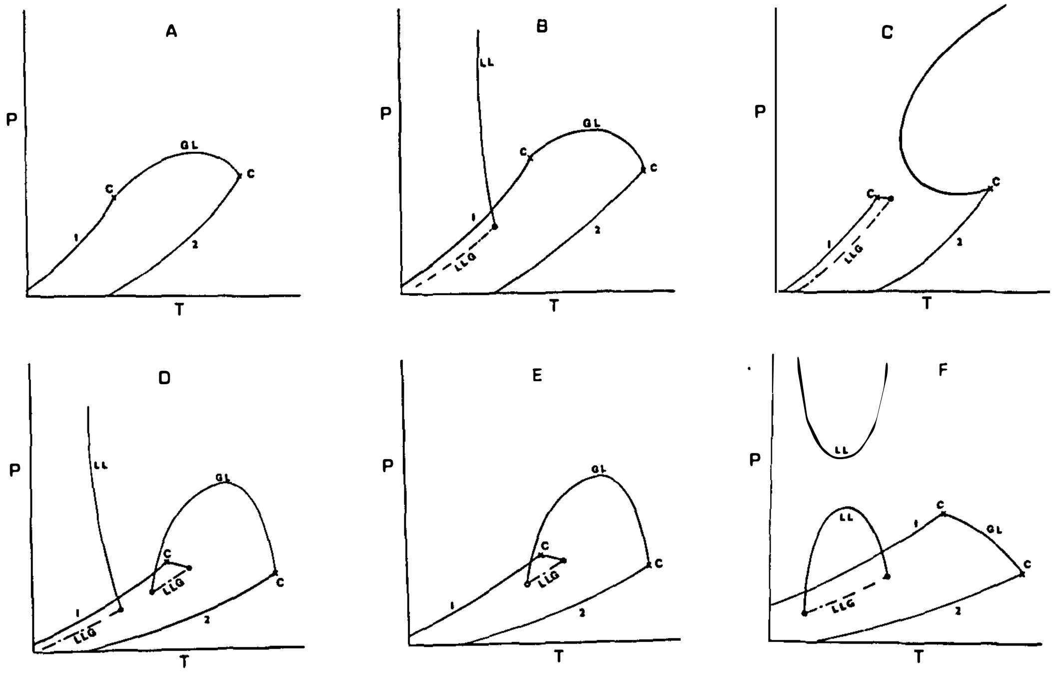

Fig. 1. Pressure-temperature projections for the six types of phase equilibria in binary mixtures. A - Type I; B - Type II; C - Type III; D - Type IV; E - Type V; F - Type VI. Lines labelled 1 and 2 are the vapor pressure of the two components; lines labelled LLG, GL and LL are three phase lines, gas-liquid critical loci and liquid-liquid critical loci respectively; points denoted C are critical points of the pure components.

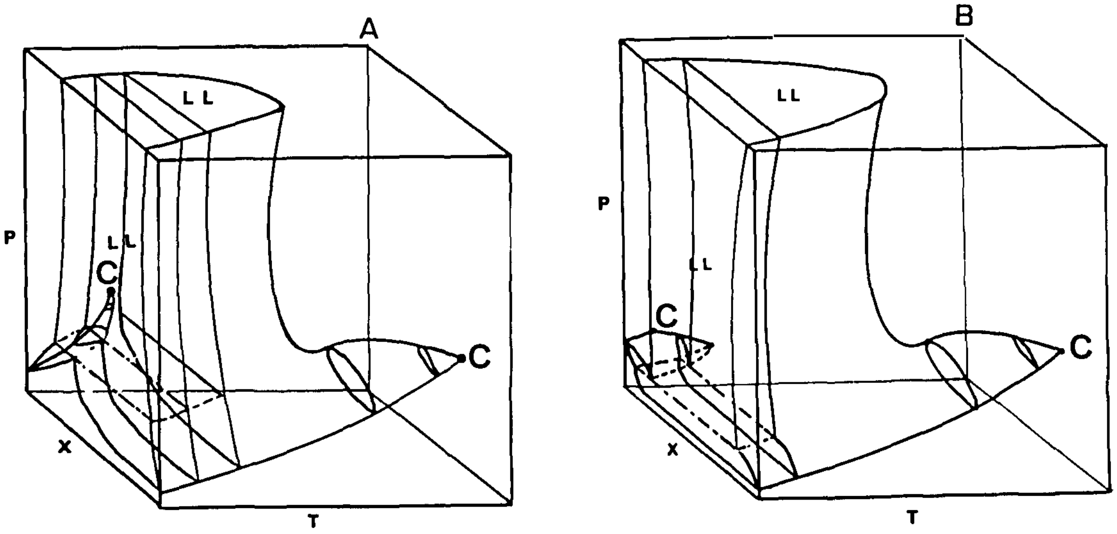

Fig. 2. Pressure-temperature-composition diagrams for two Type III systems. The three phase line is denoted -.-.-.- . The region in which two liquids coexist is denoted LL.

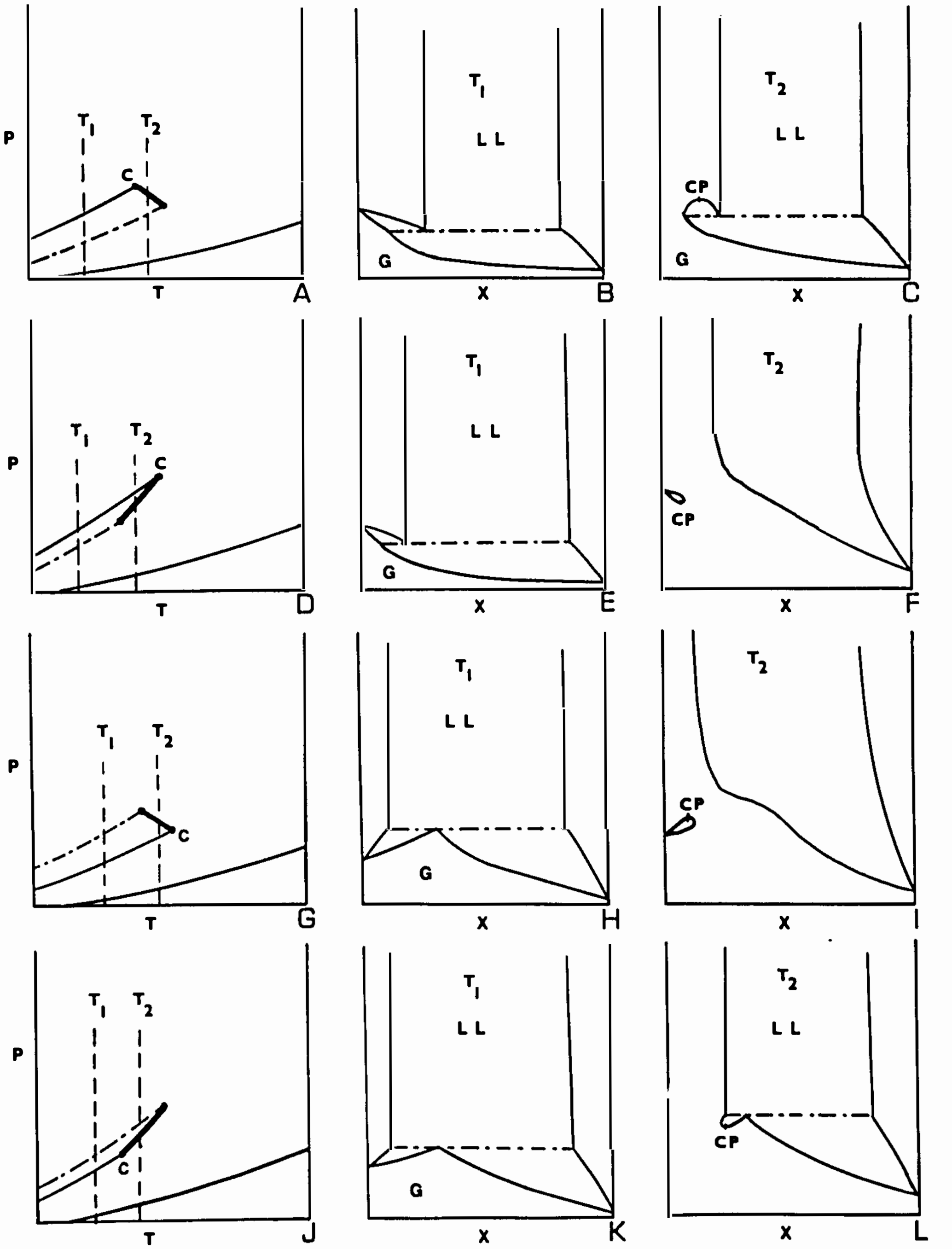

Fig. 3. The four possibilities for the relative position of the three phase line and vapor pressure curves of pure components for type III phase behavior. Figures A, D, G and J are pressure-temperature projections of the four classes. Figures B, E, H and K are the constant temperature, T_1, sections of the p,T,X diagrams; fig. C, F, I and L are analogous sections at temperature T_2. Most hydrocarbon systems have behavior illustrated in fig. 3G, 3H and 3I.

There are many sub-types of type III behavior. Consider the portion of the phase diagram in the region of the upper critical end point and the critical point of the pure component with the lower critical temperature. There are four possibilities. The three phase line could be at higher or lower pressures than the vapor pressure curve of the pure component. Each of these two cases could have the upper critical end point at a higher (or lower) temperature than the critical point. These four possibilities are illustrated in fig. 3. The position of the vapor pressure of the second component can be above or below that of the first component. In the case of hydrocarbon + water systems the two pure component vapor pressure curves sometimes cross on the pressure-temperature projection (e.g. benzene + water). Most hydrocarbons + water systems exhibit the behavior illustrated in fig. 3G. Consider fig. 3G, the three phase line is at higher pressures than the vapor pressure of the pure component (1). At a temperature, T_1, the pressure-composition diagram is shown in fig. 3H. It can be seen that depending on the pressure and overall composition it is possible to have one, two, or three phases present. At high pressures we have a fluid-fluid equilibrium which if T_1 is sufficiently low, it is reasonable to refer to as a liquid-liquid equilibrium. Although a line parallel to the composition axis at pressures between the three phase line and the vapor-pressure of component (1) cuts the boundary lines in four places, only two phases can be in equilibrium. The two phases in equilibrium will depend on the overall composition. At temperature T_2 a different situation exists in that at pressures above the critical line it is possible to have two phases present (fig. 3I). At pressures below the critical point it is possible to have two phases coexisting out of a possible four phases. Which are the two coexisting phases dependings on the overall composition. At some compositions only one phase will be present.

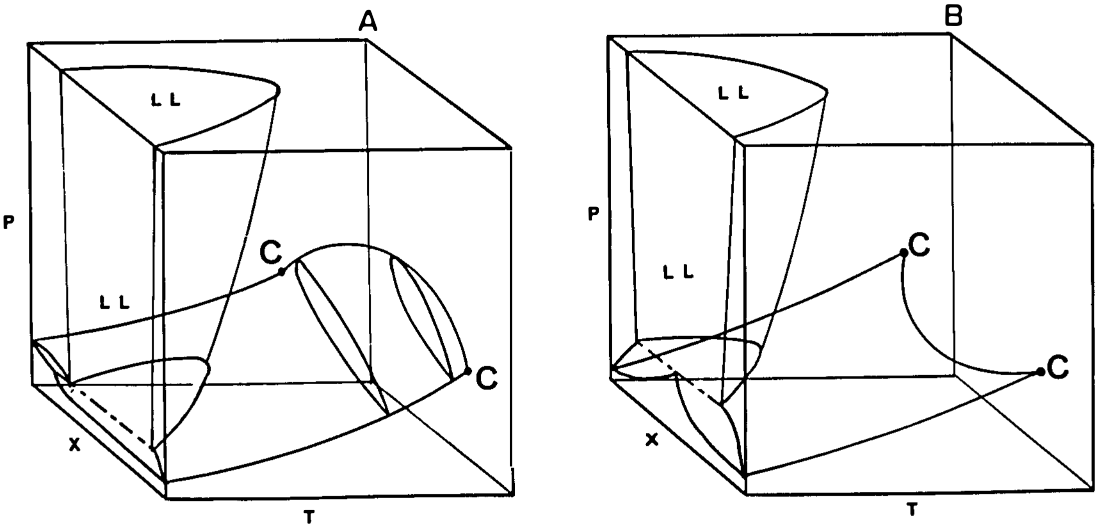

Fig. 4. Pressure, temperature, composition diagrams for two Type II systems. The three phase line is denoted -.-.-.- . The region in which two liquids coexist is denoted LL.

Although most hydrocarbon + water systems studied to date exhibit type III phase behavior it is known that some hydrocarbons of greater molecular weight, such as biphenyl exhibit type II phase behavior[6]. Figures 4A and 4B illustrate the pressure-temperature-composition diagram for two type II systems. It appears that most, if not all, hydrocarbon + water systems which exhibit type II behavior have a minimum in temperature for the gas-liquid critical curve which corresponds to the behavior illustrated in fig. 4B.

Some hydrocarbon + water systems have been observed to exhibit the phenomenon referred to as gas-gas immiscibility[6,7]. This phenomenon [5,8] occurs in type III phase behavior when the critical locus starting at the component with the highest critical temperature initially or eventually moves to high pressure at temperatures above the critical point of either component. If the critical locus always has a positive slope on the pressure-temperature projection the phenomenon is referred to as gas-gas immiscibility of the first kind (fig. 5A) whereas if the locus initially moves to lower temperatures, goes through a minimum and eventually moves to temperatures greater than the critical temperature of either component the mixture is said to exhibit gas-gas immiscibility of the second kind (fig. 5B). Gas-gas immiscibility of the second kind is exhibited by some hydrocarbon + water systems.

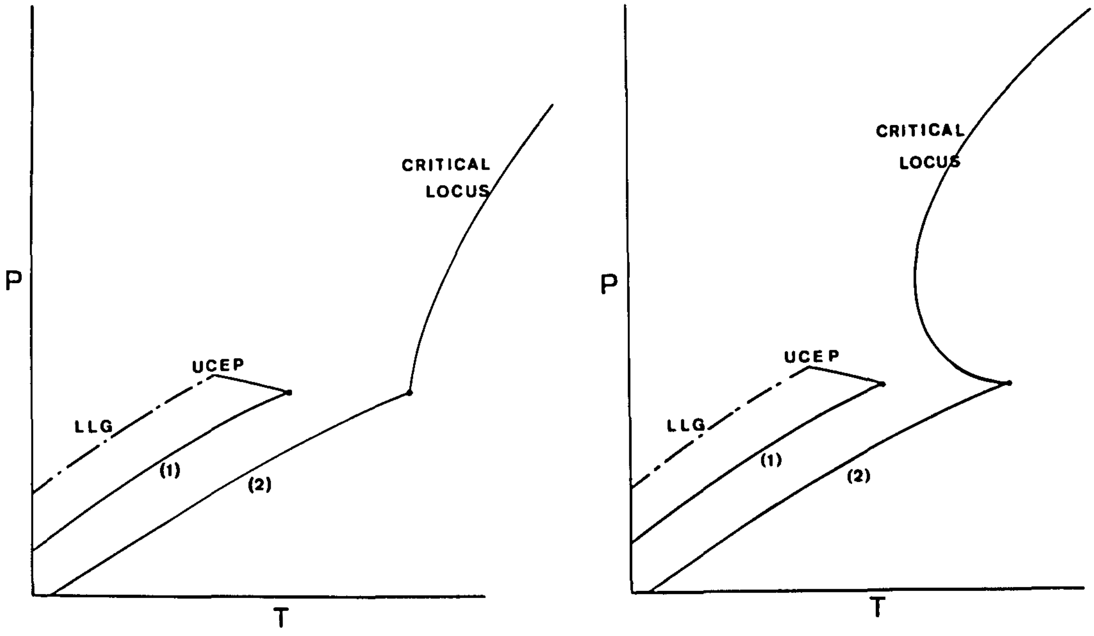

Fig. 5. Pressure, temperature projections for systems exhibiting gas-gas immiscibility. Figure 5A - immiscibility of the first kind. Figure 5B - immiscibility of the second kind.

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1. Scott, R. L.; van Konynenburg, P. H.; *Phil. Trans. Roy. Soc., London* 1980, *A298*, 495.
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8. Tsiklis, D. S.; Rott, L. A.; *Russ. Chem. Rev.* 1967, *36*, 351.

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

July 1985

CRITICAL EVALUATION:

Quantitative solubility data for the styrene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of the Styrene (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Lane (ref 1)	298-324	mutual	various[a]
Fordyce and Chapin (ref 2)	333	(1) in (2)	titration
Frilette and Hohenstein (ref 3)	298	(1) in (2)	unspecified
Andrews and Keefer (ref 4)	298	(1) in (2)	spectrophotometric
Banerjee *et al.* (ref 5)	298	(1) in (2)	HPLC

a Chemical analysis and cloud point measurements for (1) in (2). Karl Fischer and cloud point measurements for (2) in (1).

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF STYRENE (1) IN WATER (2)

All the available data (ref 1-5) are listed in Table 2. At 298K the agreement among the independent measurements (ref 1,3-5) is reasonable but not sufficient to enable the average value to be Recommended.

At other temperatures, the value of Fordyce and Chapin (ref 2) at ~ 333K is very much higher than that of Lane (ref 1). Since the latter were obtained by two independent methods and, as already noted, are in fair agreement with other determinations at 298K, the datum of Fordyce and Chapin is rejected. In the absence of confirmatory studies the data at temperatures other than 298K should be regarded as very tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Styrene; C_8H_8; [100-42-5] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985.

CRITICAL EVALUATION: (continued)

TABLE 2. Tentative Values of the Solubility of Styrene (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values	
	(g(1)/100g sln)	g(1)/100g sln	$10^5\ x_1$
283	0.29* (ref 1)	0.029	5.0
293	0.030* (ref 1)	0.030	5.2
298	0.033* (ref 1), 0.022 (ref 3), 0.030 (ref 4), 0.016 (ref 5)	0.025 ± 0.006[b]	4.3
303	0.034* (ref 1)	0.034	5.9
313	0.040* (ref 1)	0.040	6.9
323	0.046* (ref 1)	0.046	8.0
333	0.053* (ref 1), 0.95 (ref 2)[c]	0.053	9.2

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the author's two data sets, followed by averaging.

[b] Average (± σ_n) of all data; σ_n has no statistical significance.

[c] At T = 333.5K, value rejected: see text.

2. THE SOLUBILITY OF WATER (2) IN STYRENE (1)

The solubility of water in styrene has been reported in only one study (ref 1) and thus no Critical Evaluation is possible. The interested user is referred to the relevant data sheet for the experimental solubility values.

REFERENCES

1. Lane, W.H. *Ind. Eng. Chem. Anal. Ed.* 1946, *18*, 295-6.
2. Fordyce, R.G.; Chapin, E.C. *J. Am. Chem. Soc.* 1947, *69*, 581-3.
3. Frilette, V.J.; Hohenstein, W.P. *J. Polym. Sci.* 1948, *3*, 22-31.
4. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
5. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Env. Sci. Technol.* 1980, *14*, 1227-9.

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

ORIGINAL MEASUREMENTS:

Lane, W.H.

Ind. Eng. Chem. Anal. Ed. 1946, *18*, 295-6.

VARIABLES:

Temperature: 7-65°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of styrene in water

t/°C	g(1)100 g sln	10^5x_1 (compiler)
(a) Formaldehyde - Sulfuric Acid Reagent Method		
7	0.029	5.0
24	0.033	5.7
32	0.036	6.2
40	0.040	6.9
51	0.045	7.8
(b) Cloud Point Method		
15	0.025	4.3
25	0.031	5.3
44	0.040	6.9
49	0.045	7.8
56	0.050	8.6
65	0.058	10.0

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(a) The solubility of (1) in (2) was determined by means of the formaldehyde-sulfuric acid reagent, ref (1). The value shown for 7°C is the mean of three determinations, and the value for 25°C is the mean of two determinations; all other data are single determinations only.

(b) The cloud point exhibited by this system appeared to be very sharp, as the samples passed from a state in which they were cloudy within 1°C. The cloud point data are averages of from two to eight separate determinations. Cloud points at 0.025 g(1)/100 g solution were very faint.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; fresh samples; used as received.

(2) not specified.

ESTIMATED ERROR:

temp. (b) ± 0.5°C (from two to eight determinations)

REFERENCES:

1. Morris, H.E.; Stiles, R.B.; Lane, W.H. *Ind. Eng. Chem. Anal. Ed.* 1946, *18*, 294.

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

ORIGINAL MEASUREMENTS:

Lane, W.H.

Ind. Eng. Chem. Anal. Ed. 1946, *18*, 295-6.

VARIABLES:

Temperature: 6-51°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in styrene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
(a) Karl Fischer Reagent Method		
6	0.032	1.8
24	0.066	3.8
31	0.084	4.8
40	0.101	5.8
51	0.123	7.1
(b) Cloud Point Method		
14	0.040	2.3
27	0.060	3.5
34	0.080	4.6
40	0.100	5.7
45	0.120	6.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(a) A large sample of (1) containing a slight excess of (2) was shaken at a given temperature and then allowed to stand in a water bath at this temperature for 24 hr to ensure complete separation of the two phases before withdrawal of sample of the rich phase for titration of the water present with the Karl Fischer reagent.
(b) Duplicate determinations gave cloud points agreeing within 1°C, except in the case of 0.120 g(1)/100 g solution where the agreement was within about 3°C. Cloud points at 0.040 (1)/100 g solution were very faint. No more details were reported.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; fresh samples; used as received.

(2) not specified.

ESTIMATED ERROR:

soly. (a) ± 1.5% (from two determinations)

temp. (b) ± 1 to ± 3°C.

REFERENCES:

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

ORIGINAL MEASUREMENTS:

Fordyce, R.G.; Chapin, E.C.

J. Am. Chem. Soc. 1947, *69*, 581-3.

VARIABLES:

One temperature: 60.3°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of styrene in water at 60.3 C was reported to be 0.96 g(1)/ 100 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.95 g(1)/100 g sln and 1.66×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Into two stoppered 50 mL Erlenmeyer flasks were weighed two 25.000 g portions of (2). The flasks were placed in a water-bath regulated to 60.3 ± 0.02°C. Component (1) was added a drop at a time to the water samples by means of a calibrated micro-pipet and the flasks agitated after each addition. The saturation point was taken at the first appearance of the turbidity and the amount of (1) was calculated from the number of drops added.

SOURCE AND PURITY OF MATERIALS:

(1) Dow Chemical Co, N-100; redistilled.

(2) Not specified.

ESTIMATED ERROR:

temp. ±0.02°C

soly. ±0.05 g(1)/100 g sln

REFERENCES:

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

ORIGINAL MEASUREMENTS:

Frilette, V.J.; Hohenstein, W.P.

J. Polym. Sci. 1948, *3*, 22-31.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of styrene in water at 25°C was reported to be 0.022 g(1)/100 g sln.

The corresponding mole fraction, x_1, value calculated by the compilers is 3.8×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two different ways. In the first method, conjugated solutions were prepared by shaking together excess (1) with (2) and allowing the layers to separate; the aqueous layer was then analyzed for (1). To avoid the possibility of contaminating the aqueous phase by small suspended droplets a second method was utilized; a cellophane sack, filled with (2) was completely submerged in a beaker containing (2); a layer of (1) was then floated on top of (2) in the beaker. After 48 hr at 25°C, the sack was retrieved and the contents carefully removed and analyzed.

The method of analysis was not described.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1950, *72*, 5034-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of styrene in water at 25°C was reported to be 0.030 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 5.19×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; distilled shortly before use; 1 wt % of hydroquinone added as stabilizer before distillation; b.p. 76 C (78 mm Hg).

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Styrene; C_8H_8; [100-42-5]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

One temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of styrene in water was reported to be 1.54 x 10^{-3} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction (x_1) solubilities, calculated by the compiler, are 0.0160 g(1)/100 g sln and 2.77 x 10^{-5} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of styrene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by high-performance liquid chromatography using a Waters M6000A instrument fitted with a C_{18} Bondapak column. The mobile phase was a mixture of methanol/water or acetonitrile/water. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; purity not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature:	±0.2°C
Solubility:	±5.7% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) *o*-Xylene; C_8H_{10}; [95-47-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the *o*-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the *o*-Xylene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 2)	385-524	(1) in (2)	unspecified
McAuliffe (ref 3)	298	(1) in (2)	GLC
Hoegfeldt and Bolander (ref 4)	298	(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Price (ref 8)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 10)	299-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Alwani and Schneider (ref 5) have also reported data on a critical locus at high temperatures and pressures. For convenience further discussion of this system will be given in two parts.

1. SOLUBILITY OF *O*-XYLENE (1) IN WATER (2)

The high temperature, high pressure data of Guseva and Parnov (ref 2) and Alwani and Schneider (ref 5) have been obtained under quite different conditions and thus no Critical Evaluation of their data is possible. However, it may be noted that the data of Guseva and Parnov are frequently unreliable. The interested user is referred to the relevant Data Sheets for experimental values.

At atmospheric pressure all the available data are listed in Table 2 except for the value of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) and has therefore been excluded from consideration.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *o*-Xylene; C_8H_{10}; [95-47-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985.

CRITICAL EVALUATION: (continued)

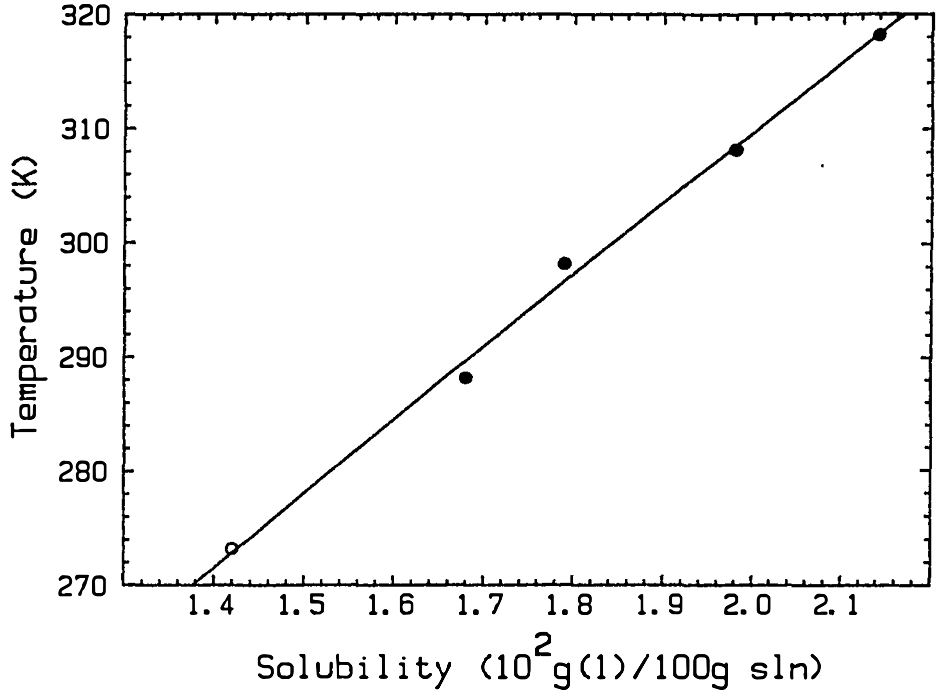

FIGURE 1: Solubility of *o*-xylene in water, selected data: ref 5 (o); ref 10 (●).

2. SOLUBILITY OF WATER (2) IN *O*-XYLENE (1)

The available solubility values for water in *o*-xylene are listed in Table 3. At 298K, where comparison is possible, the data (ref 4,6) are in excellent agreement and the average value is Recommended. The remaining datum at 273K must be regarded as Tentative in the absence of confirmatory data.

TABLE 3: Recommended (*R*) and Tentative Values of the Solubility of Water (2) in *o*-Xylene (1)

T/K	Solubility values		
	Reported values	"Best" values	
	10^2g(2)/100g sln	10^2g(2)/100g sln	10^3 x_2
273	1.85 (ref 6)	1.9	1.1
298	4.5 (ref 4), 4.56 (ref 6)	4.5 (*R*)	2.6 (*R*)

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *o*-Xylene; C_8H_{10}; [95-47-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985

CRITICAL EVALUATION: (continued)

At 298K, the data of McAuliffe (ref 3), Sutton and Calder (ref 7), Price (ref 8) and Sanemasa *et al.* (ref 10) are in excellent agreement and their average is Recommended. The values of Andrews and Keefer (ref 1) and Polak and Lu (ref 6) are markedly higher ($>3\sigma_n$) and are rejected.

At other temperatures only the data of Sanemasa *et al.* (ref 10) are available except for the 273K datum of Polak and Ly (ref 6). These data are therefore regarded as Tentative.

Selected data are plotted in Figure 1.

TABLE 2: Recommended (*R*) and Tentative Solubility Values of *o*-Xylene (1) in Water (2

T/K	Solubility values		
	Reported values	"Best" values ($\pm\ \sigma_n$)^a	
	10^2g(1)/100g sln	10^2g(1)/100g sln	$10^5\ x_1$
273	1.42 (ref 5)	1.4	2.4
288	1.68 (ref 10)	1.7	2.9
298	1.75 (ref 3), 1.705 (ref 7), 1.67 (ref 8), 1.79 (ref 10)	1.73 ± 0.05 (*R*)	2.93 (*R*)
308	1.98 (ref 10)	2.0	3.4
318	2.14 (ref 10)	2.1	3.6

a Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *o*-Xylene; C_8H_{10}; [95-47-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. July 1985

CRITICAL EVALUATION: (continued)

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1. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-7.
2. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76-9.
3. McAuliffe, C. *Nature* 1963, *200*, 1092-3; *J. Phys. Chem.* 1966, *70*, 1267-72.
4. Hoegfeldt, E.; Bolander, B. *Ark. Kemi* 1964, *21*, 161-86.
5. Alwani, Z.; Schneider, G.M. *Ber. Bunsenges.* 1969, *73*, 294-301.
6. Polak, J.; Lu, B. C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
7. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
8. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44; see also Ph.D. Dissertation, 1973, Univ. California, Riverside, CA, U.S.A., quoted in ref 10.
9. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.
10. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) o-Xylene; C_8H_{10}; [95-47-6] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-77.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of o-Xylene in water at 25°C was reported to be 0.0204 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 3.46×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 144.3-144.5°C.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [95-47-6]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Vestn. Mosk. Univ. Khim. 1963, *18*, 76-9.

VARIABLES:

Temperature: 139-251°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of o-xylene in water

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
139	0.047	0.80
162	0.093	1.58
207	0.407	6.93
251	0.960	16.42

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; n_D^{20} 1.5054.

(2) doubly distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [95-47-6]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

Nature (London) 1963, *200*, 1092-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of o-Xylene in water at 25°C was reported to be 0.0175 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 2.97×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+%; used as received.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±1.5°C

Soly. 0.0008 (std. dev. of mean)

REFERENCES:

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [95-47-6]

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

ORIGINAL MEASUREMENTS:

Hoegfeldt, E.; Bolander, B.

Ark. Kemi, 1964, *21,* 161-86.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in o-Xylene was reported to be 0.022 mol(2) L sln.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.045 g(2)/100 g sln and 0.0026.

The assumption that 1.00 L sln = 876 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration in ref 1, 2.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; 0.7% of (m-p) xylene, 0.07% of ethylbenzene; purity 99.0%; used as received.

ESTIMATED ERROR:

Temp. ±0.3 C

Soly. ±0.002 mol(2) L^{-1} sln (type of error not specified)

REFERENCES:

1. Hardy, C.J.; Greenfield, B.F.; Scargill, D. *J. Chem. Soc.* 1961, *90.*
2. Johansson, A. *Sv. Papperstidn.* 1947, *11B,* 124.

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [95-47-6]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C.-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of o-xylene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	10^5x_1 (compiler)
0(a)	142(c)	0.0142	2.41
25(b)	213(c)	0.0213	3.61

Solubility of water in o-xylene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	10^3x_2 (compiler)
0(a)	185(d)	0.0185	1.09
25(b)	456(e)	0.0456	2.68

a-e See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.
The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Organics, pure grade reagent; shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. (a) ± 0.02°C, (b) ± 0.01°C
soly. (c) ± 1.7%, (d) ± 4.7%,
(e) ± 3.1% (from two or three determinations)

REFERENCES:

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [95-47-6]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of o-xylene in water at 25°C was reported to be 170.5 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.01705 g(1)/100 g sln and 2.892×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 2.5 mg(1)/kg(2)

(the standard deviation of the mean for six replicates)

REFERENCES:

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [97-47-6]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of o-xylene in water at 25°C and at system pressure was reported to be 167.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0167 g(1)/100 g sln and 2.83×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 4.0 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [97-47-6]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of o-xylene in water at 25°C was reported to be 167.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0167 g(1)/100 g sln and 2.83×10^{-5}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostated at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 4.2 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) *o*-Xylene; C_8H_{10}; [97-47-6] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.
VARIABLES:	**PREPARED BY:**
Temperature: 15-45°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *o*-xylene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)[a]	$10^5\ x_1$ (compiler)[a]
15	1.58 ± 0.11	0.0168	2.85
25	1.68 ± 0.06	0.0179	3.04
35	1.85 ± 0.02	0.0198	3.35
45	2.00 ± 0.02	0.0214	3.64

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.1°C.

REFERENCES:

1. Kell, G.S.
   J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.;
   Deguchi, Y.; Nagai, H.
   Chem. Lett. 1981, 225-8.

COMPONENTS:

(1) o-Xylene; C_8H_{10}; [95-47-6]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of o-xylene in artificial seawater is reported to be 129.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 0.01296 g(1)/100 g sln and 2.26×10^{-5} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 1.8 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:	EVALUATOR:
(1) *m*-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986

CRITICAL EVALUATION:

Quantitative solubility data for the *m*-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the *m*-Xylene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 2)	274-313	(1) in (2)	spectrophotometric
Pryor and Jentoft (ref 3)	344-544	(1) in (2)	synthetic
Guseva and Parnov (ref 4)	400-512	(1) in (2)	unspecified[a]
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer
Englin *et al.* (ref 6)	283-303	(2) in (1)	analytical
Polak and Lu (ref 7)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 8)	298	(1) in (2)	GLC
Chernoglazova and Simulin (ref 9)	293-343	mutual	synthetic, GLC
Price (ref 10)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 11)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 12)	288-318	(1) in (2)	spectrophotometric

a The synthetic method was probably used.

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

1. SOLUBILITY OF *M*-XYLENE (1) IN WATER (2)

All the available data for the solubility of *m*-xylene in water at low temperatures ($T \le 343$K) are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 11) which does not appear to be independent of that of Price (ref 10) and has therefore been excluded from consideration.

The data are in general in reasonable agreement although with a few exceptions the agreement is insufficient for the average values to be Recommended. Selected data from Table 2 are plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *m*-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of *m*-Xylene (1) in Water (2)

T/K	Solubility values Reported values[a] $10^2 g(1)/100g$ sln	"Best" values (± σ_n)[b] $10^2 g(1)/100g$ sln	 10^5 x_1
273	2.10* (ref 2), 1.96 (ref 7)	2.03 ± 0.07 (*R*)	3.44 (*R*)
283	1.97* (ref 2)	2.0	3.4
293	1.95* (ref 2), 1.6 (ref 9) 1.60* (ref 12)	1.7 ± 0.2	2.9
298	1.73 (ref 1), 1.96 (ref 2), 1.62 (ref 7), 1.46 (ref 8), 1.7* (ref 9), 1.34 (ref 10), 1.62 (ref 12)	1.6 ± 0.2	2.7
303	1.98* (ref 2), 1.8* (ref 9), 1.65* (ref 12)	1.8 ± 0.1	3.1
313	2.19* (ref 2), 2.2 (ref 9)	2.20 (*R*)	3.73 (*R*)
323	2.6* (ref 9), 2.0* (ref 12)	2.3 ± 0.3	3.9
333	3.2* (ref 9)	3.2	5.4
343	3.5* (ref 3)	3.5	5.9

[a] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

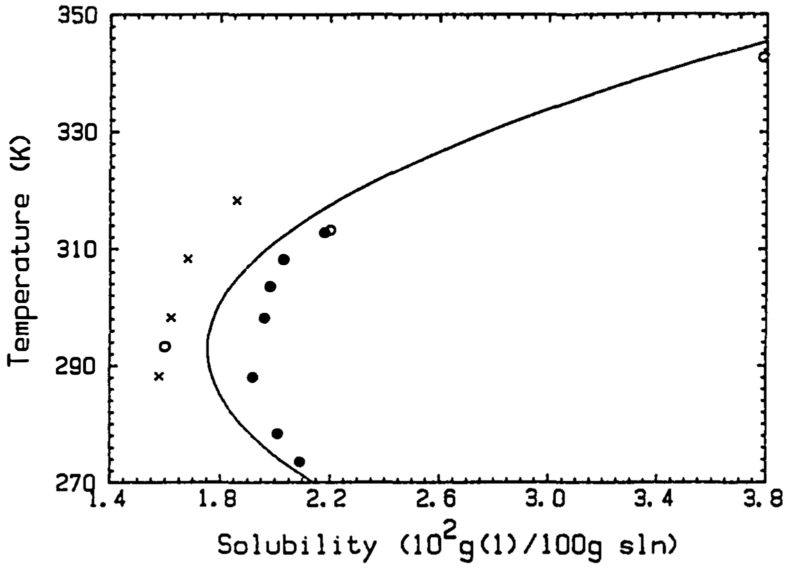

FIGURE 1. Solubility of *m*-xylene in water; selected data: ref 2 (●); ref 9 (o); ref 12 (x). Solid curve fitted to "Best" values (Table 2).

(continued next page)

COMPONENTS:

(1) *m*-Xylene; C_8H_{10}; [108-38-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION: (continued)

Table 3 summarizes thermodynamic functions calculated by application of the van't Hoff equation to the solubility data obtained over various temperature ranges. At low temperatures (T < 343K) the values of ΔH_{sln} and $\Delta C_{p,sln}$ from the data of Bohon and Claussen (ref 2) and Sanemasa *et al.* (ref 12) are in good agreement (Table 3) and are close to calorimetric values reported for similar systems (*e.g.* benzene in water, ref 13). However, the ΔH_{sln} derived from the data of Chernoglazova and Simulin (ref 9) is much too positive.

TABLE 3: Thermoydnamic Functionf for the Dissolution of *m*-Xylene in Water Derived from Solubility Data

Reference	ΔH_{sln} kJ mol^{-1}	$\Delta C_{p,sln}$ J K^{-1} mol^{-1}
Bohon and Claussen (ref 2)	2.8	386
Pryor and Jentoft (ref 3)	8.6	200
Guseva and Parnov (ref 4)	36.7	55
Chernoglazova and Simulin (ref 9)	11.4	167
Sanemasa (ref 12)	2.6	317
"Best" values (Table 2)	2.9	516

2. SOLUBILITY OF *M*-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for *m*-xylene in water at elevated temperatures (*ca.* 340-550K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 14). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of comfirmatory studies it is difficult to know which values are more reasonable. However, it may be noted that the thermodynamic functions derived from the data of Pryor and Jentoft are more reasonable than those obtained from Guseva and Parnov's work (Table 3). The interested user is referred to the relevant Data Sheets for the experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *m*-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

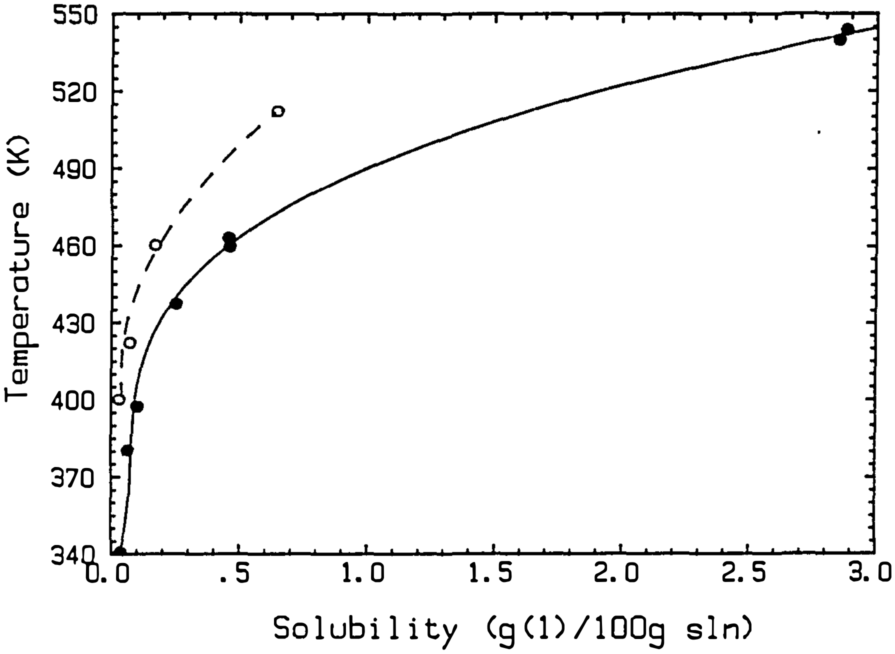

FIGURE 2. Solubility of *m*-xylene in water at elevated temperatures and system pressure: ref 3 (●); ref 4 (o).

3. SOLUBILITY OF WATER (2) IN *M*-XYLENE (1)

All the reported data for the solubility of water in *m*-xylene are collected in Table 4. The data from independent studies over a range of temperatures are in excellent agreement, enabling a number of values to be Recommended (σ_n ~ 5% relative).

Selected data from Table 4 are also plotted in Figure 3 which emphasizes the general agreement.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *m*-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

TABLE 4: Recommended (*R*) and Tentative Values of the Solubility of Water (2) in *m*-Xylene (1)

T/K	Solubility values		
	Reported values[a]	"Best" values (± σ_n)[b]	
	10^2g(2)/100g sln	10^2g(2)/100g sln	10^3x_2
273	1.88 (ref 7)	1.9	1.1
283	2.89 (ref 6), 2.8* (ref 7)	2.9 ± 0.1 (*R*)	1.7(*R*)
293	4.02 (ref 6), 3.7* (ref 7), 3.4 (ref 9)	3.7 ± 0.3 (*R*)	2.2(*R*)
298	4.4 (ref 5), 4.7* (ref 6), 4.32 (ref 7), 4.0 (ref 9)	4.4 ± 0.3 (*R*)	2.6(*R*)
303	5.36 (ref 6), 4.8 (ref 9)	5.1 ± 0.3 (*R*)	3.0(*R*)
313	6.7 (ref 9)	6.7	6.7
323	10* (ref 9)	10	5.9
333	14* (ref 9)	14	8.3
343	19* (ref 9)	19	11

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.
b Calculated by averaging where appropriate; σ_n has no statistical significance.

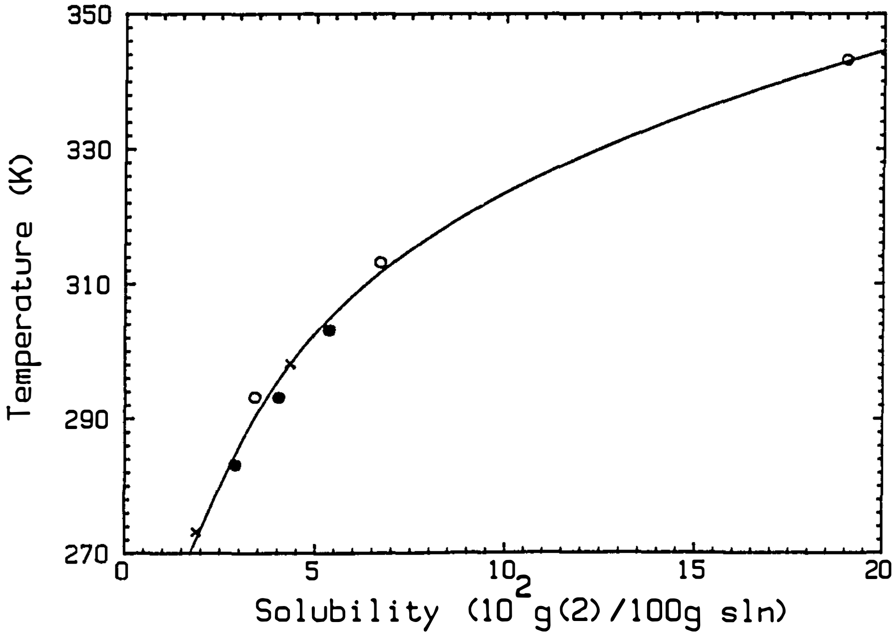

FIGURE 3. Solubility of water in *m*-xylene: ref 6 (●); ref 7 (x); ref 9 (o).

(continued next page)

COMPONENTS:

(1) *m*-Xylene; C_8H_{10}; [108-38-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION: (continued)

Application of the van't Hoff equation to the data of Englin *et al.* (ref 6) and Chernoglazova and Simulin (ref 9) gives values for ΔH_{sln} of 21.3 and 24.9 kJ mol^{-1} and for $\Delta C_{p,sln}$ of -152 and 208 J K^{-1} mol^{-1} respectively. Comparison with related systems (*e.g.* water in benzene) suggests the data of Chernoglazova and Simulin (ref 9) may be more reliable.

REFERENCES

1. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-7.

2. Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73* 1571-8.

3. Pryor, W.A.; Jentoft, R.E. *J. Chem. Eng. Data* 1961, *6*, 36-7.

4. Guseva, A.N.; Parnov, E.T. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76-9.

5. Hoegfeldt, E.; Bolander, B. *Ark. Kemi* 1964, *21*, 161-86.

6. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

7. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

8. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.

9. Chernoglazova, F.S.; Simulin, Yu.N. *Zh. Fiz. Khim.* 1976, *50*, 809; Deposited doc. 1976, VINITI 3528-75.

10. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *6*, 213-44.

11. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

12. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

13. Gill, S.J.; Nichols, N.F.; Wadso, I. *J. Chem. Thermodyn.* 1976, *8*, 445-52.

ACKNOWLEDGEMENT

The evaluator thanks Dr Brian Clare for the regression analyses and graphics.

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1949, *71*, 3644-77.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of m-Xylene in water at 25°C was reported to be 0.0173 g(1)/100 g sln. (value updated from original paper)

The corresponding mole fraction, *x*1, calculated by the compilers is 2.93 x 10-5.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. 139.5°C.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1571-8.
VARIABLES:	PREPARED BY:
Temperature: 0.4-39.6°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of m-xylene in water

t/°C	g(1)/100g sln[a] (compiler)	$10^5 x_1$ (compiler)
0.4	0.0209	3.54
5.2	0.0201	3.41
14.9	0.0192	3.25
21.0	0.0196	3.33
25.0	0.0196[b]	3.33[b]
25.6	0.0196	3.33
30.3	0.0198	3.36
34.9	0.0203	3.44
39.6	0.0218	3.69

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

[b] Given in the original paper as 0.196g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe] 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

(1) Oronite Chemical Co. was sulphonated, hydrolysed, steam distilled, washed, dried by passing through silica gel and finally distilled. Purity was judged by refractometry (no value given).

(2) Air-free conductivity water (no details given).

ESTIMATED ERROR:

Temp. ± 0.02°C
Soly. ± 0.5% relative

REFERENCES:

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Pryor, W.A.; Jentoft, R.E.

J. Chem. Eng. Data 1961, *6*, 36-7.

VARIABLES:

Temperature: 67.7-270.6°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of m-xylene in water

t/°C				
Cloud point appears	Cloud point disappears	Midpoint	10^3x_1	g(1)/100 g sln (compiler)
64.4	71.1	67.7	0.0590	0.0348
105.6	109.0	107.3	0.1127	0.0664
122.7	125.6	124.2	0.1749	0.1031
162.7	165.6	164.2	0.4265	0.2509
185.6	187.3	186.4	0.7825	0.4595
187.8	190.0	189.9	0.7762	0.4559
264.4	268.9	266.6	4.956	2.852
-	270.6	270.6	5.00	2.88

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixture of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4-liter stirred silicone oil bath, and the bath was heated until the (1) dissolved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud disappeared. The cycle was repeated three to four times until reliable appearance and disappearance temperatures for the cloud were recorded.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; 99.8% by freezing point; main impurities are isomeric xylenes; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Vestn. Mosk. Univ. Khim. 1963, *18*, 76-9.

VARIABLES:

Temperature: 127-239°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of m-xylene in water

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
127	0.031	0.53
149	0.072	1.22
187	0.168	2.85
239	0.648	11.06

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; n_D^{20} 1.4974.

(2) doubly distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Hoegfeldt, E.; Bolander, B.

Ark. Kemi, 1964, *21*, 161-86.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in m-Xylene was reported to be 0.021 mol (2) L^{-1} sln.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.044 g(2)/100 g sln and 0.0026.

The assumption that 1.00 L sln = 860 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration in ref 1, 2.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; 0.3% of ethylbenzene, 0.03% of o-Xylene; purity 99.6%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.03°C

Soly. ±0.001 mol(2) L^{-1} sln (type of error not specified)

REFERENCES:

1. Hardy, C.J.; Greenfield, B.F.; Scargill, D. *J. Chem. Soc.* 1961, *90*.
2. Johansson, A. *Sv. Papperstidn.* 1947, *11B*, 124.

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in m-Xylene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
10	0.0289	1.70
20	0.0402	2.37
30	0.0536	3.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C.-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of m-xylene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^5 x_1$ (compiler)
0(a)	196(c)	0.0196	3.32
25(b)	162(c)	0.0162	2.75

Solubility of water in m-xylene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
0(a)	188(d)	0.0188	1.11
25(b)	432(e)	0.0432	2.54

a-e See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99+%); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. (a) ± 0.02°C, (b) ± 0.01°C

soly. (c) ± 1.7%, (d) ± 4.7%,

(e) ± 3.1% (from two or three determinations)

REFERENCES:

COMPONENTS: (1) m-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of m-xylene in water at 25°C was reported to be 146.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.01460 g(1)/100 g sln and 2.48×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The concentration of (1) in (2) was determined by gas chromatography.	**SOURCE AND PURITY OF MATERIALS:** (1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 0.1°C soly. 1.6 mg(1)/kg(2) (the standard deviation of the mean for six replicates)
	REFERENCES:

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Chernoglazova, F.S.; Simulin, Yu.N.

Zh. Fiz. Khim. 1976, *50*, 809.
Deposited doc. 1976,
VINITI 3528-75.

VARIABLES:

Temperature: 20-70°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of m-Xylene in Water

t/°C	g(1)/100 g sln	$10^5\, x_1$ (compiler)
20	0.016	2.7
40	0.022	3.7
70	0.038	6.4

Solubility of Water in m-Xylene

t/°C	g(2)/100 g sln	$10^3\, x_2$ (compiler)
20	0.034	2.0
40	0.067	3.9
70	0.190	11.1

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by the synthetic method of Fuhner, ref 1. Glass tubes filled with 50-100 mL of (2) were frozen and then (1) was micropipetted. Next, the tubes were sealed and thermostatted for 6 hrs at 70°C and 72 hrs at 20°C. The solubility was followed visually. The samples were incremented at regular steps 0.005 g (1)/ 100 g (2). The mean value from 5-6 determinations was adopted.

The solubility of (2) in (1) was determined by gas chromatography. The LKhM-7a instrument equipped with a katharometer was employed.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; 99.9 purity by glc.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Fuhner, H.; *Chem. Ber.* 1924, *57*, 514.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C_8H_{10}; [108-38-3] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of m-xylene in water at 25°C and at system pressure was reported to be 134.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0134 g(1)/100 g sln and 2.27×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 2.0 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) m-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of m-xylene in water at 25°C was reported to be 134.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0134 g(1)/100 g sln and 2.27×10^{-5}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 3.4 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) *m*-Xylene; C_8H_{10}; [108-38-3]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *m*-xylene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)[a]	10^5 x_1 (compiler)[a]
15	1.49 ± 0.04	0.0158	2.68
25	1.52 ± 0.06	0.0162	2.75
35	1.57 ± 0.10	0.0168	2.85
45	1.73 ± 0.08	0.0186	3.15

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.1°C.

REFERENCES:

1. Kell, G.S.
J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.;
Deguchi, Y.; Nagai, H.
Chem. Lett. 1981, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) m-Xylene; C_8H_{10}; [108-38-3] (2) Artificial seawater (ref 1)	Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	**PREPARED BY:** M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of m-xylene in artificial seawater is reported to be 106.0 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 0.01060 g(1)/100 g sln and 1.85×10^{-5} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.6 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) *p*-Xylene; C_8H_{10}; [106-42-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the *p*-xylene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the *p*-Xylene (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 2)	274-316	(1) in (2)	spectrophotometric
Pryor and Jentoft (ref 3)	316-577	(1) in (2)	synthetic
Guseva and Parnov (ref 4)	414-531	(1) in (2)	unspecified
Hoegfeldt and Bolander (ref 5)	298	(2) in (1)	Karl Fischer
Polak and Lu (ref 6)	273,298	mutual	GLC, Karl Fischer
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Kirchnerova and Cave (ref 8)	298	(2) in (1)	Karl Fischer
Price (ref 9)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 10)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 11)	288-318	(1) in (2)	spectrophotometric

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience, further discussion of this system will be divided into three parts.

1. SOLUBILITY OF *p*-XYLENE (1) IN WATER (2)

All the available data on the solubility of *p*-xylene in water are summarized in Table 2 with the exception of the high temperature data of Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4) which are discussed in the next section. The 298K datum of Krzyzanowska and Szeliga (ref 10) has also been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 9).

The various data for *p*-xylene in water (Table 2) are in only fair agreement and none of the averaged values are Recommended. At 298K the values cluster around two values: 0.019 (ref 1, 2, 6) and 0.016 g(1)/100g sln (ref 6, 7, 9, 11). Although the values of Bohon and Claussen (ref 2) in well characterized systems are often high this is not sufficient justification for favouring the lower values (ref 7, 9, 11) at this stage. At other temperatures,

(continued next page)

COMPONENTS:

(1) *p*-Xylene; C_8H_{10}; [106-42-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of *p*-Xylene (1) in Water (2)

T/K	Solubility values Reported values[a] 10^2g(1)/100g sln	"Best" values (± σ_n)[b] 10^2g(1)/100g sln	 10^5 x_1
273	1.55[c] (ref 2), 1.64 (ref 6)	1.60 ± 0.05	2.7
283	1.97 (ref 2)	2.0	3.4
293	1.96* (ref 2), 1.60* (ref 11)	1.8 ± 0.2	3.1
298	2.00 (ref 1), 1.98 (ref 2), 1.85 (ref 6), 1.56 (ref 7), 1.57 (ref 9), 1.63 (ref 11)	1.8 ± 0.2	3.1
303	2.02* (ref 2), 1.68 (ref 11)	1.9 ± 0.2	3.2
313	2.20* (ref 2), 2.5* (ref 3), 1.75 (ref 11)	2.2 ± 0.3	3.7
323	2.8* (ref 3)	2.8	4.7
333	3.2* (ref 3)	3.2	5.4
343	3.6* (ref 3)	3.6	6.1
353	4.2* (ref 3)	4.2	7.1
363	4.8* (ref 3)	4.8	8.1

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original data.
b Obtained by averaging where appropriate; σ_n has no statistical significance.
c Refers to solubility of solid.

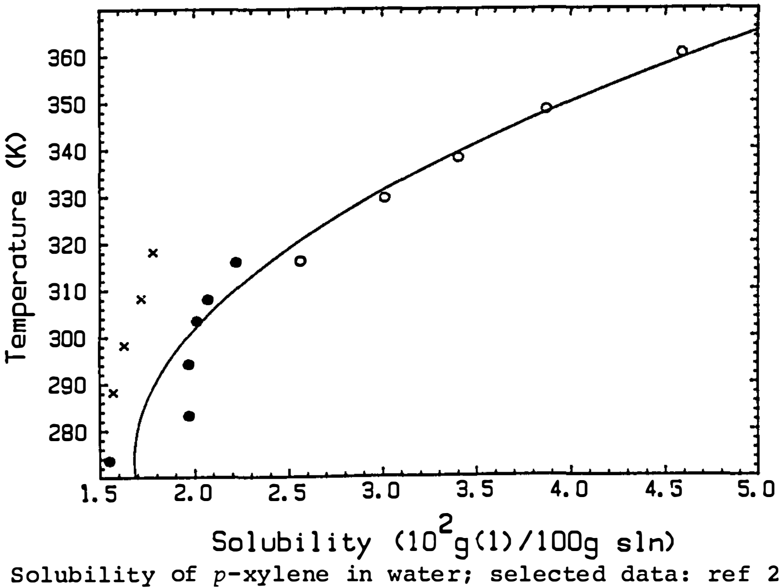

FIGURE 1. Solubility of *p*-xylene in water; selected data: ref 2 (●), ref 3 (o); ref 11 (x). Solid line drawn through "Best" values (Table 2).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *p*-Xylene; C_8H_{10}; [106-42-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

agreement is equally poor and at higher temperatures (323-363K) only the values of Pryor and Jentoft (ref 3) are available. Clearly this system warrants further investigation. Selected data have been plotted in Figure 1 which emphasizes the differences among the available data.

Thermodynamic functions derived from various data sets by application of the van't Hoff equation are summarized in Table 3.

TABLE 3: Thermodynamic Functions for the Dissolution of *p*-Xylene in Water Derived from Solubility Data

Reference	ΔH_{sln} kJ mol^{-1}	$\Delta C_{p,sln}$ J K^{-1} mol^{-1}
Bohon and Claussen (ref 2)	3.9	-211
Pryor and Jentoft (ref 3)	7.8[a] 30.4[b]	122[a] 81[b]
Guseva and Parnov (ref 4)	16.0	210
Sanemasa *et al.* (ref 11)	3.2	11
"Best" values (Table 2)	6.9	204

[a] $316 < T < 360$ K
[b] $434 < T < 568$ L

Comparison of the thermodynamic data in Table 3 with similar but better characterized hydrocarbon systems (*e.g.* benzene in water) suggests that none of the solubility data for *p*-xylene in water are very reliable (including the "Best" values).

2. SOLUBILITY OF *p*-XYLENE (1) IN WATER (2) AT ELEVATED TEMPERATURES

Solubility data for *p*-xylene in water at elevated temperatures (*ca.* 400-570K) and system pressure in sealed tubes have been reported by Pryor and Jentoft (ref 3) and Guseva and Parnov (ref 4). The results are plotted in Figure 2 and are clearly in poor agreement. In the absence of confirmatory data it is not possible to know which set is more reasonable. Thermodynamic functions derived from both data sets (Table 3) are in poor agreement and differ markedly from low *T* values. The interested user is referred to the relevant Data Sheets for the experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *p*-xylene; C_8H_{10}; [106-42-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

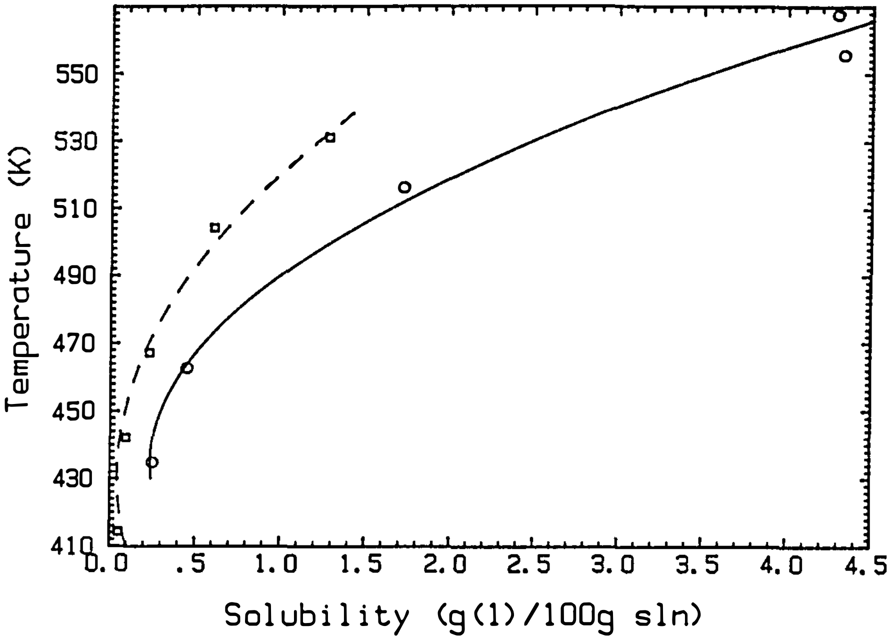

FIGURE 2. Solubility of *p*-xylene in water at elevated temperatures: ref 3 (o); ref 4 (□).

3. THE SOLUBILITY OF WATER (2) IN *p*-XYLENE (1)

The solubility of water in *p*-xylene has been determined only at 298K. All the available data are collected in Table 4. The results are in excellent agreement and the mean is Recommended.

TABLE 4: Recommended (*R*) Value of the Solubility of Water (2) in *p*-Xylene (1)

T/K	Solubility values Reported values $10^2 g(2)/100g$ sln	"Best" value (± σ_n)^a $10^2 g(2)/100g$ sln	$10^3\ x_2$
298	4.5 (ref 5), 4.40 (ref 6), 4.57 (ref 8)	4.5 ± 0.1 (*R*)	2.6 (*R*)

a Obtained by averaging; σ_n has no statistical significance.

REFERENCES

1. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-7.

2. Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1571-8.

3. Pryor, W.A.; Jentoft, R.E. *J. Chem. Eng. Data* 1961, *6*, 36-7.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *p*-Xylene; C_8H_{10}; [106-42-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

4. Guseva, A.N.: Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76-9.

5. Hoegfeldt, E.; Bolander, B. *Ark. Kemi* 1964, *21*, 161-86.

6. Polak, J.; Lu, B.C.-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

7. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.

8. Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* 1976, *54*, 3909-16.

9. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44; see also Ph.D. Dissertation 1974, University of California, Riverside, CA, U.S.A., 1973, quoted in ref 22.

10. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

11. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the regression analyses and graphics.

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1949, *71*, 3644-77.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of p-Xylene in water at 25°C was reported to be 0.0200 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 3.39×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25 C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. 138.5 C.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Bohon, R.L.; Claussen, W.F.

J. Am. Chem. Soc. 1951, *73*, 1571-8.

VARIABLES:

Temperature: 0.4-42.8°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of p-xylene in water

t/°C	g(1)/100g sln[a] (compiler)	$10^5 x_1$ (compiler)
0.4	0.0156[b]	2.64[b]
10.0	0.0188[b]	3.19[b]
10.0	0.0197	3.34
14.9	0.0195	3.31
21.0	0.0197	3.34
25.0	0.0198[c]	3.36[c]
25.6	0.0199	3.37
30.2	0.0201	3.41
30.3	0.0204	3.46
34.9	0.0207	3.51
35.2	0.0207	3.51
42.8	0.0222	3.76

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

[b] Data refer to solubility solid (1) in (2).

[c] Given in the original paper as 0.198g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co., purified by recrystallization from ethanol, washing, filtering through silica gel then distilling. Purity was determined by refractometry (no details given).

(2) Air-free conductivity water, no other details given.

ESTIMATED ERROR:

Temp. ± 0.02°C

Soly. ± 0.5% relative

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Pryor, W.A.; Jentoft, R.E.

J. Chem. Eng. Data 1961, *6*, 36-7.

VARIABLES:

Temperature: 43.0-294.5°

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of p-xylene in water

t/°C				
Cloud point appears	Cloud point disappears	Midpoint	$10^3 x_1$	g(1)/100 g sln (compiler)
42.8	43.3	43.0	0.0434	0.0256
54.4	58.3	56.4	0.0510	0.0301
61.7	68.3	65.0	0.0576	0.0340
73.9	76.7	75.3	0.0656	0.0387
85.0	89.4	87.2	0.0779	0.0459
161.7	163.3	162.5	0.4264	0.2508
186.7	189.5	188.1	0.7686	0.4514
241.6	244.9	243.2	2.9555	1.7174
280.5	284.4	282.5	7.6238	4.3326
291.6	298.3	294.5	7.5407	4.2871

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixture of (1) and (2) were carefully weighed into glass ampoules. The ampoules were sealed allowing just enough space for thermal expansion. The ampoule, observed through a telescope from behind a safety barrier, was suspended in a 4-liter stirred silicone oil bath, and the bath was heated until the (1) dissolved. On cooling, a cloud of fine (1) droplets appeared, making the suspension opaque. The temperature was raised until the cloud disappeared. The cycle was repeated three to four times until reliable appearance and disappearance temperatures for the cloud were recorded.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; 99.1% by freezing point; main impurities are isomeric xylenes; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Vestn. Mosk. Univ. Khim. 1963, *18*, 76-9.

VARIABLES:

Temperature: 141 - 258°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of p-xylene in water

t/°C	g(1)/100 g sln	10^4x_1 (compiler)
141	0.049	0.83
169	0.096	1.63
194	0.231	3.93
231	0.607	10.34
258	1.283	22.00

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; n_D^{20} 1.4958.

(2) doubly distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Hoegfeldt, E.; Bolander, B.

Ark. Kemi, 1964, *21*, 161-86.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in p-Xylene was reported to 0.022 mol(2) L^{-1} sln.

The corresponding mass percent and mol fraction, x_2, calculated by the compilers are 0.045 g(2)/100 g sln and 0.0027.

The assumption that 1.00 L sln = 857 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The water determination was carried out according to Johansson's modification of the Karl Fischer titration described in ref 1, 2.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; 0.04% of ethylbenzene; purity 99.8%; used as received.

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.3°C

Soly. ±0.002 mol(2) L^{-1} sln (type of error not specified)

REFERENCES:

1. Hardy, C.J.; Greenfield, B.F.; Scargill, D. *J. Chem. Soc.* 1961, *90*.
2. Johansson, A. *Sv. Papperstidn.* 1947, *11B*, 124.

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C.-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of p-xylene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^5 x_1$ (compiler)
0† (a)	164 (c)	0.0164	2.78
25 (b)	185 (c)	0.0185	3.14

The solubility of water in p-xylene at 25°C was reported to be 440 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0440 g(2)/100 g sln and 2.59×10^{-3}.

a-c See "Estimated Error"

†p-xylene was at supercooled liquid state.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.
The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Organics, pure grade reagent; shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. (a) ± 0.02°C, (b) ± 0.01°C
soly. (c) ± 1.7% (from two or three determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Xylene; C_8H_{10}; [106-42-3] (2) Water; H_2O; [7732-18-5]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* 1974, *54*, 3909-16.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in p-xylene at 25°C was reported to be 0.0217 mol(2)/L and x_2 = 0.00269. The corresponding mass percent calculated by the compilers is 0.0457 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) was placed in the equilibration vessel. A test tube containing 6 mL of (2) was then placed in the vessel so that the rim of the test tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag, and the jacketed vessel was emersed up to its neck in a water thermostat. Trials had shown that the stoichiometric concentration of (1) in (2) became constant within 2 days.
The stoichiometric concentration of water was determined by a conventional Karl Fischer dead-stop back-titration.

SOURCE AND PURITY OF MATERIALS:

(1) Fisher 277; purified by double crystallization.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.0002 mol(2) dm^{-3} sln
(standard deviation from 5 determinations).

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C was reported to be 156.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.01560 g(1)/100 g sln and 2.65×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 1.6 mg(1)/kg(2)
(the standard deviation of the mean for six replicates)

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C and at system pressure was reported to be 157.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0157 g(1)/100 g sln and 2.66×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 1.0 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of p-xylene in water at 25°C was reported to be 157.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0157 g(1)/100 g sln and 2.66×10^{-5}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150-mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 3.9 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) *p*-Xylene; C_8H_{10}; [106-42-3]
(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55* , 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *p*-xylene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)[a]	10^5 x_1 (compiler)[a]
15	1.48[b]	0.0157	2.67
25	1.53 ± 0.07	0.0163	2.76
35	1.61 ± 0.08	0.0172	2.92
45	1.66 ± 0.05	0.0178	3.02

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

[b] No error given.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.1°C.

REFERENCES:

1. Kell, G.S. *J. Chem. Eng. Data* 1975, *20* , 97.

2. Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. *Chem. Lett.* 1981, 225-8.

COMPONENTS:

(1) p-Xylene; C_8H_{10}; [106-42-3]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of p-xylene in artificial seawater is reported to be 110.9 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 0.01109 g(1)/100 g sln and 1.93×10^{-5} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.9 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

October 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the ethylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Ethylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Führer (ref 1)	288	(1) in (2)	titration
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Klevens (ref 3)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 4)	273-316	(1) in (2)	spectrophotometric
Filippov and Furman (ref 5)	291-323	(2) in (1)	synthetic
Morrison and Billett (ref 6)	298	(1) in (2)	analytical
Jones and Monk (ref 7)	298-308	(2) in (1)	radiotracer
McAuliffe (ref 8)	298	(1) in (2)	GLC
Guseva and Parnov (ref 9)	338-507[a]	(1) in (2)	unspecified
Englin *et al.* (ref 10)	283-303	(2) in (1)	analytical
McAuliffe (ref 11)	298	(1) in (2)	GLC
Polak and Lu (ref 14)	273,298	mutual	GLC, Karl Fischer
Brown and Wasik (ref 15)	278-293	(1) in (2)	chromatographic
Sutton and Calder (ref 16)	298	(1) in (2)	GLC
Price (ref 17)	298	(1) in (2)	GLC
Korenman and Aref'eva (ref 18)	293	(1) in (2)	titration
Korenman and Aref'eva (ref 19)	298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 20)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 21,22)	288-318	(1) in (2)	spectrophotometric
Sanemasa *et al.* (ref 23)	298	(1) in (2)	spectrophotometric
Heidman *et al.* (ref 24)	311-568[a]	mutual	GLC, Karl Fischer

[a] Pressure also varied, see Table 6.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Critical phenomena at high pressures have been reported by Alwani and Schneider (ref 12) and Roof (ref 13) and are discussed along with the high pressure solubility data (ref 9, 24) in Section 3 below. For convenience, further discussion of this system will be divided into three parts.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

In the tables which follow values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original authors' experimental data. "Best" values have been obtained by averaging all non-rejected data. Standard deviations (σ_n) have been included as a convenient measure of the spread of experimental results: they do not have any statistical significance.

1. SOLUBILITY OF ETHYLBENZENE (1) IN WATER (2)

Of the data available on the solubility of ethylbenzene in water, values of Bohon and Claussen (ref 4) and Korenman and Aref'eva (ref 18) have been rejected because they are significantly higher (by about 10%) than all other studies. The value of Price (ref 17) at 298K is markedly lower than all other studies and is also rejected. The datum of Krzyzanowska and Szeliga (ref 20) has been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 17). The remaining data are summarized in Table 2 and are generally in excellent agreement even though few studies have covered the same temperature range (which has limited the number of Recommended values). Selected data are also plotted in Figure 1.

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of Ethylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values (± σ_n)	
	10^2g(1)/100g sln	10^2g(1)/100g sln	10^5 x_1
273	1.97 (ref 14)	2.0	3.4
283	1.84* (ref 15)	1.8	3.1
293	1.84* (ref 15), 1.77 (ref 21)	1.81 ± 0.04 (*R*)	3.07 (*R*)
298	1.68 (ref 2), 1.75 (ref 3), 1.65 (ref 6), 1.59 (ref 8), 1.52 (ref 11), 1.77 (ref 14), 1.61 (ref 16), 1.8 (ref 19), 1.81 (ref 21), 1.69 (ref 22), 1.72 (ref 23)	1.69 ± 0.09 (*R*)	2.87 (*R*)
303	1.86* (ref 21)	1.9	3.2
313	2.03* (ref 21), 1.97^a (ref 24)	2.00 ± 0.03 (*R*)	3.39 (*R*)
323	2.19^a (ref 24)	2.2	3.7
333	2.47^a (ref 24)	2.5	4.2
343	2.83^a (ref 24)	2.8	4.8

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility values			
	Reported values		"Best" values ($\pm\ \sigma_n$)	
	10^2g(1)/100g sln		10^2g(1)/100g sln	$10^5\ x_1$
353	3.28^a	(ref 24)	3.3	5.6
363	3.86^a	(ref 24)	3.9	6.6
373	4.60^a	(ref 24)	4.6	7.8

a Calculated over the stated experimental range from the fitting equation given by the original authors.

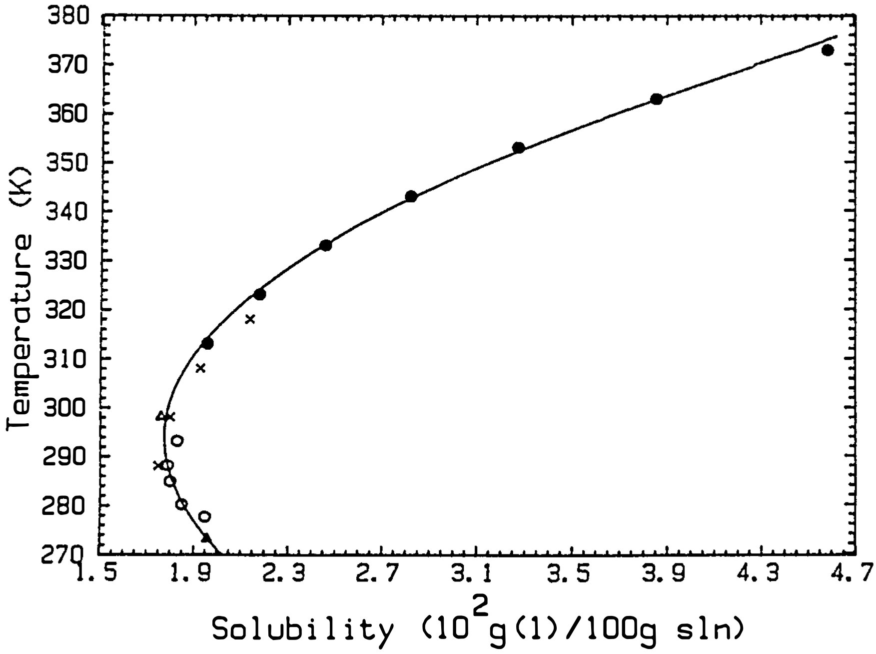

FIGURE 1: Solubility of ethylbenzene in water, selected data: ref 14 (Δ); ref 15 (o); ref 21 (x); ref 24 (●). The solid curve has been fitted to the "Best" values (Table 2).

Thermodynamic functions for the dissolution of ethylbenzene in water derived by application of the van't Hoff equation are summarized in Table 3. With the exception of the data of Brown and Wasik (ref 15) which were obtained over a limited temperature range (Table 1), the ΔH_{sln} and $\Delta C_{p,sln}$ derived from the various values are quite close to reliable calorimetric values reported for the dissolution of benzene in water. This gives added confidence to the solubility data in Table 2. (continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

TABLE 3: Thermodynamic Functions for the Dissolution of Ethylbenzene in Water Derived from Solubility Data

Reference	ΔH_{sln} kJ mol^{-1}	$\Delta C_{p,sln}$ J K^{-1} mol^{-1}
Brown and Wasik (ref 15)	11.9	1123
Sanemasa *et al.* (ref 21)	3.6	319
Sanemasa *et al.* (ref 22)	3.9	230
Heidman *et al.* (ref 24)	4.5	213
"Best" values (Table 2)	2.1	275

2. SOLUBILITY OF WATER (2) IN ETHYLBENZENE (1)

With the exception of the data of Jones and Monk (ref 7) which are reported in v/v fractions, all the available values for the solubility of water in ethylbenzene are summarized in Table 4 below. Unfortunately, few of the determinations cover the same temperature range. Where comparison is possible at lower temperatures ($T \leq 298$K) independent determinations are in reasonable agreement. At higher temperatures ($T > 298$K) the values of Filippov and Furman (ref 5) and Heidman *et al.* (ref 24) show an increasing divergence with increasing temperature (Figure 2).

TABLE 4: Recommended (R) and Tentative Values of the Solubility of Water (2) in Ethylbenzene (1)

T/K	Solubility values		
	Reported values	"Best" values ($\pm \sigma_n$)	
	10^2g(2)/100g sln	10^2g(2)/100g sln	10^3 x_2
273	1.78 (ref 14)	1.8	1.1
283	2.75 (ref 10)	2.8	1.7
293	3.3* (ref 5), 3.73 (ref 10)	3.5 ± 0.2	2.1
298	4.2* (ref 5), 4.4* (ref 10), 4.42 (ref 14)	4.3 ± 0.1 (R)	2.5 (R)
303	5.9* (ref 5), 5.02 (ref 10)	5.5 ± 0.5	3.2
313	9.6* (ref 5), 7.2^a (ref 24)	8 ± 1	5
323	13.3* (ref 5), 9.68^a (ref 24)	11 ± 2	6
333	12.9^a (ref 24)	13	8
343	16.9^a (ref 24)	17	10
353	21.9^a (ref 24)	22	13
363	28.0^a (ref 24)	28	17
373	35.6^a (ref 24)	36	21

---

[a] Calculated over the stated experimental range by the fitting equation given by the original authors.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; 100-41-4 (2) Water; H_2O; 7732-18-5	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986

CRITICAL EVALUATION: (continued)

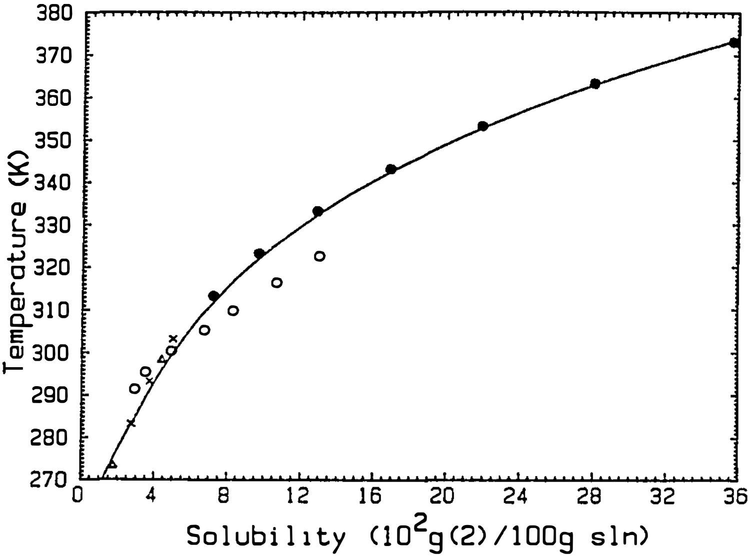

FIGURE 2. Solubility of water in ethylbenzene: ref 5 (o); ref 10 (x); ref 14 (Δ); ref 24 (●). Solid line is fitted to "Best" values from Table 4.

Thermodynamic functions derived by application of the van't Hoff equation to the various data sets are summarized in Table 5.

TABLE 5: Thermodynamic functions for the Dissolution of Water in Ethylbenzene Derived from Solubility Data

Reference	ΔH_{sln} kJ mol^{-1}	$\Delta C_{p,sln}$ J K^{-1} mol^{-1}
Filippov and Furman (ref 5)	45.2	-809
Englin *et al.* (ref 10)	22.0	91
Heidman *et al.* (ref 24)	24.4	33

The thermodynamic functions derived from the data of both Englin *et al.* (ref 10) and Heidman *et al.* (ref 24) are comparable to those obtained for related, well characterized systems (*e.g.* water in benzene) whereas the values of Filippov and Furman (ref 5) are not. Further investigation of this system is clearly warranted.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.

CRITICAL EVALUATION: (continued)

3. MUTUAL SOLUBILITIES OF ETHYLBENZENE (1) AND WATER (2) AT ELEVATED TEMPERATURES

To clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram for this system. On such a diagram (Figure 3) phases with the same value of pressure and temperature but different composition will be located at the same point. The general typology of the phase diagram of this system is similar to that of benzene + water (except that the vapor pressure of ethylbenzene is considerably less than that of benzene). Ethylbenzene + water has type III phase behaviour (using Scott and von Konynenberg's classification (ref 25, 26). This type of phase behaviour is characterized by two critical loci, with one starting at the critical point of the pure component with the higher critical temperature (water in this case) and eventually approaching high pressures. The other critical locus starts at the critical point of the other pure component (ethylbenzene) and ends on a three phase (liquid-liquid-vapor) line at a critical end point.

The *p-T* projection of the *p-T-x* diagram for this system is shown schematically in Figure 3.

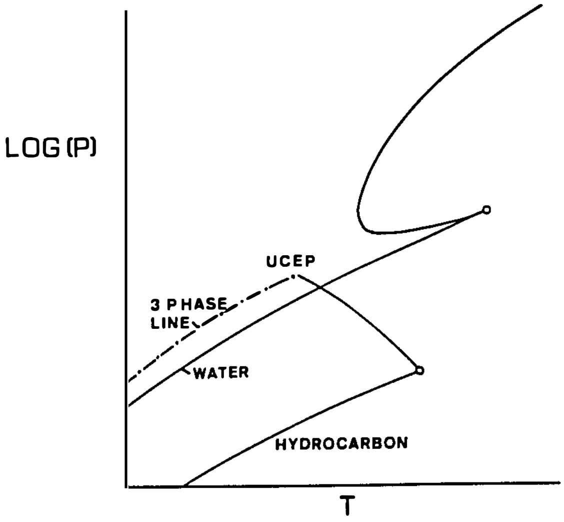

FIGURE 3. Pressure-temperature projection for ethylbenzene/water.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia. October 1986.

CRITICAL EVALUATION: (continued)

It is important to note that the three phase line on a p-T projection corresponds to three lines on the p-T-x diagram. In the region above the three phase line on the p-T projection, the pressure is greater than the vapor pressure and then a maximum of two liquid phases is possible. There may be one or two liquid phases depending on the overall composition. To the left of the critical line starting at the least volatile component it is possible to have one or two phases present depending on the overall composition.

Solubilities in the ethylbenzene + water system have been studied at elevated pressures in the publications listed in Table 6.

TABLE 6: Solubility Studies of the Ethylbenzene (1) - Water (2) System at Elevated Pressures

Reference	p/kPa	T/K	Solubility
Guseva and Parnov (ref 9)	-[a]	338-507	(1) in (2)
Alwani and Schneider (ref 12)	1.8-2.0	348-387	critical locus
Roof (ref 13)	-[b]	-[b]	-[b]
Heidman *et al.* (ref 24)	0.1-10.7[c]	311-568	mutual

a Unspecified but presumably at pressures on the three phase line.
b Critical point of unknown composition.
c Along three phase line.

The data of Guseva and Parnov (ref 9) are thought to be unreliable. The solubilities reported by these workers are considerably larger than values obtained by other workers for the systems water + benzene, + hexane, + ethylcyclohexane and + octane. The data of Heidman *et al.* (ref 24) are classified as Tentative for measurements along the three phase line. However, it should be pointed out that there is some discrepancy between the critical end point properties (574.3K, 11.2 MPa) reported by Roof (ref 13) and those reported by Heidman *et al.* (568.1K, 10.68 MPa). Nevertheless, the thermodynamic functions derived from the data of Heidman *et al.* are in reasonable agreement with those derived from lower temperature data (Table 3) and also with those of related hydrocarbons (*e.g.* benzene in water).

Alwani and Schneider (ref 12) have reported values of the critical properties along the critical curve starting at the critical point of ethylbenzene (*cf.* Figure 3).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986

CRITICAL EVALUATION: (continued)

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COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Fuhner, H.

Ber. Dtsch. Chem. Ges. 1924, *57*, 510-5.

VARIABLES:

One temperature: 15°C

PREPARED BY:

A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 15°C was reported to be 0.014 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 2.4×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm^3 (2) until a completely clear solution was no longer obtained at the experimental temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; commercial grade; used as received.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. <u>1950</u>, *72*, 5034-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 0.0168 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 2.85×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; fractionally distilled; b.p. 136.0°C.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 0.175 g(1) L^{-1} sln and 0.00164 mol(1) L^{-1} sln.

The corresponding mass percent and mole fraction calculated by the compiler are 0.0175 g(1)/100 g sln and $x_1 = 2.9 \times 10^{-5}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1571-8.
VARIABLES:	PREPARED BY:
Temperature: 0.4-42.8°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

t/°C	g(1)/100g sln[a] (compiler)	$10^5 x_1$ (compiler)
0.4	0.0219	3.71
5.2	0.0213	3.61
20.7	0.0207	3.51
21.2	0.0207	3.51
25.0	0.0208[b]	3.53
25.6	0.0209	3.54
30.2	0.0211	3.58
34.9	0.0221	3.75
42.8	0.0231	3.92

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

[b] Given in the original paper as 0.208g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

(1) Koppers Co., purified by redistillation, several washings, and passing through silica gel. Purity was determined by refractometry (no values given).

(2) Air-free conductivity water, no other details given.

ESTIMATED ERROR:

Temp. ± 0.02°C
Soly. ± 0.5% relative

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Filippov, T.S.; Furman, A.A.

Zh. Prikl. Khim. 1952, *25*, 895-7.

VARIABLES:

Temperature: 18.2-49.5°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in ethylbenzene

t/°C	g(2)/100 g sln	10^3x_2 (compiler)
18.2	0.0296	1.74
18.3	0.0308	1.81
19.7	0.0327	1.92
22.3	0.0352	2.07
23.4	0.0360	2.12
24.2	0.0388	2.28
27.2	0.0494	2.91
29.8	0.0595	3.50
31.6	0.0648	3.81
32.1	0.0679	4.05
34.2	0.0745	4.38
35.1	0.0777	4.56
36.6	0.0835	4.90
38.8	0.0917	5.38
41.5	0.1005	5.90
43.1	0.1070	6.27
47.2	0.1225	7.18
49.5	0.1300	7.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Weighed amounts of both components were placed in glass tubes, 40 mm across and 65 mm long, and shaken. Clear and cloud points were observed 5-6 times to within 0.2-0.3°C.

SOURCE AND PURITY OF MATERIALS:

(1) source unspecified; distilled; no turbidity if cooled to -10 or -20°C.

(2) twice distilled.

ESTIMATED ERROR:

temp: ± 0.3°C
soly: not specified

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	Morrison, T.J.; Billett, F. *J. Chem. Soc.* 1952, 3819-22.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 0.00155 mol(1)/1000 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by compilers are 0.0165 g(1)/100 g sln and $x_1 = 2.8 \times 10^{-5}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

After an excess of (1) had been shaken with about 1 dm^3 of (2) for about a week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through to drive off the (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustions were taken.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; purest obtainable material; distilled; purity not specified.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. ± 1% (mean of large numbers of determinations)

REFERENCES:

COMPONENTS: (1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Jones, J.R.; Monk, C.B. *J. Chem. Soc.* 1963, 2633-5.
VARIABLES: Temperature: 25-35°C	**PREPARED BY:** A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of Water in Ethylbenzene

t/°C	10^4 mL (2)/mL (1)
25	3.7
30	4.3
35	5.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL aliquot was reshaken for 4 hrs. with 5 mL H_2O in a 10 mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quencing effects (due to solvent) on the scintillator.

SOURCE AND PURITY OF MATERIALS:

(1) Laboratory grade; dried over $CaCl_2$ and fractionally distilled

(2) Not specified.

ESTIMATED ERROR:

Soly. ±5% to ±1%
(average deviation)

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

Nature (London) 1963, *200*, 1092-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 0.0159 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 2.70×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+%; used as received.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±1.5°C
Soly. 0.0008 (std. dev. of mean)

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Zh. Fiz. Khim. 1964, *38*, 805-6.

VARIABLES:

Temperature: 115.0 - 233.5°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

t/°C	g(1)/100 g sln	$10^4 x_1$ (compiler)
115.0	0.0513	0.871
140.5	0.119	2.02
170.5	0.355	6.04
210.0	0.661	11.27
233.5	1.129	19.33

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Ethylbenzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0275	1.62
20	0.0373	2.19
30	0.0502	2.95

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS: (1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 152 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0152 g(1)/100 g sln and 2.57 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 8 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C.-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	10^4x_1 (compiler)
0(a)	197(c)	0.0197	3.34
25(b)	177(c)	0.0177	3.00

Solubility of water in ethylbenzene

$t/°C$	mg(2)/kg(1)	g(2)/100 g sln (compiler)	10^3x_2 (compiler)
0(a)	178(d)	0.0178	1.05
25(b)	442(e)	0.0442	2.60

[a-e] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis.

The solubility of water in the organic layer was determined by Karl Fischer titration and the solubility of hydrocarbon in the water layer was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99+%); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. (a) ± 0.02°C, (b) ± 0.01°C

soly. (c) ± 1.7%, (d) ± 4.7%, (e) ± 3.1% (from two or three determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	Brown, R.L.; Wasik, S.P. *J. Res. Natl. Bur. Stds. A.* 1974, *78*, 453-60.
VARIABLES:	**PREPARED BY:**
Temperature: 4.5-20.1°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of Ethylbenzene in Water

t/°C	g(1)/100 g sln[a]	$10^5\ x_1$ (compiler)
4.5	0.0196 ± 0.0004	3.33
6.3	0.0192 ± 0.0004	3.26
7.1	0.0186 ± 0.0006	3.16
9.0	0.0187 ± 0.0004	3.18
11.8	0.0181 ± 0.0005	3.07
12.1	0.0183 ± 0.0004	3.11
15.1	0.0180 ± 0.0005	3.06
17.9	0.0184 ± 0.0005	3.12
20.1	0.018 ± 0.0004[b]	3.1

[a] Errors given as standard deviations.

[b] Typographical error in original publication, digit missing in fourth decimal place.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. Basically, the hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 cm of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99 mole per cent purity; source and methods of purification not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.01°C

Solubility: See Table above.

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 161.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.01612 g(1)/100 g sln and 2.734×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.9 mg(1)/kg(2)
(the standard deviation of the mean for six replicates)

REFERENCES:

COMPONENTS: (1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C and at system pressure was reported to be 131.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0131 g(1)/ 100 g sln and 2.22×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 1.4 mg(1)/kg(2)

REFERENCES:

COMPONENTS: (1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. *87*:87654.
VARIABLES: One temperature: 20°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 20°C was reported to be 0.21 g(1) L^{-1} (2).
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.021 g(1)/100 g sln and 3.6 x 10^{-5}. The assumption that 1 dm^3 sln = 1 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 100-500 mL(2) was placed in a glass cylinder and 10-50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5-1.5 min.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* 1978, *51*, 957-8.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 0.18 g(1) L^{-1} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.018 g(1)/100 g sln and 3.1×10^{-5}. The assumption that 1.00 L^{-1} = 1.00 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 200-500 mL (2) was placed in a ground-joint glass cylinder and 20-50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Soly. 0.01 g(1) L^{-1} sln (std. dev. from 6 determinations).

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 131.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0131 g(1)/100 g sln and 2.22×10^{-5}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 3.4 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Chem. Lett. 1981, 225-8.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

t/°C	g(1)/L	g(1)/100 g sln[a]	10^4x_1[a]
15	0.176 ± 0.009	0.0176	2.99
25	0.181 ± 0.006	0.0182	3.09
35	0.194 ± 0.006	0.0195	3.31
45	0.215 ± 0.004	0.0217	3.69

[a] Assuming the solution density to be that of pure water at the same temperature (ref. 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, generated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

SOURCE AND PURITY OF MATERIALS:

(1) analytical reagent grade used as purchased.

(2) redistilled.

ESTIMATED ERROR:

soly. : given above

REFERENCES:

1. CRC Handbook of Chemistry and Physics, R.C. Weast, Editor, CRC Press, Florida, 63rd edn, 1982, pF-11.

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)^a	$10^5\ x_1$ (compiler)^a
15	1.51 ± 0.08	0.0160	2.72
25	1.59 ± 0.05	0.0169	2.87
35	1.54 ± 0.05	0.0176	2.99
45	1.83 ± 0.05	0.0196	3.33

a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.01°C.

REFERENCES:

1. Kell, G.S.
J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.;
Deguchi, Y.; Nagai, H.
Chem. Lett. 1981, 225-8.

COMPONENTS: (1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* 1984, *57*, 1539-44.
VARIABLES: One Temperature: 25°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 1.62×10^{-3} mol(1)/dm^3 sln. Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 0.0172 g(1)/100 g sln, $x_1 = 2.92 \times 10^{-5}$, calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectrophotometry.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade source and purity not stated, used without further purification.

(2) Deionized and redistilled; no further details given.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]
(2) Water, H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Heidman, J.L.; Tsonopoulos, C.;
Brady, C.J.; Wilson, G.M.
A. I. Ch. E. J. 1985, *31*, 376-84.

VARIABLES:

Temperature: 311-568 K
Pressure: 0.01-10.7 MPa

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

T/K	p /MPa	$10^4 x_1$	g(1)/100 g sln (compiler)
311.5	-[a]	0.32	0.019
367.6	0.111	0.86	0.051
423.4	0.627	2.19	0.129
479.5	2.32	6.0	0.35
536.1	6.50	32.5	1.88
552.8	8.59	37.5	2.17

a Not specified.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography.

(2) Distilled; no details given.

ESTIMATED ERROR:

soly. ± 5%, relative precision of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

1. Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* 1983, *29*, 990-9.

(1) Ethylbenzene; C_8H_{10}; [100-41-4]
(2) Water, H_2O; [7732-18-5]

(continued)

Solubility of water in ethylbenzene

T/K	p /MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
310.9	0.0091[a]	0.43	0.073
367.6	0.111	1.86	0.320
423.4	0.627	5.96	1.06
479.5	2.32	16.3	3.20
536.1	6.50	40.8	10.5
550.4	8.27	47.2	13.2
568.1[b]	10.68[b]	69.1[b]	27.5

a Estimated by the authors from pure component data.
b Three phase critical point.

The three phase critical point was reported to be 568.1 ± 0.6 K, 10.68 ± 0.04 MPa and $x_1 = 5.83 \times 10^{-3}$ (3.34 g(1)/100 g sln, compiler).

The authors also report an equation providing a fit of their own and literature data over the range 273-568 K, *viz.*

$$\ln x_1 = -185.1695 + 7348.55/T + 26.34525 \ln T$$

$$\ln x_2 = -0.37215 - 4.4626\ (T_r^{-1} - 1) - 0.38596\ (1 - T_r)^{1/3} - 2.59850\ (1 - T_r)$$

where $T_r = T/568.1$

COMPONENTS:

(1) Ethylbenzene; C_8H_{10}; [100-41-4]

(2) Artificial seawater

ORIGINAL MEASUREMENTS:

Brown, R.L.; Wasik, S.P.

J. Res. Natl. Bur. Stds. A. 1974, *78*, 453-60.

VARIABLES:

Temperature: 0-20°C

Salinity: 34.42 g salts/kg sln

PREPARED BY:

G.T. Hefter and D.G. Shaw

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in artificial seawater

t/°C	g(1)/100 g sln[a]	$10^5 x_1$ (compiler)
0.19	0.0140 (0.0002)	2.44
5.32	0.0133 (0.0003)	2.31
10.05	0.0129 (0.0003)	2.25
14.96	0.0125 (0.0003)	2.18
20.04	0.0122 (0.0003)	2.12

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography.

The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 L of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99 mole per cent purity; source and methods of purification not specified.

(2) Prepared according to ref 1. Purity not specified.

ESTIMATED ERROR:

Temperature: ±0.01 K

Solubility: see Table above

REFERENCES:

1. Sverdrup, H.U.; Johnson, M.W.; Fleming, R.H.; The Oceans, 1942, Prentice-Hall, Englewood Cliffs, New Jersey, p186.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C_8H_{10}; [100-41-4] (2) Artificial seawater (ref 1)	Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	**PREPARED BY:** M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in artificial seawater is reported to be 111.0 mg (1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 0.01110 g(1)/100 g sln and 1.9×10^{-5} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 1.3 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS: (1) 4-Vinyl-1-cyclohexene; C_8H_{12}; [100-40-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 4-vinyl-1-cyclohexene in water at 25°C was reported to be 50 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.005 g(1)/100 g sln and 8.3×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.	**SOURCE AND PURITY OF MATERIALS:** (1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled. **ESTIMATED ERROR:** temp. ± 1.5°C soly. 5 g(1)/10^6 g(2) (standard deviation of mean) **REFERENCES:**

COMPONENTS:

(1) 1-Propenylcyclopentane; C_8H_{14}; [5623-78-9]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

One temperature: 30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in 1-propenylcyclopentane at 30°C was reported to be 0.0383 g(2)/100 g sln. The corresponding value mole fraction, x_2, calculated by the compilers is 2.34×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) 1-Octyne; C_8H_{14}; [629-05-0]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and
A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-octyne in water at 25°C was reported to be 24 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0024 g(1)/100 g sln and 4.4 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.8 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) 1,1,3-Trimethylcyclopentane; C_8H_{16}; [4516-69-2]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclopentane in water at 25°C and at system pressure was reported to be 3.73 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.73×10^{-4} g(1)/100 g sln and 5.99×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±1°C

Soly. ±0.17 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,1,3-Trimethylcyclopentane; C_8H_{16}; [4516-69-2] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclopentane in water at 25°C was reported to be 2.04 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 2.04 x 10^{-4} g(1)/100 g sln and 3.27 x 10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.	(1) not specified. (2) not specified. **ESTIMATED ERROR:** soly. 0.10 mg(1)/kg(2) (standard deviation from 7-9 determinations). **REFERENCES:**

COMPONENTS:

(1) Isopropylcyclopentane; C_8H_{16}; [3875-51-2]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in isopropylcyclopentane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
10	0.0059	3.68
20	0.0102	6.35
30	0.0159	9.90

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) Propylcyclopentane; C_8H_{16}; [2040-96-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of propylcyclopentane in water at 25°C and at system pressure was reported to be 2.04 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.04 x 10^{-4} g(1)/100 g sln and 3.27 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.10 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) Propylcyclopentane; C_8H_{16};
[2040-96-2]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12,* 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of propylcyclopentane in water at 25°C was reported to be 1.77 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.77×10^{-4} g(1)/100 g sln and 2.84×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.07 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) cis-1,2-Dimethylcyclohexane; C_8H_{16}; [2207-01-4]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of cis-1,2-dimethylcyclohexane in water at 25°C was reported to be 6.0 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00060 g(1)/100 g sln and 9.6×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.8 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) 1,4-Dimethylcyclohexane; C_8H_{16}; [589-90-2]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Vestn. Mosk. Univ. Khim. 1964, *19*, 77-8.

VARIABLES:

Temperature: 57-240°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 1,4-dimethylcyclohexane in water

t/°C	g(1)/100 g(2)	g(1)/100 g sln (compiler)	10^4x_1 (compiler)
57	0.0017	0.0017	0.027
105	0.0056	0.0056	0.090
165	0.0263	0.0263	0.422
240	0.257	0.257	4.120

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-trans-Dimethylcyclohexane; C_8H_{16}; [2207-04-7] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,4-trans-dimethylcyclohexane in water at 25°C and at system pressure was reported to be 3.84 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.84 x 10^{-4} g(1)/100 g sln and 6.16 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.17 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 1,4-Dimethylcyclohexane; C_8H_{16}; [589-90-2]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,4-dimethylcyclohexane in water at 25°C was reported to be 3.84 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 3.84×10^{-4} g(1)/100 g sln and 6.16×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.12 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. May 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the ethylcyclohexane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Ethylcyclohexane (1) - Water (2) System

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	352-486	(1) in (2)	unspecified[a]
Heidman *et al.* (ref 2)	311-561	mutual	GLC, Karl Fischer

a Probably using the synthetic method.

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system is in two parts.

1. SOLUBILITY OF ETHYLCYCLOHEXANE (1) IN WATER (2)

This system almost certainly exhibits type III phase behaviour (see introductory material at the beginning of this volume). The phase diagram is similar to that of ethylbenzene and water.

The solubility of ethylcyclohexane in water at elevated temperatures and system pressures along the three phase equilibrium line have been investigated by Guseva and Parnov (ref 1) and Heidman *et al.* (ref 2). Their results are summarized in Table 2 and plotted in Figure 1. The agreement is very poor. However, it may be noted (ref 1) that the values reported by Guseva and Parnov at higher temperatures approach those of cyclohexane which is unreasonable. It may also be noted that the data of Guseva and Parnov often differ markedly from Recommended values in other systems. The data of Heidman *et al.* are thus considered Tentative.

Heidman *et al.* report a three phase critical end point at 561.4 ± 0.6 K, 9.93 ± 0.04 MPa and $x_1 = 3.35 \times 10^{-3}$ (2.05 g(1)/100g sln, Evaluator).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. May 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Solubility Values for Ethylcyclohexane (1) in Water (2) at the Three-Phase Equilibrium Pressure

T/K	Solubility values		
	Reported values[a]	"Best" values[b]	
	$10^2 g(1)/100g$ sln	$10^2 g(1)/100g$ sln	$10^4 x_1$
313	0.066 (ref 2)	0.07	0.01
323	0.074 (ref 2)	0.07	0.011
333	0.086 (ref 2)	0.07	0.014
343	0.10 (ref 2)	0.10	0.016
353	0.5 (ref 1), 0.13 (ref 2)	0.13	0.020
363	0.8 (ref 1), 0.16 (ref 2)	0.16	0.026
373	1.3 (ref 1), 0.21 (ref 2)	0.21	0.034
393	2.2 (ref 1), 0.55 (ref 2)	0.55	0.088
413	3.7 (ref 1), 0.95 (ref 2)	0.95	0.15
433	6.5 (ref 1), 1.6 (ref 2)	1.6	0.26
453	16.0 (ref 1), 2.8 (ref 2)	2.8	0.45
473	27.0 (ref 1), 5.5 (ref 2)	5.5	0.9
493	16 (ref 2)	16	2.2
513	34 (ref 2)	34	5.2
533	65 (ref 2)	65	10.4
553	150 (ref 2)	150	24.0

[a] All data obtained by graphical or algebraic interpolation by the Evaluator of the authors' original data.

[b] Rounded values from ref 2; data from ref 1 not included in "Best" values, see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. May 1986.

CRITICAL EVALUATION: (continued)

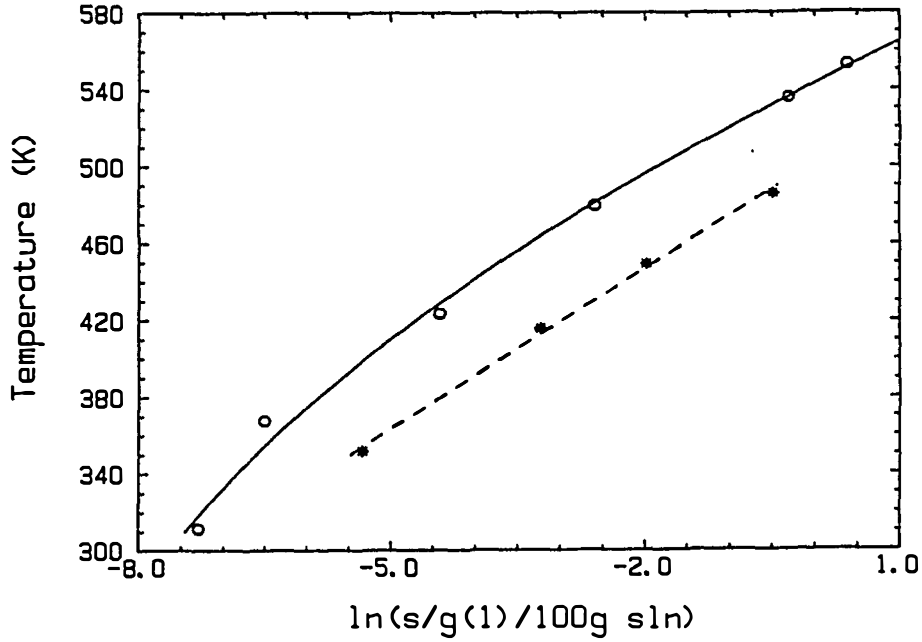

FIGURE 1. Solubility of ethylcyclohexane in water at elevated temperatures and equilibrium pressures: ref 1 (x); ref 2 (o).

2. SOLUBILITY OF WATER (2) IN ETHYLCYCLOHEXANE (1)

As only the data of Heidman *et al.* (ref 2) are available on the solubility of water in ethylcyclohexane (Table 1) no Critical Evaluation of water is possible. The interested user is referred to the appropriate Data Sheet for the experimental values.

REFERENCES

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1964, *12*, 77-8.
2. Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. *A.I.Ch.E.J.* 1985, *31*, 376-84.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics and Dr Colin Young for his comments on the phase behaviour of this system.

COMPONENTS:

(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Vestn. Mosk. Univ. Khim. 1964, *19*, 77-8.

VARIABLES:

Temperature: 79-213°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of ethylcyclohexane in water

t/°C	g(1)/100 g(2)	g(1)/100 g sln (compiler)	10^4x_1 (compiler)
79	0.0048	0.0048	0.077
142.5	0.0398	0.0398	0.639
176	0.138	0.138	2.22
213	0.66	0.62	9.96

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76.

COMPONENTS:

(1) Ethylcyclohexane; C_8H_{16}; [1678-91-7]

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

ORIGINAL MEASUREMENTS:

Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M.

A. I. Ch. E. J. 1985, *31*, 376-84.

VARIABLES:

Temperature: 311-561 K

Pressure: 0.01-9.9 MPa

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of ethylcyclohexane in water

T/K	p /MPa	10^4 x_1	10^2 g(1)/100 g sln (compiler)
311.5	-[a]	0.011	0.068
367.6	0.117	0.024	0.15
423.4	0.647	0.20	1.2
479.5	2.36	1.21	7.5
536.1	6.69	11.8	73
552.8	8.83	23.7	146

[a] Not specified.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography.

(2) Distilled; no details given.

ESTIMATED ERROR:

soly. ± 5%, relative precision of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

1. Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* 1983, *29*, 990-9.

(1) Ethylcyclohexane, C_8H_{16}; [1678-91-7]
(2) Water, H_2O; [7732-18-5]

(continued)

Solubility of water in ethylcyclohexane

T/K	p /MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
310.9	0.0099^a	0.081	0.0130
367.6	0.117	0.65	0.104
423.4	0.647	3.0	0.48
479.5	2.36	10.7	1.89
536.1	6.69	29.0	6.15
552.8	8.83	41.4	10.2
561.4^b	9.93^b	60.3^b	19.6

a Estimated by the authors from pure component data.
b Three phase critical point.

The three phase critical point was reported to be 561.4 ± 0.6 K, 9.93 ± 0.04 MPa and $x_1 = 3.35 \times 10^{-3}$ (1.05 g(1)/100 g sln, compiler).

The authors also report an equation which fits their own and related literature data over the range 273-561 K, *viz.*

$$\ln x_1 = -334.2468 + 14105.21/T + 47.93102 \ln T$$

$$\ln x_2 = -0.50980 - 7.4603\ (T_r^{-1} - 1) - 0.67885\ (1 - T_r)^{1/3} + 0.44796\ (1 - T_r)$$

where $T_r = T/561.4$

COMPONENTS:

(1) Cyclooctane; C_8H_{16}; [292-64-8]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclooctane in water at 25°C was reported to be 7.9 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 1.27×10^{-6}.

The same value is also reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 1.8 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:

(1) 1-Octene; C_8H_{16}; [111-66-0]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and
A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-octene in water at 25°C was reported to be 2.7 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00027 g(1)/100 g sln and 4 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.2 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS: (1) 1-Octene; C_8H_{16}; [111-66-0] (2) Water; H_2O [7732-18-5]	**ORIGINAL MEASUREMENTS:** Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 1-octene in water was reported to be 1.979×10^{-4} mol L^{-1} at 25°C.[a] Assuming a solution density of 1.00 g mL^{-1} the corresponding mass percent and mole fraction (x_1) solubilities calculated by the compilers are respectively, 0.00222 g(1)/100 g sln and 3.63×10^{-6}.

Solubility data are also presented as a function of temperature in various salt solutions.

[a] It should be noted that although the authors state that the solubility refers to "water" the context in the paper is ambiguous and the data were probably obtained in 0.001 mol L^{-1} HNO_3 solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson, Coleman and Bell; 99%

(2) Not specified

ESTIMATED ERROR:

Temp. ± 0.05K
Soly. not specified.

REFERENCES:

COMPONENTS: (1) 2-Octene; C_8H_{16}; [111-67-1] (2) Water; H_2O; [7732-18-5]	ORIGINAL MEASUREMENTS: Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9.
VARIABLES: Temperature: 15-25°C	PREPARED BY: M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of 2-octene in 0.001 mol/L HNO_3 solution.

t/°C	10^4 mol/L sln[a]	10^3 g(1)/100 g sln[b] (compiler)	10^6 x_1 (compiler)
15	2.92 ± 0.14	3.3	5.3
20	2.51 ± 0.16	2.8	4.5
25	2.16 ± 0.15	2.4	3.9

[a] Uncertainties stated to be "standard deviations from means".

[b] Assuming a solution density of 1.00 g mL^{-1} at all temperatures.

Compiler's note: Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause olefin solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol L^{-1} HCl.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: 15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.	SOURCE AND PURITY OF MATERIALS: (1) Prepared by dehydration of 2-octanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography. (2) Not specified.
	ESTIMATED ERROR: Temp. ± 0.05 K Soly. see table above.
	REFERENCES:

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,2,4-Trimethylpentane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Berkengeim (ref 1)	273-313	(2) in (1)	Karl Fischer
Baker (ref 2)	unspecified	(1) in (2)	radiotracer
Englin *et al.* (ref 3)	273-323	(2) in (1)	analytical
McAuliffe (ref 4)	298	(1) in (2)	GLC
Polak and Lu (ref 5)	273,298	mutual	GLC, Karl Fischer
Budantseva *et al.* (ref 6)	293	mutual	unspecified
Price (ref 7)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 8)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediatley following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF 2,2,4-TRIMETHYLPENTANE (1) IN WATER (2)

Very few data are available for the solubility of 2,2,4-trimethylpentane in water making critical evaluation difficult. The datum of Baker (ref 2) is rejected as the temperature was not specified. All other reported values are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 8) which does not appear to be independent of that of Price (ref 7) and has therefore been excluded from consideration.

At 298K where comparisons are possible, the values of McAuliffe (ref 4) and Polak and Lu (ref 5) are in reasonable agreement. The value reported by Price (ref 7) is much lower. Although Price's data for many hydrocarbons in water are normally reliable, many of his values for the higher hydrocarbons are lower than other studies. However, in the absence of confirmatory studies it is not reasonable to reject Price's value at this stage. However, it has not been included in the calculation of the "Best" values at 298K.

At other temperatures the "Best" values should be regarded with caution in the absence of confirmatory studies.

(continued next page)

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of 2,2,4-Trimethylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values (± σ_n)[a]	
	10^4g(1)/100g sln	10^4g(1)/100g sln	10^7 x_1
273	2.46 (ref 5)	2.5	3.9
293	2 (ref 6)	2	3
298	2.44 (ref 4), 2.05 (ref 5) 1.14 (ref 7)	2.2 ± 0.2[b]	3.5[b]

[a] Obtained by averaging where appropriate; σ_n has no statistical significance.

[b] Average of data from ref 4 and 5 only, see text.

2. SOLUBILITY OF WATER (2) IN 2,2,4-TRIMETHYLPENTANE (1)

The various reported values of the solubility of water in 2,2,4-trimethylpentane are collected in Table 3 and plotted in Figure 1.

The data are generally in poor agreement and the averaged "Best" values must be regarded with caution pending further studies. Generally, for many other systems investigated by these authors, the data of Englin *et al.* (ref 3) are reliable at T < 300K but are too high at higher temperatures. Application of the van't Hoff equation to the data of Englin *et al.* and Bergengeim (ref 1) gives values of ΔH_{sln} = 41.9 and 20.1 kJ mol^{-1} and $\Delta C_{p,sln}$ = -100 and -1950 J K^{-1} mol^{-1} respectively. Comparison of these data with other systems suggests that the values of Englin *et al.* are more realistic (although probably high at T > 300K). This system clearly warrants further investigation.

TABLE 3: Tentative Values of the Solubility of Water (2) in 2,2,4-Trimethylpentane (1)

T/K	Solubility values		
	Reported values[c]	"Best" values (± σ_n)[a]	
	10^3g(2)/100g sln	10^3g(2)/100g sln	10^4 x_2
273	1.7* (ref 1), 3.1 (ref 3), 2.3 (ref 5)	2.4 ± 0.6	1.5
283	3.7 (ref 1), 5.9 (ref 3), 4.5* (ref 5)	4.7 ± 0.9	2.9
293	5.5 (ref 1), 11.5 (ref 3), 6.5* (ref 5), 7.9 (ref 6)	8 ± 2	5

(Table 3 continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,4-Trimethylpentane; C_8H_{18} [540-84-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986

CRITICAL EVALUATION: (continued)

Table 3 (continued)

T/K	Solubility values		
	Reported values[c]	"Best" values (± σ_n)[a]	
	10^3g(2)/100g sln	10^3g(2)/100g sln	10^4 x_2
298	6.2* (ref 1), 15.3* (ref 3), 8.0 (ref 5)	10 ± 4	6
303	7.0* (ref 1), 20.1 (ref 3)	20[b]	10[b]
313	8.0 (ref 1)		
323	53.8 (ref 3)	50[b]	30[b]

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[a] Best values obtained by averaging where appropriate; σ_n has no statistical significance.

[b] Order of magnitude values only, see text.

[c] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

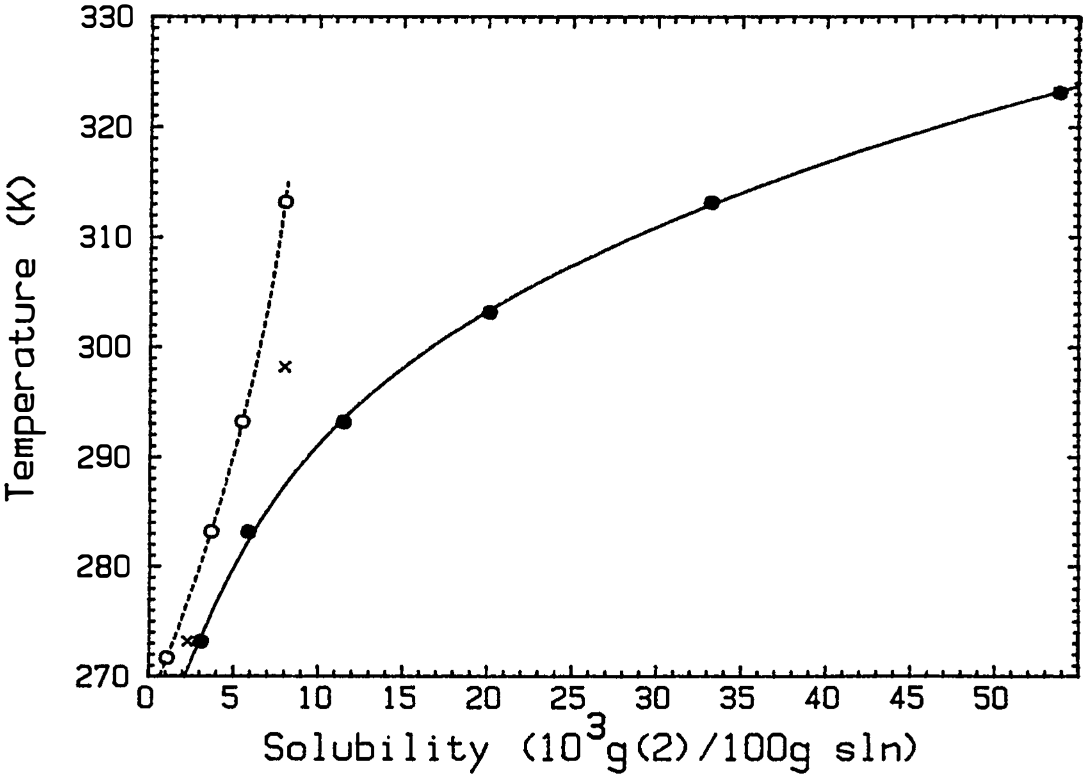

FIGURE 1. Solubility of water in 2,2,4-trimethylpentane: ref 1 (o); ref 3 (●); ref 5 (x).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Berkengeim, T.I. *Zavod. Lab.* 1941, *10*, 592-4.
2. Baker, E.G. *Geochim. Cosmochim. Acta* 1960, *19*, 309-17.
3. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
4. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
5. Polak, J.; Lu, B.C.-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
6. Budantseva, L.A.; Lesteva, T.M.; Nemtsov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344, Deposited doc. 1976, VINITI 437-76.
7. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
8. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Marie-Claire Haulait-Pirson for comments and Dr Brian Clare for the graphics and regression analyses.

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

Berkengeim, T.I.

Zavod. Lab. 1941, *10*, 592-4.

VARIABLES:

Temperature: (-1.5) - 40°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubilitv of water in 2,2,4-trimethylpentane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
-1.5	0.0011	0.697
10	0.0037	2.35
20	0.0055	3.49
40	0.0080	5.07

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (2) in (1) was determined by the Karl Fischer reagent method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; d_D^{20} 0.6947; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	Baker, E.G. *Geochim. Cosmochim. Acta* 1960, *19*, 309-17.
VARIABLES:	**PREPARED BY:**
One temperature: not specified	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water was reported to be 0.0009 mL (1) L^{-1} (2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The procedure is described in ref 1.

SOURCE AND PURITY OF MATERIALS:

not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints* 1958, *3*, N°4, C61.

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 0-50°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2,2,4-trimethylpentane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
0	0.0031	1.97
10	0.0059	3.74
20	0.0115	7.29
30	0.0201	12.74
40	0.0332	21.02
50	0.0538	34.03

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 25°C was reported to be 2.44 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 3.85×10^{-7}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C

soly. 0.12 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* 1963, *200*, 1092.
2. McAuliffe, C. *Am. Chem. Soc., Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

mw = [illegible]

Solubility of 2,2,4-trimethylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0^a	2.46^c	3.88×10^{-7}
25^b	2.05^c	3.23×10^{-7}

Solubility of water in 2,2,4-trimethylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0^a	23^d	1.46×10^{-4}
25^b	80^e	5.07×10^{-4}

[a-e] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02°C; b) ± 0.01°C
soly. c) ± 4%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S.

Zh. Fiz. Khim. 1976, *50*, 1344. *Deposited doc.* 1976, VINITI 437-76.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 20°C was reported to be $x_1 = 3 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is about 2×10^{-4}g(1)/100 g sln.

The solubility of water in 2,2,4-trimethylpentane at 20°C was reported to be $x_2 = 4.4 \times 10^{-4}$.

The corresponding mass percent value calculated by the compiler is 7.9×10^{-3} (2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Nothing specified in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS: (1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 25°C and at system pressure was reported to be 1.14 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.14×10^{-4} g(1)/100 g sln and 1.80×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.02 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,4-trimethylpentane in water at 25°C was reported to be 1.14 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.14×10^{-4} g(1)/100 g sln and 1.80×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.04 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,3,4-trimethylpentane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,3,4-Trimethylpentane (1) - Water (2) System

Reference	T/K	Solubility	Method
Polak and Lu (ref 1)	273,298	mutual	GLC, Karl Fischer
Price (ref 2)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF 2,3,4-TRIMETHYLPENTANE (1) IN WATER (2)

All the available data on the solubility of 2,3,4-trimethylpentane in water are collected in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 3) which does not appear to be independent of that of Price (ref 2) and has thus been excluded from consideration.

At 298K, the datum of Polak and Lu (ref 1) is much higher than that reported by Price (ref 2), as for many other hydrocarbon systems investigated by these authors. In the absence of other independent studies it is not possible to prefer either datum.

TABLE 2: Tentative Values of the Solubility of 2,3,4-Trimethylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	10^4g(1)/100g sln	10^4g(1)/100g sln	10 x_1
273	2.34 (ref 1)	2.3	
298	2.30 (ref 1), 1.36 (ref 2)	1.8 ± 0.5	

^{a} Obtained by simple averaging, σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2,3,4-TRIMETHYLPENTANE (1)

As only one study of the solubility of water in 2,3,4-trimethylpentane has been reported (ref 1) no Critical Evaluation is possible. The interested user is referred to the appropriate Data Sheet for experimental values. However, it may be noted that the solubility of water in other hydrocarbons reported by Polak and Lu (ref 1) are normally reliable.

REFERENCES

1. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.
2. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
3. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

COMPONENTS:

(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2,3,4-trimethylpentane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	2.34^c	3.69×10^{-7}
25^b	2.30^c	3.62×10^{-7}

Solubility of water in 2,3,4-trimethylpentane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	20^d	1.27×10^{-4}
25^b	74^e	4.69×10^{-4}

[a-e] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02°C; b) ± 0.01°C
soly. c) ± 4%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:

(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3,4-trimethylpentane in water at 25°C and at system pressure was reported to be 1.36 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.36×10^{-4} g(1)/100 g sln and 2.14×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.03 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 2,3,4-Trimethylpentane; C_8H_{18}; [565-75-3]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3,4-trimethylpentane in water at 25°C was reported to be 1.36 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.36×10^{-4} g(1)/100 g sln and 2.14×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.05 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) 2,3-Dimethylhexane; C_8H_{18}; [584-94-1]

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

ORIGINAL MEASUREMENTS:

Baker, E.G.

Geochim. Cosmochim. Acta 1960, *19*, 309-17.

VARIABLES:

One temperature: not specified

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3-dimethylhexane in water was reported to be 0.0002 mL(1)/L(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The procedure is described in ref 1.

SOURCE AND PURITY OF MATERIALS:

not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints* 1958, *3*, N°4, C61.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylhexane; C_8H_{18}; [589-43-5] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 42-6.
VARIABLES:	**PREPARED BY:**
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2,4-dimethylhexane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
10	0.0053	3.36
20	0.0098	6.21
30	0.0180	11.41

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) 3-Methylheptane; C_8H_{18}; [589-81-1]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylheptane in water at 25°C and at system pressure was reported to be 0.792 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 7.92×10^{-5} g(1)/100 g sln and 1.25×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.028 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 3-Methylheptane; C_8H_{18};
[589-81-1]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylheptane in water at 25°C was reported to be 0.792 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 7.92×10^{-5} g(1)/100 g sln and 1.25×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.04 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter,* School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the *n*-octane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Octane (1) - Water (2) System

Reference	T/K	Solubility	Method
Führer (ref 1)	289	(1) in (2)	titration
Black *et al.* (ref 2)	293	(2) in (1)	radiotracer
Baker (ref 3)	unspecified	(1) in (2)	radiotracer
Englin (ref 4)	283-303	(2) in (1)	analytical
McAuliffe (ref 5)	298	(1) in (2)	GLC
Nelson and De Ligny (ref 6)	278-318	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 9)	298	(1) in (2)	GLC
Polak and Lu (ref 10)	273,298	mutual	GLC, Karl Fischer
Budantseva *et al.* (ref 11)	293	mutual	unspecified
Price (ref 12)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 13)	298	(1) in (2)	GLC
Skripka (ref 14)	498-538^a	(2) in (1)	unspecified
Jonsson *et al.* (ref 15)	288-308	(1) in (2)	partition coefficient
Heidman *et al.* (ref 16)	311-539^a	mutual	synthetic

a High pressure data

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition critical phenomena have been investigated by Roof (ref 8). These are considered along with solubility data at high pressures in Section 3 below.

For convenience further discussion of this system will be in three parts.

1. THE SOLUBILITY OF OCTANE (1) IN WATER (2)

Agreement amongst the independent determinations of the solubility of octane in water is not particularly good and no data have been Recommended.

At 298K the value reported by Price (ref 11) is substantially lower than all other studies (ref 5,9,10,15) and has been rejected. At higher temp-

(continued next page

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*Section 3 was written with C.L. Young, Department of Physical Chemistry, University of Melbourne, Australia.

COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

eratures the values of Price (ref 12) are also considerably lower than those of Heidman *et al.* (ref 16). In the absence of confirmatory studies, it is not reasonable to reject Price's data outright but they have not been used in the calculation of "Best" values. Application of the van't Hoff equation to both data sets gives values of ΔH_{sln} = -3.3 (ref 12) and +13.3 (ref 16) kJ mol^{-1} and $\Delta C_{p,sln}$ = 568 (ref 12) and 284 (ref 16) J K^{-1} mol^{-1}. Neither set of values are close to those reported for related systems although those of Heidman *et al.* are somewhat more reasonable.

At other temperatures the data of Führer (ref 1), Nelson and De Ligny (ref 6), and Budantseva *et al.* (ref 11) are markedly higher than all other studies and are therefore rejected. All the remaining data are summarized in Table 2 and selected data are plotted in Figure 1.

It is interesting to note that the averaged "Best" value at 298K is very close to the value which would be predicted by an extrapolation of the lower *n*-alkane solubilities.

TABLE 2: Tentative Values of the Solubility of Octane (1) in Water (2)

T/K	Solubility values Reported values $10^4 g(1)/100g$ sln	"Best" values (± σ_n)^a $10^4 g(1)/100g$ sln	 $10^7 x_1$
273	1.35 (ref 10)	1.4	2.2
293	0.628 (ref 15)	0.63	0.99
298	0.66 (ref 5), 0.70 (ref 9), 0.85 (ref 10), 0.615 (ref 15)	0.71 ± 0.09	1.1
303	0.46^b (ref 12), 0.612 (ref 15)	0.61	0.96
313	0.52^b (ref 12), 0.80^c (ref 16)	0.8	1.3
323	0.61^b (ref 12), 0.96^c (ref 16)	1.0	1.6
333	0.74^b (ref 12), 1.2^c (ref 16)	1.2	1.9
343	0.91^b (ref 12), 1.5^c (ref 16)	1.5	2.4
353	1.0^b (ref 12), 1.99^c (ref 16)	2.0	3.2
363	1.1^b (ref 12), 2.67^c (ref 16)	2.7	4.3
373	1.2^b (ref 12), 3.66^c (ref 16)	3.7	5.8

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

TABLE 2 (continued)

T/K	Solubility values Reported values 10^4g(1)/100g sln	"Best" values (± σ_n)[a] 10^4g(1)/100g sln	 10^7 x_1
393	4.5[b] (ref 12), 7.23[c] (ref 16)	7.2	11
413	9.5[b] (ref 12), 15.1[c] (ref 16)	15	24
433	12.0[b] (ref 12), 22.2[c] (ref 16)	22	35

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[a] Obtained by averaging where appropriate; σ_n has no statistical significance. Data from ref 12 have been excluded in the calculation of "Best" values, see text.

[b] Obtained by the Evaluator by graphical interpolation of the author's original data.

[c] Calculated from the authors' fitting equation over the range of their experimental values.

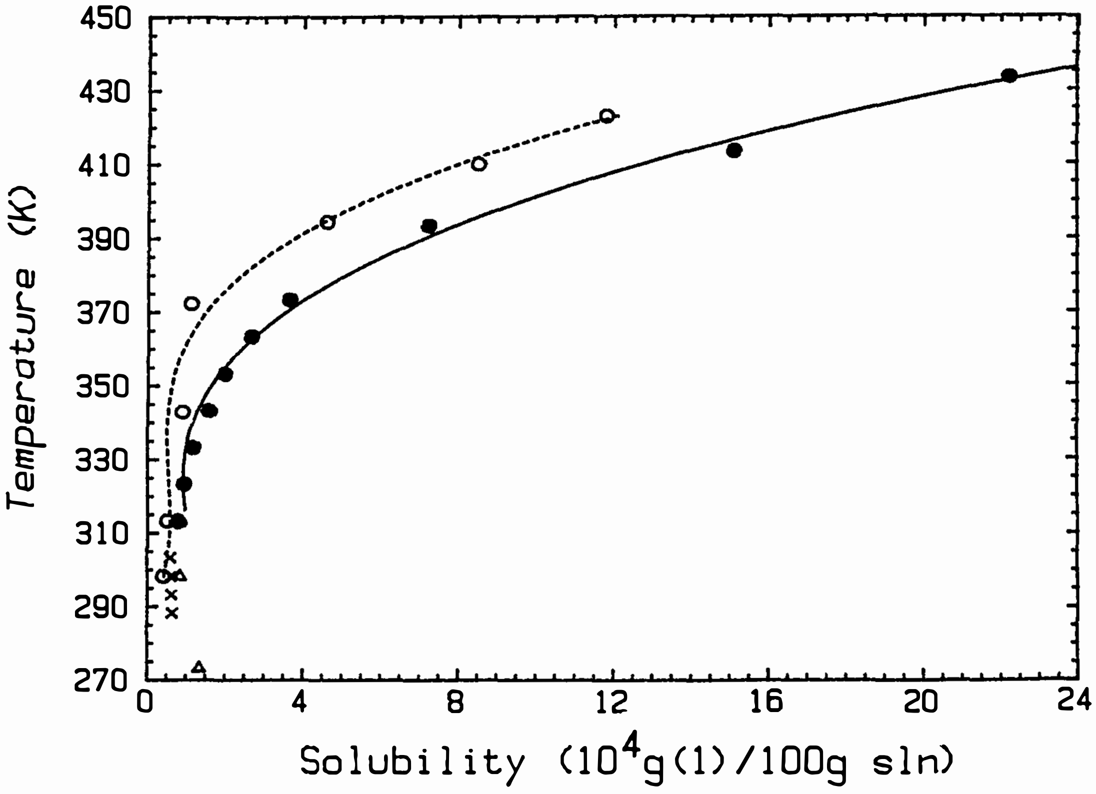

FIGURE 1. Solubility of octane in water, selected data: ref 10 (△); ref 12 (o); ref 15 (x); ref 16 (●).

(continued next page)

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

October 1986.

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN OCTANE (1)

Only limited data are available for the solubility of water in *n*-octane and agreement amongst independent determinations is only fair. The datum of Black *et al.* (ref 2) is much higher than all other values and is therefore rejected. The remaining data are collected in Table 3 and plotted in Figure 2.

TABLE 3: Tentative Values of the Solubility of Water (2) in Octane (1)

T/K	Solubility values		
	Reported values 10^2g(2)/100g sln	"Best" values (± σ_n)^a 10^2g(2)/100g sln	 10^4 x_2
273	0.23 (ref 9)	0.2	1
283	0.51 (ref 4)	0.5	3
293	0.95 (ref 4), 0.68 (ref 10)	0.8 ± 0.1	5
298	1.26^b (ref 4), 0.79 (ref 9)	1.0 ± 0.2	6
303	1.68 (ref 4)	1.7	11
313	1.58^c (ref 14)	1.6	10
323	2.40^c (ref 14)	2.4	15
333	3.54^c (ref 14)	3.5	22
343	5.14^c (ref 14)	5.1	32
353	7.30^c (ref 14)	7.3	46
363	10.2^c (ref 14)	10	63
373	14.0^c (ref 14)	14	89

[a] Obtained by averaging where appropriate; σ_n has no statistical significance.

[b] Obtained by graphical interpolation (Evaluator) of authors' original data.

[c] Calculated (Evaluator) from fitting equation given by authors, over the range of their experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

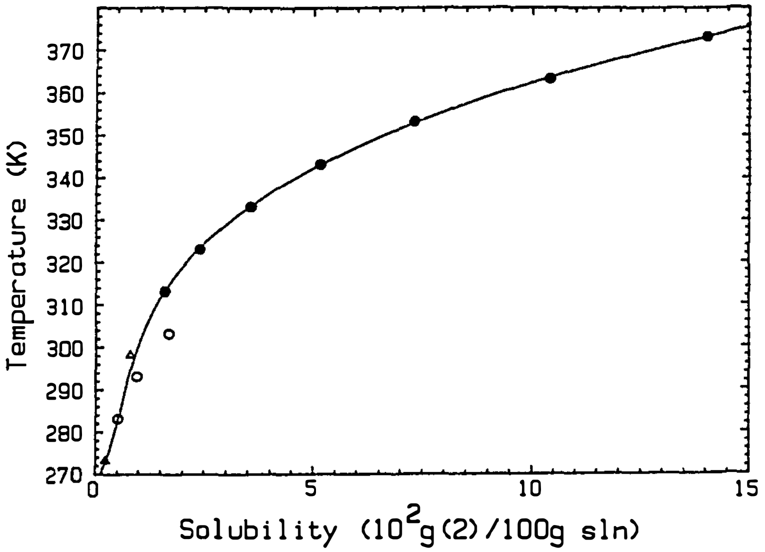

FIGURE 2. Solubility of water in octane; ref 4 (o); ref 10 (Δ); ref 16 (●). Solid line has been fitted to "Best" values in Table 3.

3. SOLUBILITY STUDIES OF THE OCTANE (1) - WATER (2) SYSTEM AT ELEVATED PRESSURES

This system exhibits phase behaviour which is topographically similar to that of benzene + water, *i.e.*, it belongs to type III phase behaviour using Scott and von Konynenburg's (ref 17) classification (see Figure 3 and the Introduction to this volume).

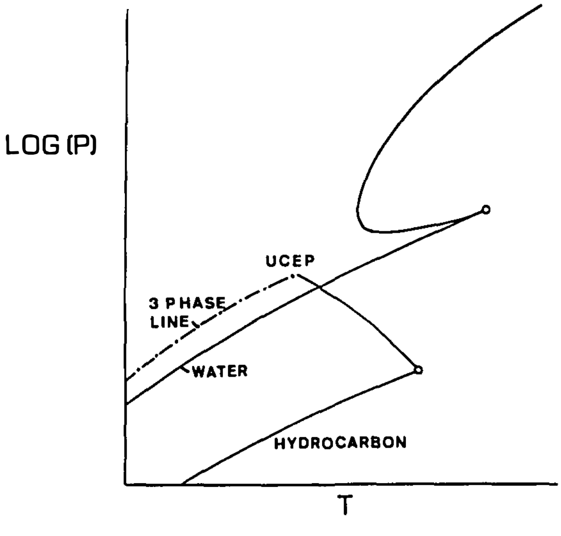

FIGURE 3. Pressure-temperature projection of the equilibrium pressure-temperature composition surface for type III phase behaviour.

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COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

Quantitative solubility data on the octane - water system at elevated pressures have been reported in the studies listed in Table 4.

TABLE 4. Solubility Studies of the Octane (1) - Water (2) System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Roof (ref 8)	-[a]	-[a]	-[a]
Price (ref 12)	-[b]	298-423	(1) in (2)
Skripka (ref 14)	3.5-78.5	498-538	(2) in (1)
Heidman *et al.* (ref 16)	0.01-8.9[b]	311-539	mutual

a Critical point of unspecified composition.
b Along the three-phase line.

As can be seen from Table 4 data have not generally been obtained under comparable conditions, making Critical Evaluation difficult. However, it may be noted that the solubility of 9.95 g(2)/100g sln of water in octane at 7.4 MPa and 538.2 K reported by Skripka (ref 14) differs markedly from the value of 14.9 g(2)/100g sln reported at 7.41 MPa and 539.1 K by Heidman *et al.* (ref 16). Further studies are necessary before any preference can be expressed for either data set. Previous mention (Section 1 above) has already been made of the fact that the solubilities of octane in water reported by Heidman *et al.* (ref 16) are much higher than those of Price (ref 12).

On the other hand the properties of the critical end point (Figure 3) reported by Roof: 7.41 MPa and 540.4 K, are in good agreement with those reported by Heidman *et al.* (ref 16): 7.41 MPa and 539.1 K.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Führer, H. *Chem. Ber.* 1924, *57*, 510-5.
2. Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 537-48.
3. Baker, E.G. *Geochim. Cosmochim. Acta* 1960, *19*, 309-17.
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16. Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. *A.I.Ch.E.J.* 1985, *31*, 376-84.
17. Scott, R.L.; van Konynenburg, P.H. *Phil. Trans. Roy. Soc.* London 1980, *A298*, 495.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

*NOTE ADDED IN PROOF

Delete ref 7.

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Führer, H.

Ber. Dtsh. Chem. Ges. 1924, *57*, 510-5.

VARIABLES:

One temperature: 16°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of octane in water at 16°C was reported to be 0.002 mL(1)/100 mL sln or 0.0014 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler is 0.22×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100 or 1000 cm^3 of (2) until a completely clear solution was obtained at the experimental temperature.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; commercial grade; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 537-43.
VARIABLES:	**PREPARED BY:**
One temperature: 20°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in octane at 20°C and at a total saturation pressure of 1 atm was reported to be 0.0142 g(2)/100 g(1). The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.0142 g(2)/100 g sln and 9.0×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method described in ref 1 in which tritium oxide acts as a tracer, was used.
Air saturated with radioactive water vapor was bubbled through the (1) sample until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred in the counter through equilibration with ethanol vapor.

SOURCE AND PURITY OF MATERIALS:

(1) Ohio State University under an American Petroleum Institute project; purity not specified; used as received.

(2) not specified.

ESTIMATED ERROR:

soly. a few percent (type of error not specified).

REFERENCES:

1. Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* 1948, *16*, 45.

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Baker, E.G.

Geochim. Cosmochim. Acta 1960, *19*, 309-17.

VARIABLES:

One temperature: not specified.

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of octane in water was reported to be 0.09×10^{-6} mL(1)/mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined after ultrafiltration using the procedure described in ref 1.

SOURCE AND PURITY OF MATERIALS:

not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprint* 1958, *3*, N°4, C61.

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in octane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
10	0.0051	3.24
20	0.0095	6.03
30	0.0168	10.65

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of octane in water at 25°C was reported to be 0.66 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 1.04×10^{-7}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C

soly. 0.06 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* 1963, *200*, 1092.

2. McAuliffe, C. *Am. Chem. Soc., Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water, H_2O; [7732-18-5]	Nelson, H.D.; De Ligny, C.L. *Rec. Trav. Chim. Pays-Bas* 1968, *87*, 528-44.
VARIABLES:	**PREPARED BY:**
Temperature: 5-45°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of octane in water

$t/°C$	10^7x_1	mg(1)/kg sln (compiler)
5.0	2.6 ± 0.6	1.65
15.0	1.4 ± 0.6	0.89
45.0	2.9 ± 0.6	1.84

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturation vessel is drawn in the original paper. (2) was saturated with (1) via the vapor phase: a few drops of (1) were put on the bottom of a tight-fitting flask containing a small flask filled with water. Complete saturation was reached by shaking overnight in an upright position. Samples were taken from the aqueous solution with a microsyringe through the septum and injected into the gas chromatograph equipped with a flame ionization detector. The gas chromatographic conditions are described in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka purum.

(2) tap-water was refluxed for 8 hours in the presence of $KMnO_4$ and KOH and distilled. The whole process was repeated once more.

ESTIMATED ERROR:

soly.: error given above (standard deviation)

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Krasnoshchekova, P.Ya.; Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of octane in water at 25°C was reported to be $x_1 = 1.0 \times 10^{-7}$.
The corresponding mass percent calculated by the compiler is 7.0×10^{-5} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; purity not specified.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of octane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0^a	1.35^c	2.13×10^{-7}
25^b	0.85^c	1.34×10^{-7}

Solubility of water in octane

t/°C	mg(2)/kg sln	x_2 (compiler)
0^a	23^d	1.46×10^{-4}
25^b	79^e	5.01×10^{-4}

[a-e] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02°C; b) ± 0.01°C
soly. c) ± 4%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S.

Zh. Fiz. Khim. 1976, *50*, 1344. *Deposited doc.* 1976, VINITI 437-76.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of octane in water at 20°C was reported to be $x_1 \approx 2 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is about 0.0001 g(1)/100 g sln.

The solubility of water in octane at 20°C was reported to be $x_2 = 4.3 \times 10^{-4}$.

The corresponding mass percent calculated by the compiler is 0.007 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Nothing specified in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

Temperature: 25-149.5°C

PREPARED BY:

F. Kapuku

EXPERIMENTAL VALUES:

Solubility of octane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	10^7x_1 (compiler)
25.0	0.431 ± 0.012	0.0000431	0.680
40.1	0.524 ± 0.021	0.0000524	0.826
69.7	0.907 ± 0.042	0.0000907	1.43
99.1	1.12 ± 0.07	0.000112	1.77
121.3	4.62 ± 0.22	0.000462	7.29
136.6	8.52 ± 0.34	0.000852	13.4
149.5	11.80 ± 0.7	0.00118	18.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C

soly. range of values given above

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

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

ORIGINAL MEASUREMENTS:

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

VARIABLES:

Temperature: 225-265°C
Pressure: 3.5-78.5 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in octane

t/°C	*p*/kg cm^{-2}	*p*/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
225	36	3.5	0.166	3.04
	100	9.8	0.137	2.44
	200	19.6	0.109	1.89
	300	29.4	0.098	1.68
	400	39.2	0.091	1.55
	500	49.0	0.088	1.50
	600	58.8	0.084	1.42
	700	68.6	0.080	1.35
	800	78.5	0.075	1.26
240	50	4.9	0.216	4.16
	100	9.8	0.193	3.63
	200	19.6	0.164	3.00
	300	29.4	0.149	2.69
	400	39.2	0.140	2.50
	500	49.0	0.132	2.34
	600	58.8	0.126	2.22
	700	68.6	0.122	2.14
	800	78.5	0.117	2.05

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, chemical reagent grade; purity not specified; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Gazov. Prom.* 1971, *4*, 6.

(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	Skripka, V.G. *Tr. Vses. Neftegazov. Nauch. Issled. Inst.* 1976, *61*, 139-51. Sultanov, R.G.; Skripka, V.G. *Zh. Fiz. Khim.* 1973, *47*, 1035.

t/°C	*p*/kg cm^{-2}	*p*/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
265	75	7.4	0.412	9.95
	100	9.8	0.350	7.83
	200	19.6	0.254	5.10
	300	29.4	0.224	4.35
	400	39.2	0.207	3.95
	500	49.0	0.194	3.66
	600	58.8	0.183	3.41
	700	68.6	0.172	3.19
	800	78.5	0.163	2.98

COMPONENTS: (1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice),* 1978, *12*, 413-7.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of octane in water at 25°C was reported to be 0.431 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 4.31×10^{-5} g(1)/100 g sln and 6.80×10^{-8}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.02 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C_8H_{18}; [111-65-9] (2) Water; H_2O; [7732-18-5]	Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, *9*, 279-86.
VARIABLES:	**PREPARED BY:**
Temperature: 15-35°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of octane in water

t/°C	mg(1)/kg sln	10^5g(1)/100g sln (compiler)	10^7x_1 (compiler)
15	0.653	6.53	1.03
20	0.628	6.28	0.99
25	0.615	6.15	0.97
30	0.612	6.12	0.96
35	0.620	6.20	0.98

[a] Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapour concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analysed by gas chromatography. The method and apparatus are described in detail in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka, > 99.8%, used as received.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Vejrosta, J.; Novak, J.; Jonsson, J.A. *Fluid Phase Equil.* 1982, *8*, 25-35.

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]
(2) Water, H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M. *A. I. Ch. E. J.* 1985, *31*, 376-84.

VARIABLES:

Temperature: 311-553 K
Pressure: 0.01-7.4 MPa

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of octane in water

T/K	p /MPa	$10^5\ x_1$	10^2 g(1)/100 g sln (compiler)
310.9	0.0103[a]	0.012	0.0076
366.5	0.117[a]	0.048	0.030
422.0	0.655	0.38	0.24
479.5	2.51	4.0	2.5
536.1	7.03	35	22
552.8	8.86	60[b]	38

a Estimated by the authors from pure component data
b Above three-phase equilibrium point.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography.

(2) Distilled; no details given.

ESTIMATED ERROR:

soly. ± 5%, relative precision of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

1. Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* 1983, *29*, 990-9.

(1) Octane; C_8H_{18}; [111-65-9]
(2) Water, H_2O; [7732-18-5]

(continued)

Solubility of water in octane

T/K	p /MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
310.9	0.0103[a]	0.100	0.0158
366.5	0.117	0.62	0.098
422.0	0.655	3.94	0.622
477.6	- [b]	12.6	2.22
533.1	- [b]	38.7	9.05
539.1[c]	7.41	52.7[c]	14.9
550.4[d]	-	54.9[d]	16.1

[a] Estimated by the authors from pure component data.
[b] Not specified.
[c] Three phase critical point.
[d] Above three phase critical point.

The three phase critical point was reported to be 539.1 ± 0.6 K, 7.37 ± 0.04 MPa and $x_1 = 4.61 \times 10^{-4}$ (0.292 g(1)/100 g sln, compiler).

The authors also report equations which fit their own and literature data over the range 273-539 K, *viz.*

$$\ln x_1 = -343.1497 + 13862.49/T + 49.24609 \ln T$$

$$\ln x_2 = -0.66037 - 7.1130\ (T_r^{-1} - 1) - 0.67885\ (1 - T_r)^{1/3} - 1.43381\ (1 - T_r)$$

where $T_r = T/539.1$

COMPONENTS:	EVALUATOR:
(1) Octane; C_8H_{18}; [111-65-9] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of octane (1) in seawater (2) has been reported in two works:

Authors	Method	T/K	Salinity· g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	2.5×10^{-4}
Freegarde *et al.* (ref 2)	GLC	?	?	1×10^{-4}

Because temperature and salinity are not specified, the data of Freegarde *et al.* are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of octane in pure water at 298 K.

SOLUBILITY OF OCTANE (1) IN SEAWATER (2)
DOUBTFUL VALUE

T/K	g salts/kg sln	g(1)100 g sln
298	6	2.5×10^{-4}

REFERENCES

1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.

2. Freegarde, M.; Hatchard, C.G.; Parker, C.A. *Lab. Pract.* 1971, *20*, 35-40.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octane; C_8H_{18}; [111-65-9] (2) Seawater (composition not specified)	Freegarde, M.; Hatchard, C.G.; Parker, C.A. *Lab Pract.* 1971, *20*, 35-40.
VARIABLES:	**PREPARED BY:**
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of octane was reported to be 1.0 mg/L. The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 1.0×10^{-4} g(1)/100 g sln and 1.6×10^{-7}, assuming a solution density of 1.02 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

None given except that analysis was done using gas chromatography.

SOURCE AND PURITY OF MATERIALS:

not given.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Octane; C_8H_{18}; [111-65-9]

(2) Seawater

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.;
Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-8.

VARIABLES:

One temperature: 25°C
Salinity: 6 g/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of octane in seawater was reported to be 2.5×10^{-4} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 4.0 \times 10^{-7}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

SOURCE AND PURITY OF MATERIALS:

(1) "chemically pure"

(2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Indan; C_9H_{10}; [496-11-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. February 1986.

CRITICAL EVALUATION:

Quantitative solubility studies for indan (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of Indan (1) in Water (2)

Reference	T/K	Method
Price (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data in these publications are compiled in the Data Sheets immediately following this evaluation. No data have been reported on the solubility of water in indan.

The data of Price (ref 1) and Mackay and Shiu (ref 2) are in good agreement (Table 2) although the relative uncertainty (± 10%) is too large for the mean to be Recommended given the relatively high solubility. Further studies are required.

TABLE 2: Tentative Value of the Solubility of Indan (1) in Water (2)

T/K	Solubility value		
	Reported value $10^2 g(1)/100g$ sln	"Best" value ($\pm\sigma_n$) $10^2 g(1)/100g$ sln	 $10^5 x_1$
298	0.889 (ref 1), 1.091 (ref 2)	1.0 ± 0.1	1.5

REFERENCES

1. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) Indan; C_9H_{10}; [496-11-7]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of indan in water at 25°C and at system pressure was reported to be 88.9 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00889 g(1)/100 g sln and 1.35×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 2.7 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Indan; C_9H_{10}; [496-11-7] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of indan in water at 25°C was reported to be 109.1 mg(1) dm^{-3} sln and $x_1 = 1.665 \times 10^{-5}$.

The corresponding mass percent calculated by the compiler is 0.01091 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 1.02 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 1,2,3-Trimethylbenzene; C_9H_{12}; [526-73-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

December 1986

CRITICAL EVALUATION:

Quantitative solubility data for 1,2,3-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,2,3-trimethylbenzene.

TABLE 1: Quantitative Solubility Studies of 1,2,3-Trimethylbenzene (1) in Water (2)

Reference	*T*/K	Method
Sutton and Calder (ref 1)	298	GLC
Sanemasa *et al.* (ref 2)	288-318	spectrophotometry

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The available data are summarized in Table 2. At 298K, the only temperature where comparison is possible, the data of Sutton and Calder (ref 1) and Sanemasa *et al.* (ref 2) are in reasonable agreement (Table 2) and their average may be considered as the Tentative solubility.

At other temperatures, only the data of Sanemasa *et al.* are available so no Critical Evaluation is possible. Nevertheless, it may be noted that for other hydrocarbons in water the data of Sanemasa *et al.* are normally reliable.

TABLE 2: Tentative Values of the Solubility of 1,2,3-Trimethylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values ($\pm \sigma_n$)[a]	
	10^3g(1)/100g sln	10^3g(1)/100g sln	10^6 x_1
288	5.99 (ref 2)	6.0	9.0
298	7.52 (ref 1), 6.27 (ref 2)	6.9 ± 0.5	10
308	7.22 (ref 2)	7.2	11
318	8.52 (ref 2)	8.5	13

[a] Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,2,3-Trimethylbenzene; C_9H_{12}; [526-73-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. December 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.

2. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

COMPONENTS:

(1) 1,2,3-Trimethylbenzene; C_9H_{12}; [526-73-8]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of 1,2,3-trimethylbenzene in water at 25°C was reported to be 75.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00752 g(1)/100 g sln and 1.126×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell purified by distillation through a Vigreaux Column; 94.4% purity determined by gas chromatography.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±0.1°C

Soly. 0.6 (the standard deviation of the mean for six replicates).

REFERENCES:

COMPONENTS:

(1) 1,2,3-Trimethylbenzene; C_9H_{12}; [526-73-8]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 1,2,3-trimethylbenzene in water

t /°C	10^4 mol(1)/dm^3 sln	10^3 g(1)/100 g sln (compiler)[a]	10^6 x_1 (compiler)[a]
15	4.98 ± 0.19	5.99	8.97
25	5.20 ± 0.32	6.27	9.40
35	5.97 ± 0.41	7.22	10.8
45	7.02 ± 0.19	8.52	12.8

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), no stated purity, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.

temp. ± 0.01°C.

REFERENCES:

1. Kell, G.S. *J. Chem. Eng. Data* 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. *Chem. Lett.* 1981, 225-8.

COMPONENTS: (1) 1,2,3-Trimethylbenzene; C_9H_{12}; [526-73-8] (2) Artificial seawater (ref 1)	**ORIGINAL MEASUREMENTS:** Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	**PREPARED BY:** M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of 1,2,3-trimethylbenzene in artificial seawater is reported to be 48.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 4.86×10^{-3} g(1)/100 g sln and 7.47×10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.5 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:	EVALUATOR:
(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985.

CRITICAL EVALUATION:

Quantitative solubility data for 1,2,4-trimethylbenzene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of 1,2,4-Trimethylbenzene (1) in Water (2)

Reference	*T*/K	Method
McAuliffe (ref 1)	298	GLC
Sutton and Calder (ref 2)	298	GLC
Price (ref 3)	298	GLC
Krzyzanowska and Szeliga (ref 4)	298	GLC
Sanemasa *et al.* (ref 5)	288-318	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data have been reported for the solubility of water in 1,2,4-trimethylbenzene.

All the available data are collected in Table 2 with the exception of that of Krzyzanowska and Szeliga (ref 4) which does not appear to be independent of that of Price (ref 3) and thus has been excluded from consideration. At 298K the only temperature where comparison is possible, the data are in excellent agreement so that the mean can be Recommended, although interestingly the value of Price (ref 3) is somewhat lower than those reported by other workers as for many of the higher hydrocarbons investigated by this author. At other temperatures only the data of Sanemasa *et al.* (ref 5) are available and must thus be regarded as Tentative.

TABLE 2: Recommended (R) and Tentative Values of the Solubility of 1,2,4-Trimethylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values 10^3g(1)/100g sln	"Best" values $(\pm\sigma_n)^a$ 10^3g(1)/100g sln	$10^6\ x_1$
288	5.23 (ref 5)	5.2	7.8
298	5.7 (ref 1), 5.90 (ref 2), 5.19 (ref 3), 5.65 (ref 5)	5.6 ± 0.3 (*R*)	8.4 (*R*)
308	6.21 (ref 5)	6.2	9.3
318	6.93 (ref 5)	6.9	10

a Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985

CRITICAL EVALUATION: (continued)

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
2. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
4. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.
5. Sanemasa, I.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at 25°C was reported to be 57 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0057 g(1)/100 g sln and 8.5 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 4 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at 25°C was reported to be 59.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00590 g(1)/100 g sln and 8.83×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.8 mg(1)/kg(2)
(the standard deviation of the mean for six replicates)

REFERENCES:

COMPONENTS:

(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at 25°C and at system pressure was reported to be 51.9 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00519 g(1)/100 g sln and 7.77×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 1.2 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water at 25°C was reported to be 51.9 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00519 g(1)/100 g sln and 7.78×10^{-6}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 1.6 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) 1,2,4-Trimethylbenzene; C_9H_{12};
[95-63-6]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in water

t /°C	10^4 mol(1)/dm^3 sln	10^3 g(1)/100 g sln (compiler)^a	10^6 x_1 (compiler)^a
15	4.35 ± 0.12	5.23	7.84
25	4.69 ± 0.07	5.65	8.48
35	5.14 ± 0.20	6.21	9.32
45	5.71 ± 0.07	6.93	10.4

a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating strea was used to vaporize li to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 95.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.01°C.

REFERENCES:

1. Kell, G.S.
J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.;
Deguchi, Y.; Nagai, H.
Chem. Lett. 1981, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6] (2) Artificial seawater (ref 1)	Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES:	**PREPARED BY:**
One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of 1,2,4-trimethylbenzene in artificial seawater is reported to be 39.6 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 3.96×10^{-3} g(1)/100 g sln and 6.09×10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.5 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) Mesitylene; C_9H_{12}; [108-67-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

August 1985

CRITICAL EVALUATION:

Quantitative solubility data for the mesitylene (1) - water (2) system have reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Mesitylene (1) - Water (2) System

REFERENCE	*T*/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	residue volume
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 3)	391-484	(1) in (2)	unspecified
Englin *et al.* (ref 4)	293-313	(2) in (1)	analytical
Sutton and Calder (ref 5)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 6)	288-318	(1) in (2)	spectrophotometric
Sanemasa *et al.* (ref 7)	288-318	(1) in (2)	spectrophotometric

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF MESITYLENE (1) IN WATER (2)

All the available data on the solubility of mesitylene in water at low temperatures (288-318K) are summarized in Table 2, except for the rejected values referred to below.

At 298K, the only temperature where comparison is possible, the datum of Sutton and Calder (ref 5) is in good agreement with the values reported by Sanemasa *et al.* (ref 6,7) enabling the mean to be Recommended. The datum of Andrews and Keefer (ref 2) is markedly higher than the other studies (ref 5,6,7) and is rejected as is the approximate value of Booth and Everson (ref 1).

At other temperatures only the two data sets of Sanemasa *et al.* (ref 6,7) are available and must thus be considered as Tentative.

At the elevated temperatures (*ca.* 390-480K) and system pressure only the data of Guseva and Parnov (ref 3) are available and thus no Critical Evaluation is possible. However, it may be noted that solubilities reported by Guseva and Parnov are not always reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. August 1985.

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of Mesitylene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values ($\pm \sigma_n$)	
	10^3g(1)/100g sln	10^3g(1)/100g sln	$10^6\ x_1$
288	4.56 (ref 6), 4.60 (ref 7)	4.6	6.9
298	4.82 (ref 5), 4.95 (ref 6) 5.00 (ref 7)	4.89 ± 0.08^a(*R*)	7.4 (*R*)
308	5.42 (ref 6), 5.49 (ref 7)	5.4	8.2
318	5.65 (ref 6), 5.89 (ref 7)	5.7	8.7

a Obtained by simple averaging; σ_n has no statistical significance.

2. THE SOLUBILITY OF WATER (2) IN MESITYLENE (1)

The solubility of water in mesitylene has been reported only by Englin *et al.* (ref 4) and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for experimental values. However, it may be noted that for other hydrocarbon systems studies by Englin *et al.* their results are generally reliable at T < 300K but are higher than Recommended values at higher temperatures.

REFERENCES

1. Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
2. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
3. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* 1963, *18*, 76-9.
4. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
5. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
6. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Chem. Lett.* 1981, 225-8.
7. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.
8. Alwani, Z.; Schneider, G.M. *Ber. Bunsenges. Phys. Chem.* 1969, *73*, 294-301.

NOTE ADDED IN PROOF

Alwani and Schneider (ref 8) have also reported a critical locus of the mesitylene-water system.

COMPONENTS: (1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of mesitylene in water at 25°C was reported to be less than 0.02 g(1)/100 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant-temperature water bath and weighed quantities of (1) were added to this solution. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes and then centrifuged for 5 minutes. After this treatment, the volume of residue was determined directly.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP or highest commercial grade; used as received.

(2) distilled.

ESTIMATED ERROR:

soly. ± 0.1 mL(1)/100 mL(2).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Mesitylene; C_9H_{12}; [108-67-8] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of mesitylene in water at 25°C was reported to be 0.0097 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 1.45×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; fractionally distilled; b.p. 165.0°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Mesitylene; C_9H_{12}; [108-67-8]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Vestn. Mosk. Univ. Khim. 1963, *18*, 76-9.

VARIABLES:

Temperature: 118-211°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of mesitylene in water

t/°C	g(1)/100 g sln	$10^4 x_1$ (compiler)
118	0.007	0.10
144	0.013	0.19
187	0.041	0.61
211	0.078	1.17

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; n_D^{20} 1.49945.

(2) doubly distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Mesitylene; C_9H_{12}; [108-67-8]

(2) Water· H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-40°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Mestitylene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
20	0.0291	1.94
30	0.0393	2.62
40	0.0519	3.45

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Mesitylene; C_9H_{12}; [108-67-8]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of mesitylene in water at 25°C was reported to be 48.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00482 g(1)/100 g sln and 7.22×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.3 (the standard deviation of the mean for six replicates).

REFERENCES:

COMPONENTS:

(1) Mesitylene; C_9H_{12}; [108-67-8]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Chem. Lett. 1981, 225-8.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of mesitylene in water

t/°C	g(1)/L	g(1)/100 g sln[a]	$10^6 x_1$[a]
15	0.0456 ± 0.0010	0.00456	6.82
25	0.0495 ± 0.0015	0.00495	7.41
35	0.0542 ± 0.0033	0.00542	8.11
45	0.0565 ± 0.0031	0.00565	8.46

[a] calculated by compiler assuming a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, generated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a pump. The circulation rate was 2 L/min. Solubility equilibria were attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred into funnels to which 10 mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported. The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. The solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

SOURCE AND PURITY OF MATERIALS:

(1) analytical reagent grade used as purchased.

(2) redistilled.

ESTIMATED ERROR:

soly. : given above

REFERENCES:

COMPONENTS:

(1) Mesitylene (1,3,5-Trimethylbenzene); C_9H_{12}; [108-67-8]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 1,3,5-trimethylbenzene in water

t /°C	10^4 mol(1)/dm^3 sln	10^3 g(1)/100 g sln (compiler)^a	10^6 x_1 (compiler)^a
15	3.83 ± 0.15	4.60	6.90
25	4.15 ± 0.22	5.00	7.50
35	4.55 ± 0.23	5.49	8.22
45	4.85 ± 0.32	5.89	8.83

a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 97.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.1°C.

REFERENCES:

1. Kell, G.S.
   J. Chem. Eng. Data 1975, *20*, 97.
2. Sanemasa, I.; Araki, M.;
   Deguchi, Y.; Nagai, H.
   Chem. Lett. 1981, 225-8.

COMPONENTS: (1) Mesitylene (1,3,5-Trimethylbenzene); C_9H_{12}; [108-67-8] (2) Artificial seawater (ref 1)	**ORIGINAL MEASUREMENTS:** Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	**PREPARED BY:** M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of 1,3,5-trimethylbenzene in artificial seawater is reported to be 31.3 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 3.13×10^{-3} g(1)/100 g sln and 4.81×10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.2 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

January 1986.

CRITICAL EVALUATION:

Quantitative solubility studies of the cumene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Cumene (1) - Water (2) System

Reference	T/K	Solubility	Method
Stearns *et al.* (ref 1)	298	(1) in (2)	turbidimetric
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Glew and Robertson (ref 3)	298-354	(1) in (2)	spectrophotometric
McAuliffe (ref 4)	298	(1) in (2)	GLC
Englin *et al.* (ref 5)	273-323	(2) in (1)	analytical
McAuliffe (ref 6)	298	(1) in (2)	GLC
Sutton and Calder (ref 7)	298	(1) in (2)	GLC
Price (ref 8)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 9)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 10)	288-318	(1) in (2)	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. THE SOLUBILITY OF CUMENE (1) IN WATER (2)

With the exception of the rejected values referred to below and the datum of Krzyzanowska and Szeliga (ref 9) which does not appear to be independent of that of Price (ref 8) all the available data on the solubility of cumene in water are summarized in Table 2.

At 298K where the most data are available, agreement is only fair. The values of Stearns *et al.* (ref 1), Andrews and Keefer (ref 2) and Glew and Robertson (ref 3) are much higher than other studies (ref 4,6,7,8,10) and are rejected.

At other temperatures the values of Glew and Robertson are again in only fair agreement with those of Sanemasa *et al.* (ref 10), but in the absence of confirmatory studies it is not possible to express a preference for either data set, and the averaged "Best" values should be regarded as Tentative. Selected data are also plotted in Figure 1

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cumene; C_9H_{12}; [98-82-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Cumene (1) in Water (2)

T/K	Solubility values Reported values[a] 10^3g(1)/100g sln	"Best" values (± σ_n)[b] 10^3g(1)/100g sln	 $10^5\ x_1$
288	5.95 (ref 10)	6.0	0.90
298	5.3 (ref 4), 5.0 (ref 6), 6.53 (ref 7), 4.83 (ref 8), 6.15 (ref 10)	5.6 ± 0.7	0.84
303	8.3* (ref 3), 6.5* (ref 10)	7.4 ± 0.9	1.11
313	9.0* (ref 3), 7.3* (ref 10)	8.2 ± 0.9	1.23
323	10.0* (ref 3), 8.0* (ref 10)	9 ± 1	1.3
333	11.5* (ref 3)	12	1.8
343	13.5* (ref 3)	14	2.1
353	16.1* (ref 3)	16	2.4

[a] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

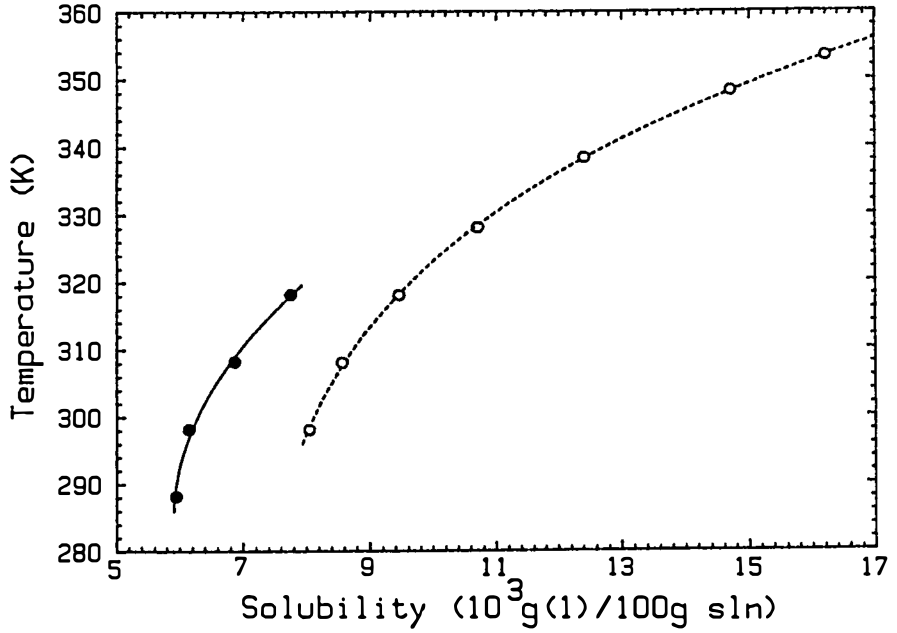

FIGURE 1. Solubility of cumene in water, selected data: ref 3(o); ref 10 (●).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cumene; C_9H_{12}; [98-82-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. January 1986.

CRITICAL EVALUATION: (continued)

Interestingly, application of the van't Hoff equation to both data sets gives values of ΔH_{sln} = 3.5 (ref 3) and 5.1 (ref 10) kJ mol^{-1} and $\Delta C_{p,sln}$ = 291 (ref 3) and 382 (ref 10) J K^{-1} mol^{-1}. Comparison of these values with those of related systems suggests both solubility data sets are reasonable.

2. THE SOLUBILITY OF WATER (2) IN CUMENE (1)

Quantitative solubilities of water in cumene have been reported only in the study of Englin *et al.* (ref 5) and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet following this Critical Evaluation for the experimental values. However, it may be noted that for other hydrocarbon systems studied by these authors, the data of Englin *et al.* are generally reliable at T < 300K but higher than Recommended values at higher temperatures.

REFERENCES

1. Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkin, L.D. *J. Chem. Phys.* 1947, *15*, 496-507.
2. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
3. Glew, D.N.; Robertson, R.E. *J. Phys. Chem.* 1956, *60*, 332-7.
4. McAuliffe, C. *Nature* 1963, *200*, 1092-3.
5. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1966, *10*, 1267-75.
6. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
7. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
8. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
9. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.
10. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for graphics and regression analyses.

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D.

J. Chem. Phys. 1947, *15*, 496-507.

VARIABLES:

Temperature: 25°C

PREPARED BY:

A. Maczynski and D. Shaw

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C was reported to be 0.017 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compiler is 2.5×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

temp. ± 3°C.

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1950, *72*, 5034-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C was reported to be 0.0073 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 1.09×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 151.5-152.0°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Glew, D.N.; Robertson, R.E.

J. Phys. Chem. 1956, *60*, 332-7.

VARIABLES:

Temperature: 298-353 K

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of cumene in water

T/K	$10^5\ x_1$	g(1)/100 g sln (compiler)
298.086	1.2050	0.00804
303.134	1.2416	0.00829
308.068	1.2825	0.00856
313.108	1.3446	0.00897
318.055	1.4162	0.00945
323.052	1.5037	0.01004
328.066	1.6011	0.01069
333.133	1.7221	0.01149
338.315	1.8624	0.01243
343.470	2.0302	0.01355
348.247	2.2064	0.01472
353.359	2.4212	0.01616

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was floated on the surface of the main body of the water and the aqueous solution was pumped steadily in a closed circuit through the quartz absorption cell where its absorbance was measured. From these values the solubility of (1) in (2) was calculated.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. White Label; distilled in an atmosphere of nitrogen; b.p.range 0.2°C, passed repeatedly through a fresh column of Fisher activated alumina,

(2) distilled; passed through a demineralizing column.

ESTIMATED ERROR:

temp. ± 0.002 K

soly. ± 1.00% at 25°C and ± 1.25% at 80°C (standard error)

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

Nature (London) 1963, *200*, 1092-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C was reported to be 0.0053 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compilers is 7.9×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer.
A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was injected directly into a gas liquid chromatograph.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+%; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.0005 (standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 0-50°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Cumene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
0	0.0156	1.04
10	0.0219	1.46
20	0.0303	2.02
30	0.0407	2.71
40	0.0550	3.66
50	0.0710	4.72

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and
A. Szafranski

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C was reported to be 50 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0050 g(1)/100 g sln and 7.5 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 5 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C was reported to be 65.3 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00653 g(1)/100 g sln and 9.78×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.8 (the standard deviation of the mean for six replicates)

REFERENCES:

COMPONENTS:

(1) Cumene; C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C and at system pressure was reported to be 48.3 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00483 g(1)/100 g sln and 7.23 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 1.2 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Cumene; C_9H_{12}; [98-82-8] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cumene in water at 25°C was reported to be 48.3 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00483 g(1)/100 g sln and 7.24 x 10^{-6}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) Cumene (Isopropylbenzene); C_9H_{12}; [98-82-8]

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

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of isopropylbenzene in water

t /°C	10^4 mol(1)/dm^3 sln	10^3 g(1)/100 g sln (compiler)[a]	10^6 x_1 (compiler)[a]
15	4.95 ± 0.28	5.95	8.92
25	5.10 ± 0.45	6.15	9.22
35	5.68 ± 0.22	6.87	10.3
45	6.38 ± 0.24	7.75	11.6

[a] Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.01°C.

REFERENCES:

1. Kell, G.S. *J. Chem. Eng. Data* 1975, *20*, 97.
2. Sanemasa, I.; Araki, M.; Deguchi, Y.; Nagai, H. *Chem. Lett.* 1981, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cumene; C_9H_{12}; [98-82-8] (2) Artificial seawater (ref 1)	Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES:	**PREPARED BY:**
One temperature: 25.0°C One salinity: 34.5 g salts/kg sln	M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of cumene (isopropylbenzene) in artificial seawater is reported to be 42.5 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 4.25×10^{-3} g(1)/100 g sln and 6.54×10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.2 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:	EVALUATOR:
(1) Propylbenzene, C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for propylbenzene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in propylbenzene.

TABLE 1: Quantitative Solubility Studies of Propylbenzene (1) in Water (2)

Reference	*T*/K	Method
Führer (ref 1)	288	volumetric
Stearns *et al.* (ref 2)	298	turbidimetric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Guseva and Parnov (ref 5)	359-495	synthetic
Krasnoshchekova and Gubergrits (ref 7)	298	GLC
Sanemasa *et al.* (ref 8)	288-318	spectrophotometric
Sanemasa *et al.* (ref 9)	298	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

Guseva and Parnov (ref 5) have reported solubility data for propylbenzene in water at elevated temperatures (359-495K) and system pressure. Alwani and Schneider (ref 6) have studied phase equilibria in the propylbenzene - water system at 600-678K and 20-200 MPa. In the absence of confirmatory studies no Critical Evaluation of these data is possible; however, it may be noted that data reported by Guseva and Parnov (ref 5) for other hydrocarbon - water systems are generally not reliable. The interested user is referred to the relevant Data Sheets for experimental results.

All other data for the solubility of propylbenzene in water are summarized in Table 2 except for the 298K data of Führer (ref 1) and Klevens (ref 4) which are very much higher than all other studies (ref 3,7,8,9) and are rejected. The remaining data at 298K, the only temperature where comparison is possible, are in only fair agreement.

At other temperatures only the values of Sanemasa *et al.* (ref 8) are available. Thus all solubility values in Table 2 must be considered Tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Propylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values (± σ_n)[a]	
	$10^3 g(1)/100g$ sln	$10^3 g(1)/100g$ sln	$10^6\ x_1$
288	4.66 (ref 8)	4.7	7.0
298	5.5 (ref 3), 7.0 (ref 7) 5.10 (ref 8), 4.52 (ref 9)	5.5 ± 0.9	8.2
308	5.50 (ref 8)	5.5	8.2
318	6.41 (ref 8)	6.4	9.6

[a] Obtained by averaging where appropriate; σ_n has no statistical significance.

REFERENCES

1. Fuhner, H. *Chem. Ber.* 1924, *57*, 510-4.
2. Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, L.D. *J. Chem. Phys.* 1947, *15*, 496-507.
3. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
4. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
5. Guseva, A.N.; Parnov, E.I. *Zh. Fiz. Khim.* 1964, *38*, 805-6.
6. Alwani, Z.; Schneider, G.M. *Ber. Bunsenges. Phys. Chem.* 1969, *73*, 294-301.
7. Krasnoshchekova, R.Y.; Gubergrits, M.Y. *Vodnye. Resursy.* 1975, *2*, 170-3.
8. Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, J. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.
9. Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* 1984, *57*, 1539-44.

COMPONENTS:

(1) Propylbenzene; C_9H_{12}; [103-65-1]

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

ORIGINAL MEASUREMENTS:

Fuhner, H.

Ber. Dtsch. Chem. Ges. 1924, *57*, 510-5.

VARIABLES:

One temperature: 15°C

PREPARED BY:

A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 15°C was reported to be 0.006 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 9×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm^3 (2) until a completely clear solution was no longer obtained at the experimental temperature.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; commercial grade; used as received,

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D. *J. Chem. Phys.* 1947, *15*, 496-507.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	A. Maczynski and D. Shaw

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.012 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler is 1.8×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photometer. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

temp. ± 3°C.

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.0055 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 8.2×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 157.8-158.1°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.12 g(1) L^{-1} sln and 0.001 mol(1) L^{-1} sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Propylbenzene; C_9H_{12}; [103-65-1]

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

ORIGINAL MEASUREMENTS:

Guseva, A.N.; Parnov, E.I.

Zh. Fiz. Khim. 1964, *38*, 805-6.

VARIABLES:

Temperature: 85.8-222.0°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of propylbenzene in water

t/°C	g(1)/100 g sln	$10^5 x_1$ (compiler)
85.8	0.0132	1.98
114.5	0.0166	2.49
140.5	0.0321	4.81
188.0	0.087	13.04
222.0	0.245	36.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The measurements were made in sealed glass tubes. No details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Vodnye. Resursy.* 1975, *2*, 170-3.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 0.070 mg(1) cm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0070 g(1)/100 g sln and 1.05 x 10^{-5}. The assumption that 1.00 cm^{-3} sln = 1.00 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by glc.
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.

SOURCE AND PURITY OF MATERIALS:

(1) described in ref (1).

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C

REFERENCES:

1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Propylbenzene; C_9H_{12}; [103-65-1]
(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;
Deguchi, T.; Nagai, H.
Bull. Chem. Soc. Jpn. 1982, *55*, 1054-62.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water

t /°C	10^4 mol(1)/dm^3 sln	10^3 g(1)/100 g sln (compiler)^a	10^6 x_1 (compiler)^a
15	3.88 ± 0.15	4.66	6.99
25	4.23 ± 0.12	5.10	7.64
35	4.55 ± 0.07	5.50	8.25
45	5.28 ± 0.17	6.41	9.61

a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm^3 of (2) and 10-20 cm^3 of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask containing (2). Five 10 cm^3 aliquots were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UV-spectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), no stated purity, used without further purification.

(2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
temp. ± 0.1°C.

REFERENCES:

1. Kell, G.S.
   J. Chem. Eng. Data 1975, *20*, 97.

2. Sanemasa, I.; Araki, M.;
   Deguchi, Y.; Nagai, H.
   Chem. Lett. 1981, 225-8.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Propylbenzene; C_9H_{12}; [103-65-1] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* 1984, *57*, 1539-44.
VARIABLES:	PREPARED BY:
One Temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of propylbenzene in water at 25°C was reported to be 3.76×10^{-4} mol(1)/dm^3 sln. Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 4.52×10^{-3} g(1)/100 g sln, $x_1 = 6.78 \times 10^{-6}$, calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectrophotometry.

SOURCE AND PURITY OF MATERIALS:

(1) Analytical reagent grade source and purity not stated, used without further purification.

(2) Deionized and redistilled; no further details given.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* 1982, *55*, 1054-62.

COMPONENTS:

(1) 1,8-Nonadiyne; C_9H_{12}; [2396-65-8]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,8-nonadiyne in water at 25°C was reported to be 125 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0125 g(1)/100 g sln and 1.9×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C

soly. 3 g(1)/10^6 g(2) (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Nonyne; C_9H_{16}; [3452-09-3] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-nonyne in water at 25°C was reported to be 7.2 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00072 g(1)/100 g sln and 1.0 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum or Columbia Chemical; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.5 g(1)/10^6 g(2)
(standard deviation of mean)

REFERENCES:

COMPONENTS:

(1) Butylcyclopentane; C_9H_{18}; [2040-95-1]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in Butylcyclopentane

t/°C	g(2)/100 g sln	10^4 x_2 (compiler)
10	0.0056	3.93
20	0.0095	6.66
30	0.0151	10.58

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hrs. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 1,1,3-Trimethylcyclohexane; C_9H_{18}; [3073-66-3]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclohexane in water at 25°C and at system pressure was reported to be 1.77 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.77×10^{-4} g(1)/100 g sln and 2.53×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.05 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 1,1,3-Trimethylcyclohexane; C_9H_{18}; [3073-66-3]

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

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, *12*, 413-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,1,3-trimethylcyclohexane in water at 25°C was reported to be 0.115 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.15×10^{-5} g(1)/100 g sln and 1.64×10^{-8}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.02 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the 2,2,5-trimethylhexane (1) and water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 2,2,5-Trimethylhexane (1) - Water (2) System

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF 2,2,5-TRIMETHYLHEXANE (1) IN WATER (2)

All the available data on the solubility of 2,2,5-trimethylhexane in water are summarized in Table 2.

At 298K,the only temperature where comparison is possible,the values of McAuliffe (ref 1) and Polak and Lu (ref 2) are in poor agreement (Table 2). The only other value available is that of Polak and Lu at 273K. Thus all solubility values must be regarded as very Tentative in the absence of confirmatory studies.

TABLE 2: Tentative Values of the Solubility of 2,2,5-Trimethylhexane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values ($\pm \sigma_n$)^a	
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10^7 x_1$
273	1.79 (ref 2)	0.8	1.1
298	1.15 (ref 1), 0.54 (ref 2)	0.8 ± 0.3	1.1

a Obtained by averaging where appropriate; σ_n has no statistical signigicance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. December 1985.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN 2,2,5-TRIMETHYLHEXANE (1)

Only the data of Polak and Lu (ref 2) are available for the solubility of water in 2,2,5-trimethylhexane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values; however, it may be noted that the data of Polak and Lu (ref 2) are generally reliable.

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

2. Polak, J.; Lu, B.C.-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

COMPONENTS:

(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9]

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

ORIGINAL MEASUREMENTS:

McAuliffe, C.

J. Phys. Chem. 1966, *70*, 1267-75.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2,5-trimethylhexane in water at 25°C was reported to be 1.15 mg (1)/kg sln.
The corresponding mole fraction, x_1, calculated by the compiler, is 1.62×10^{-7}.
The same value is also reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250 mL glass bottle, 10-20 mL of (1) was vigorously shaken for 1 hr or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. In the case of shaking, the solution was allowed to stand for 2 days to permit separation of small (1) droplets. Absence of emulsion was checked microscopically. A 50 μL sample of the (1) saturated water was withdrawn with a Hamilton Syringe and injected into the fractionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; 99+% purity; used as received.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C
soly. 0.008 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:

(1) 2,2,5-Trimethylhexane; C_9H_{20}; [3522-94-9]

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

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C-Y.

Can. J. Chem. 1973, *51*, 4018-23.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2,2,5-trimethylhexane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	0.79^c	1.11×10^{-7}
25^b	0.54^c	7.58×10^{-8}

Solubility of water in 2,2,5-trimethylhexane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	25^d	1.78×10^{-4}
25^b	75^d	5.34×10^{-4}

[a-e] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by gas chromatography. The solubility of (2) in (1) was determined by Karl Fischer titration. 50 mL of (1) together with 50 mL of (2) were placed in a 125 mL Hypovial closed with a Teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr or was kept in the bath without stirring for at least 7 days before samples were taken for analysis. Details of the analysis are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02°C; b) ± 0.01°C
soly. c) ± 4%; d) ± 4.7%;
e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:

(1) 2,6-Dimethylheptane; C_9H_{20}; [1072-05-5]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-50°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in 2,6-dimethylheptane

t/°C	g(2)/100 g sln	$10^4\ x_2$ (compiler)
10	0.0053	3.77
20	0.0091	6.48
30	0.0160	11.39
40	0.0301	21.40
50	0.0465	33.02

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 2-Methyloctane; C_9H_{20}; [3221-61-2]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in 2-methyloctane

$t/°C$	g(2)/100 g sln	$10^4\ x_2$ (compiler)
10	0.0052	3.70
20	0.0090	6.41
30	0.0156	11.10

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 3-Methyloctane; C_9H_{20}; [2216-33-3]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in 3-methyloctane

t/°C	g(2)/100 g sln	$10^4\ x_2$ (compiler)
10	0.0050	3.56
20	0.0087	6.20
30	0.0155	11.03

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) 4-Methyloctane; C_9H_{20}; [2216-34-4] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 4-methyloctane in water at 25°C and at system pressure was reported to be 0.115 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.15×10^{-5} g(1)/100 g sln and 1.6×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.011 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Methyloctane; C_9H_{20}; [2216-34-4] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 4-methyloctane in water at 25°C was reported to be 0.115 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.15×10^{-5} g(1)/100 g sln and 1.61×10^{-8}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.02 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) Nonane; C_9H_{20}; [111-84-2]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2. Tentative Solubility Values for Nonane (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values ($\pm\ \sigma_n$)[b]	
	10^5g(1)/100g sln	10^5g(1)/100g sln	$10^8\ x_1$
293	2.89 (ref 8)	2.9	4.1
298	2.2 (ref 2), 0.71 (ref 5), 1.22 (ref 6), 2.72 (ref 8)	1.7 ± 0.8	2.4
303	1.4* (ref 6)	1.4	2.0
313	1.7* (ref 6)	1.7	2.4
323	2.2* (ref 6)	2.2	3.1
333	2.6* (ref 6)	2.6	3.7
343	3.1* (ref 6)	3.1	4.4
353	3.4* (ref 6)	3.4	4.8
363	3.7* (ref 6)	3.7	5.2
373	4.2* (ref 6)	4.2	5.9
383	8.0* (ref 6)	8.0	11
393	16* (ref 6)	16	22
403	32* (ref 6)	32	45

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the author's original data.

b Obtained by averaging where appropriate; σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN NONANE (1)

Only the single point data of Schatzberg (ref 1) at 298K and Benkovski *et al.* (ref 3) at 303K are available for the solubility of water in nonane and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for the experimental values; however, it may be noted that the data of Schatzberg (ref 1) are generally reliable.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.

2. McAuliffe, C. *Science* 1969, *163*, 478-9.

3. Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M. *Tr. Inst. Khim. Nefti Prir. Solei Alkad. Nauk Kaz. SSR* 1970, *2*, 25-32.

4. Roof, J.G. *J. Chem. Eng. Data* 1970, *15*, 301-3.

5. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-7.

(continued next page)

COMPONENTS:

(1) Nonane; C_9H_{20}; [111-84-2]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the nonane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of the Nonane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Schatzberg (ref 1)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 2)	298	(1) in (2)	GLC
Benkovski *et al.* (ref 3)	303	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 5)	298	(1) in (2)	GLC
Price (ref 6)	298-410	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 7)	298	(1) in (2)	GLC
Jonsson *et al.* (ref 8)	288,293	(1) in (2)	partition coeff.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Roof (ref 4) has also reported a three phase critical point of unspecified composition at 555K and 8.5 MPa. For convenience further discussion of this system will be in two parts.

1. SOLUBILITY OF NONANE (1) IN WATER (2)

All the data available for the solubility of nonane in water are summarized in Table 2 with the exception of the datum of Krzyzanowska and Szeliga (ref 7) which does not appear to be independent of that of Price (ref 6) and has therefore been excluded from consideration.

At 298K, the only temperature where comparison is possible, the agreement between the various studies is poor (Table 2) and the average must be regarded as Tentative only. Interestingly, the average value of 1.7×10^{-5} g(1)/100g sln is, however, quite close to the value of 2.0×10^{-5} g(1)g sln predicted by extrapolation of the lower *n*-alkane solubilities.

At other temperatures only the data of Jonsson *et al.* (ref 8) at 293K and Price (ref 6) at 303-410K are available and thus no Critical Evaluation is possible. There are also insufficient independent data to warrant plotting.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

6. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

7. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *34*, 413-7.

8. Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, *9*, 279-86.

COMPONENTS: (1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in nonane at 25°C was reported to be 79 mg(2)/kg sln corresponding to a mole fraction, x_2, of 5.6×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; research grade; 99.69 mole%; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. 0-6% (deviations from the mean)

REFERENCES:

COMPONENTS: (1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** McAuliffe, C. *Science* 1969, *163*, 478-9.
VARIABLES: One temperature: 25°C	**PREPARED BY:** F. Kapuku

EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be 0.220 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.2×10^{-5} g(1)/100 g sln and 3.09×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: (1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaker for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	**SOURCE AND PURITY OF MATERIALS:** (1) not specified. (2) distilled. **ESTIMATED ERROR:** soly. ± 0.021 mg(1)/kg(2) **REFERENCES:**

COMPONENTS:

(1) Nonane; C_9H_{20}; [111-84-2]

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

ORIGINAL MEASUREMENTS:

Benkovski, V.G.; Nauruzov, M.H.; Bogoslovskaya, T.M.

Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR 1970, *2*, 25-32.

VARIABLES:

One temperature: 303 K

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in nonane at 303 K was reported to be 0.0045 g(2)/100 g sln.

The corresponding mole fraction, x_2, value calculated by compiler is 0.00032.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equal volumes of (1) and (2) were placed in a glass cylinder and periodically shaken for 6 h, then sampled and analyzed by the Karl Fischer method.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; purified; purity not specified.

(2) distilled.

ESTIMATED ERROR:

Not specified

REFERENCES:

COMPONENTS:

(1) Nonane; C_9H_{20}; [111-84-2]

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

ORIGINAL MEASUREMENTS:

Krasnoshchekova, P.Ya.; Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be $x_1 = 1.00 \times 10^{-8}$.
The corresponding mass percent calculated by the compiler is 7.1×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; purity not specified.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Nonane; C_9H_{20}; [111-84-2]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

Temperature: 25-136.6°C

PREPARED BY:

F. Kapuku

EXPERIMENTAL VALUES:

Solubility of nonane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
25.0	0.122 ± 0.007	0.0000122	1.71
69.7	0.309 ± 0.019	0.0000309	4.34
99.1	0.420 ± 0.034	0.0000420	5.90
121.3	1.70 ± 0.11	0.000170	23.9
136.6	5.07 ± 0.25	0.000507	71.2

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and insured saturation (in 2 to 4 days) of the aqueous phase. High-temperature solubility work was carried out in the ovens of the gas chromatograph. The solutions were contained in 75 mL double ended stainless steel sample cylinders. Modified Micro Linear Valves sealed the bottom of the cylinder and allowed syringe access to the solution during sampling. The sample is then transferred to the gas chromatograph equipped with dual flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C

soly. range of values given above

REFERENCES:

COMPONENTS: (1) Nonane; C_9H_{20}; [111-84-2] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of nonane in water at 25°C was reported to be 0.122 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 1.22×10^{-5} g(1)/100 g sln and 1.71×10^{-8}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.01 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) Nonane; C_9H_{20}; [111-84-2]

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

ORIGINAL MEASUREMENTS:

Jonsson, J.A.; Vejrosta, J.; Novak, J.

Fluid Phase Equil. 1982, *9*, 279-86.

VARIABLES:

Temperature: 15-20°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of nonane (1) in water (2)

t/°C	mg(1)/kg sln	10^5g(1)/100g sln (compiler)	10^8x_1 (compiler)
15	0.289	2.89	4.05
20	0.272	2.72	3.81

Solubility values were calculated by the authors from their smoothed air-water partition coefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Air-water partition coefficients were measured by saturating a portion of water by a stream of nitrogen containing a known vapor concentration of (1). After equilibration, the dissolved (1) was adsorbed in a porous polymer trap and the entrapped (1) analyzed by gas chromatography. The method and apparatus are described in detail in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka, > 99%, used as received.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Vejrosta, J.; Novak, J.; Jonsson, J.A. *Fluid Phase Equil.* 1982, *8*, 25-35.

COMPONENTS: (1) Nonane; C_9H_{20}; [111-84-2] (2) Seawater	**ORIGINAL MEASUREMENTS:** Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln	**PREPARED BY:** M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of nonane in seawater was reported to be 4.3×10^{-5} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 6.0 \times 10^{-8}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.	**SOURCE AND PURITY OF MATERIALS:** (1) "chemically pure" (2) distilled water plus salt mixture. **ESTIMATED ERROR:** not specified. **REFERENCES:**

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Quantitative data for the solubility of naphthalene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Studies of the Solubility of Naphthalene (1) in Water (2)

Reference	*T*/K	Method
Hilpert (ref 1)	273,298	gravimetric
Mitchell (ref 2)	288,298	interferometric
Andrews and Keefer (ref 3)	298	spectrophotometric
Klevens (ref 4)	298	spectrophotometric
Bohon and Claussen (ref 5)	273-316	spectrophotometric
Wauchope and Getzen (ref 6)	273-348	spectrophotometric
Eganhouse and Calder (ref 7)	298	GLC
Mackay and Shiu (ref 8)	298	spectrofluorometric
Schwarz and Wasik (ref 9)	285-298	spectrophotometric
Schwarz (ref 10)	282-305	spectrophotometric
May *et al.* (ref 11)	298	HPLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data appear to have been published on the solubility of water in naphthalene.

Despite the low solubility of naphthalene in water the published data are in excellent agreement. With the exception of the 298K data of Mitchell (ref 2) and Klevens (ref 4) which differ markedly from other studies, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of Naphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values^a	"Best" values $(\pm\ \sigma_n)^b$	
	10^3g(1)/100g sln	10^3g(1)/100g sln	$10^6\ x_1$
273	1.9 (ref 1), 1.37 (ref 5), 1.37 (ref 6)	1.5 ± 0.2	2.1
283	1.94 (ref 5), 2.0* (ref 6), 1.87* (ref 10)	1.9 ± 0.1 (*R*)	2.7 (*R*)

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March, 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility values Reported values[a] $10^3 g(1)/100g$ sln	"Best" values (± σ_n)[b] $10^3 g(1)/100g$ sln	 $10^6\ x_1$
293	2.86* (ref 5), 2.8* (ref 6), 2.62* (ref 10)	2.8 ± 0.1 (R)	3.9 (R)
298	3.0 (ref 1), 3.15 (ref 3), 3.44 (ref 5), 3.12 (ref 6), 3.13 (ref 7), 3.17 (ref 8), 3.00 (ref 9), 3.03 (ref 10), 3.17 (ref 11)	3.1 ± 0.1 (R)	3.9 (R)
303	4.3* (ref 5), 3.7* (ref 6), 3.48* (ref 10)	3.8 ± 0.3	5.3
313	6.6* (ref 5), 5.5* (ref 6)	6.1 ± 0.6	8.6
323	8.24* (ref 6)	8.2	12
333	13.0* (ref 6)	13	18
343	20.0* (ref 6)	20	28
348	25.8 (ref 6)	26	37

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

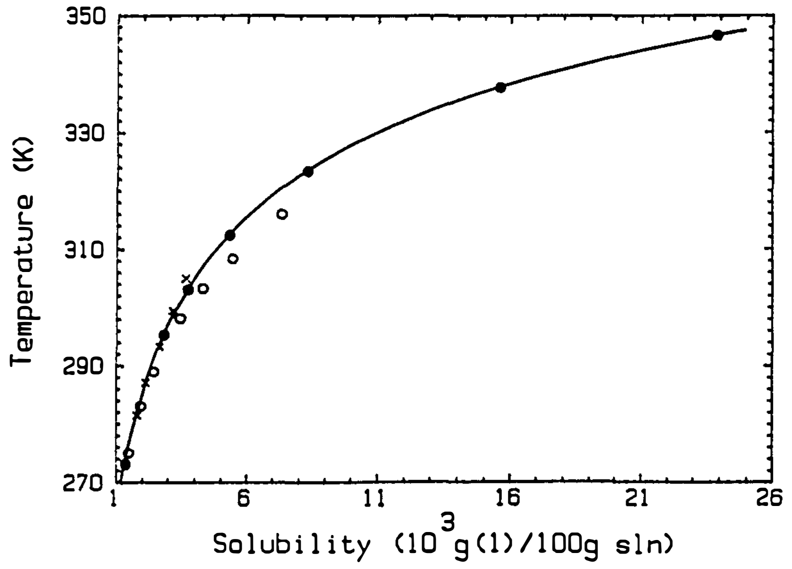

FIGURE 1. Solubility of naphthalene in water, selected data: ref 5 (o); ref 6 (●); ref 10 (x). Solid curve fitted through "Best" values (Table 2).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March, 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Hilpert, S. *Angew. Chem.* 1916, *29*, 57-9.
2. Mitchell, S. *J. Chem. Soc.* 1926, *129*, 1333-6.
3. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-77.
4. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283.
5. Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1571-8.
6. Wauchope, R.D.; Getzen, F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
7. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
8. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
9. Schwarz, F.P.; Wasik, S.P. *J. Chem. Eng. Data* 1977, *22*, 270-3.
10. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
11. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Hilpert, S.

Angew. Chem. 1916, *29*, 57-9.

VARIABLES:

Temperature: 0 and 25°C

PREPARED BY:

A. Maczynski and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of naphthalene in water

t/°C	10^3 g(1)/100 g sln	$10^6 x_1$
0	1.9	2.7
25	3.0	4.2

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A sample of (1) was shaken with 1000 g(2) until saturation and then filtered. The filtrate was steam distilled to drive away (1) which was collected and presumably weighed.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Mitchell, S.

J. Chem. Soc. London 1926, 1332-6.

VARIABLES:

Temperature: 15 and 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of naphthalene in water

t/°C	g(1) L^{-1} (2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
15	0.022	0.0022	3.1
25	0.040	0.0040	5.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

For this study an interferometer of the type described in ref (1) was constructed.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Jamin *Ann. Chim. Phys.* 1958, *52*, 171.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1949, *71*, 3644-77.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 0.00315 g(1)/100 g sln.

The corresponding mole fraction, x_1, value calculated by compiler is 4.42×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co., best grade; recrystallized from ethanol; mp. 80.5°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 0.0125 g(1) L^{-1} sln and 9.75 x 10^{-5} mol(1) L^{-1} sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding values calculated by the compiler are 0.00125 g(1)/100 g sln and mole fraction, x_1, = 1.76 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1571-8.
VARIABLES: Temperature: 0-42.8°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of naphthalene in water

t/°C	10^3g(1)/100g sln[a] (compiler)	$10^6 x_1$
0.0	1.37	1.92
0.4	1.37	1.92
0.5	1.38	1.94
0.9	1.46	2.05
1.9	1.50	2.11
9.4	1.96	2.75
10.0	1.94	2.72
14.9	2.34	3.29
15.9	2.46	3.45
19.3	2.80	3.93
25.0	3.44[b]	4.83[b]
25.6	3.58	5.03
30.1	4.30	6.04
30.2	4.39	6.16
35.2	5.45	7.65
36.0	5.48	7.69
42.8	7.35	10.3

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

[b] Given in the paper as 0.0344g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least anothe 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

(1) Allied Chemical & Dye Corp., purified by vacuum distillation.

(2) Air-free conductivity water, no other details given.

ESTIMATED ERROR:

Temp. ± 0.02°C

Soly. ± 0.5% relative

REFERENCES:

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-75°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of naphthalene in water

t/°C	mg(1)/kg(2)		g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
	experiment	smoothed with (std dev)		
0.0		13.7(0.2)	0.00137	1.93
22.2	28.8, 29.1, 28.8	28.3	0.00283	3.98
24.5	30.8(2), 30.1(2), 30.7	30.7	0.00307	4.31
25.0		31.2(0.2)	0.00312	4.38
29.9	38.1, 38.2, 38.3	37.3	0.00373	5.24
30.3	38.1, 37.6, 37.6	37.8	0.00378	5.31
34.5	44.6, 43.8	44.3	0.00443	6.23
39.2	52.6, 52.8	53.3	0.00533	7.49
40.1	54.8	55.0	0.00550	7.73
44.7	66.0, 65.5, 65.3	66.2	0.00662	9.30
50.0		82.4(0.4)	0.00824	11.58
50.2	78.6	83.1	0.00831	11.68
55.6	106	105	0.0105	14.8
64.5	166, 151, 157	156	0.0156	21.9
73.4	240, 247, 244	239	0.0239	33.6
75.0		258(3)	0.0258	36.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. see experimental values above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 31.3 mg(1)/kg(2) and 2.43 x 10^{-4} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.13 x 10^{-3} g(1)/100 g sln and 4.40 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc.
A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) double distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.4 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 31.7 mg(1) dm^{-3} sln and $x_1 = 4.46 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00317 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.26 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.4-31.8°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of naphthalene in water

t/°C	10^4 mol(1) L^{-1}	10^3 g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
8.4	1.40 ± 0.02	1.79	2.52
11.1	1.49 ± 0.03	1.91	2.68
14.0	1.66 ± 0.05	2.13	2.99
17.5	1.88 ± 0.03	2.41	3.39
20.2	2.07 ± 0.02	2.65	3.73
23.2	2.22 ± 0.03	2.85	4.00
25.0	2.36 ± 0.02	3.03	4.25
26.3	2.48 ± 0.02	3.18	4.47
29.2	2.68 ± 0.02	3.44	4.83
31.8	2.83 ± 0.02	3.63	5.10

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99.9 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P.; Wasik, S.P. *J. Chem. Eng. Data* 1977, *22*, 270-3.
VARIABLES:	**PREPARED BY:**
Temperature: 12-25°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of naphthalene in water

t/°C	10^4 mol(1) L^{-1}	10^3 g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
12	1.57	2.01	2.83
18	1.90	2.43	3.42
25	2.34	3.00	4.21

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

SOURCE AND PURITY OF MATERIALS:

(1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%.

(2) distilled from $KMnO_4$ and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ±0.1°C
soly. ±2 x 10^{-6} mol(1) dm^{-3}

REFERENCES:

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of naphthalene in water at 25°C was reported to be 31.69 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, values calculated by compiler are 0.003169 g(1)/100 g sln and 4.425 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.23 mg(1)/100 kg(2)
(standard deviation)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:	EVALUATOR:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of naphthalene (1) in seawater (2) has been reported in six works:

Authors	Method	T/K	Salinity g salts/kg sln	10^3 g(1)/100 g sln
Paul (ref 1)	uv spectral	298	30.59	2.53
Gordon and Thorne (ref 2)	uv spectral	298	35.0	2.36
Gordon and Thorne (ref 3)	uv spectral	298	31.7	2.47
Eganhouse and Calder (ref 4)	GLC	298	35	2.20
Schwarz (ref 5)	uv spectral	298	30	2.17
May *et al.* (ref 6)	HPLC	298	35.0	2.29

At 298 K and a salinity of 35 g salts/kg sln the data of Gordon and Thorne (ref 2), Eganhouse and Calder, and May *et al.* are in good agreement. Therefore the mean value, 2.29 x 10^{-3}, is adopted as the recommended value at this temperature and salinity. Since the value of Schwarz is lower than would be expected with decreasing salinity, it is considered doubtful. At 298 K and a salinity of 31 g salts/kg sln the data of Paul and of Gordon and Thorne (ref 3) are in fair agreement. Therefore their mean is adopted as a tentative value. Gordon and Thorne (ref 2) and May *et al.* report data for a range of salinities using the Setschenow equation. Schwarz reports data over the temperature range 281 to 303 K. However, since this data at 298 K appears low, the usefulness of this work is diminished.

SOLUBILITY OF NAPHTHALENE (1) IN SEAWATER (2)
RECOMMENDED(r) AND TENTATIVE(t) VALUES

T/K	g salts/kg sln	10^3 g(1)/100 g sln
298	35 (r)	2.29
298	31 (t)	2.5

REFERENCES

1. Paul, M.A. *J. Amer. Chem. Soc.* 1952, *74*, 5274-7.
2. Gordon, J.E.; Thorne, R.L. *J. Phys. Chem.* 1967, *71*, 4390-9.
3. Gordon, J.E.; Thorne, R.L. *Geochim. Cosmochim. Acta* 1967, *31*, 2433-43.
4. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
5. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
6. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

(2) Sodium chloride; NaCl; [7732-14-5]

(3) Water; H_2O; [7647-18-5]

ORIGINAL MEASUREMENTS:

Paul, M.A.

J. Am. Chem. Soc. 1952, *74*, 5274-7.

VARIABLES:

One temperature: 25°C

Salinity: 13-64 g(3)/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

Solubility of Naphthalene in Aqueous Sodium Chloride

g-mol(3)/L^{-1}	g(2)/kg sln*	10^4 g-mol(1)/L^{-1}	10^3 Mass %*	10^6 x_1*
0.214	12.40	2.37	3.01	4.27
0.440	25.31	2.00	2.52	3.61
0.535	30.59	2.02	2.53	3.64
0.771	43.70	1.68	2.09	3.02
1.101	61.63	1.38	1.69	2.48

*Calculated by compilers using density and other physical data for NaCl solutions from ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibration flask: 50-mL glass-stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until excess hydrocarbon had recrystallized. The flask was then placed into a water bath thermostatically controlled at 25.00 ± 0.05°C for at least 48 hr, and shaken occasionally during that time. Samples were withdrawn with a 10-ml transfer pipet, diluted appropriately and analyzed using a spectrophotometer in the ultra-violet region of the spectrum.

SOURCE AND PURITY OF MATERIALS:

(1) recrystallized from menthanol

(2) reagent grade, dried at 120°C before weighing

(3) redistilled

Sources not specified.

ESTIMATED ERROR:

temp. ± 0.05°C

soly. ± 1 %

REFERENCES:

1. Weast, R.C.; *CRC Handbook of Chemistry and Physics*, 59th Edition; CRC Press 1978, pp D299-D300.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

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

ORIGINAL MEASUREMENTS:

Gordon, J.E.; Thorne, R.L.

J. Phys. Chem. 1967, *71*, 4390-9.

VARIABLES:

One temperature: 24.91°C

Salinity: 0-108 g(2)/kg sln

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_sC_s$$

where, S_o is the solubility of naphthalene in water (mol/L)

S is the solubility of naphthalene in solution (mol/L)

K_s is the Setschenow constant (L/mol)

C_s is the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-2 mol/L, $\log S_o = -3.590 \pm 0.004$ (95% confidence limit) and $K_s = 0.220 \pm 0.0041$ (95% confidence limit).

The corresponding mass percent and mole fraction, x_1 at salinity = 35 g(2)/kg sln calculated by the compilers are 2.36×10^{-3} g(1)/100 g sln and 3.48×10^{-6} assuming a solution density of 1.025 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solutions were prepared by equilibrating excess (1) in salt water in sealed ampols for 24 hrs. After filtration the absorbance was measured with a UV spectrophotometer at three wavelengths.

SOURCE AND PURITY OF MATERIALS:

(1) recrystallized four times and sublimed or zone refined, 99.99+% pure,

(2) analytical reagent grade,

(3) distilled from potassium permanganate and redistilled from all glass still.

ESTIMATED ERROR:

temp. ± 0.03°C

soly. see above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthalene; $C_{10}H_8$; [91-20-3] (2) natural seawater	Gordon, J.E.; Thorne, R.L. *Geochim. Cosmochim. Acta*, 1967, *31*, 2433-43.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 10-32 g/kg sln	W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

Salinity[b] g/kg sln	Chlorosity (‰)	Treatment[a]	log S Observed	$10^4 S^b$ g-mol(1)/ dm^3	10^3 mass ratio[b] g(1)/100 g sln	10^6 mole fraction[b] x_1
31.8	17.96	MF	-3.715	1.93	2.47	3.47
			-3.717	1.92	2.46	3.45
31.8	17.96	GFF	-3.713	1.94	2.48	3.49
			-3.712	1.94	2.49	3.49
31.9	18.00	CENT	-3.704	1.98	2.53	3.56
			-3.708	1.96	2.51	3.53
31.5	17.81	MF	-3.721	1.90	2.44	3.42
			-3.722	1.91	2.45	3.41
31.8	17.95	GFF	-3.719	1.90	2.43	3.44
			-3.722	1.91	2.45	3.41
31.7	17.72	MF	-3.715	1.93	2.47	3.45
			-3.716	1.92	2.465	3.46
31.5	17.80	GFF	-3.719	1.91	2.45	3.41
			-3.720	1.905	2.44	3.43
9.8	5.45	MF	-3.630	2.344	3.005	4.22
			-3.630	2.344	3.005	4.22

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Detail given in reference (1). Saturated solutions were prepared by equilibrating excess naphthalene and salt solution in an ampoule with shaking for 24 hours. The filtered saturated solution was analyzed by a UV Spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

Naphthalene: 99.99 + % from James Hinton, Valparaiso, Florida

Salts: Analytical reagent grade from Mallinckrodt

Natural Seawater: collected at West Falmouth, Buzzards Bay, Quicks Hole and Mashapaquit Creek, Massachusetts

ESTIMATED ERROR:

Solubility ± 3% (Authors)

Temperature ± 0.03°C (Authors)

REFERENCES:

1. Gordon, J.E.; Thorne, R.L. *J. Phys. Chem.* 1967, *71*, 4390.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

(2) natural seawater

ORIGINAL MEASUREMENTS:

Gordon, J.E.; Thorne, R.L.

Geochim. Cosmochim. Acta 1967, *31*, 2433-43.

Experimental Values: (continued)

Salinity[b] g/kg sln	Chlorosity (°/₀₀)	Treatment[a]	log S Observed	$10^4 S$[b] g-mol(1)/ dm^3	10^3 mass ratio[b] g(1)/100 g sln	10^6 mole fraction[b] X 1
9.8	5.45	GFF	-3.629	2.35	3.01	4.23
			-3.632	2.33	2.99	4.20

[a] MF, membrane (0.45μ) filtered;
GFF, glass fiber filtered;
CENT, centrifuged

Temperature = 24.91°C

[b] Values calculated by compiler.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$ [91-20-3]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40* 555-61.

VARIABLES:

One temperature: 25.0°C

Salinity: 35 g/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of naphthalene in seawater is reported to be 22.0 mg/kg sln. The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 2.20 x 10^{-3} g(1)/100 g sln and 3.18 x 10^{-6}.

Graphical results for other salinities are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium flask: 1 L Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ hr at 215 rpm on a New Brunswick gyrotary shaker; a 24 hr stationary equilibrium period followed. Hydrocarbons were extracted with doubly-distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard.

Analysis: gas chromatography

SOURCE AND PURITY OF MATERIALS:

(1) analytical grade salts for artificial seawater solution, reagent grade.

water: doubly distilled

ESTIMATED ERROR:

temperature: ± 0.5°C

soly: ± 0.293 (95% confidence interval).

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]
(2) Sodium chloride; NaCl; [7647-14-5]
(3) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.6-31.8°C
Salinity: 30 g(2)/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of naphthalene in 0.5 g-mol(2)/dm^3

t/°C	10^4 mol(1)/L sln
8.6	0.84
11.1	0.92
14.0	1.09
17.1	1.23
20.0	1.37
23.0	1.58
25.0	1.73
31.8	2.22

The corresponding mass percent and mole fraction x_1, at 25.0°C calculated by the compilers are 2.17×10^{-3} g(1)/100 g sln and 3.13×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of naphthalene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of naphthalene to an air-tight 1x1 cm quarts fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 315 nm. The Spectrofluorimeter employed a ratio-photon counting mode where naphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of naphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

Naphthalene: purity > 99 mole %
Sodium chloride: reagent grade
Ethanol: reagent grade
Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.

ESTIMATED ERROR:

Solubility ± 3.3% (author)
Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:

(1) Naphthalene; $C_{10}H_8$; [91-20-3]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman D.H.

Anal. Chem. <u>1978</u>, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of naphthalene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_sC_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, K_s = 0.213 with S_o = 31.69.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 2.29×10^{-3} g(1)/100 g sln and 3.29×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C
K_s ± 0.001
S_o ± 0.23

REFERENCES:

COMPONENTS:

(1) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-244.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,2,4,5-tetramethylbenzene in water at 25°C and at system pressure was reported to be 3.48 mg(1)/kg(2). The corresponding mass per cent and mole fraction, x_1, calculated by the compiler are 3.48×10^{-4} g(1)/100 g sln and 4.67×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out using a Hewlett-Packard Model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±1°C

Solubility: ±0.28 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,2,4,5-tetramethylbenzene in water at 25°C was reported to be 3.48 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 3.48×10^{-4} g(1)/100 g sln and 4.67×10^{-7}.

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system (see previous page). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 μL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.1 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) *p*-Cymene; $C_{10}H_{14}$; [99-87-5]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the *p*-cymene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the *p*-Cymene (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	volumetric
Englin *et al.* (ref 2)	283-303	(2) in (1)	analytical
Banerjee *et al.* (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF *p*-CYMENE (1) IN WATER (2)

Only two solubility values are available, both at 298K, but they are in poor agreement. The value of 0.04g(1)/100g sln reported by Booth and Everson (ref 1) is more than an order of magnitude greater than the value of 2.34×10^{-3} g(1)/100g sln reported by Banerjee *et al.* (ref 3). On the basis of comparison with similar systems the value of Banerjee *et al.* is more realistic.

2. SOLUBILITY OF WATER (2) IN *p*-CYMENE (1)

Only the values of Englin *et al.* (ref 2) are available and so no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al.* are generally reliable at $T < 300$K but somewhat high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

REFERENCES

1. Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pyranishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
3. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.

COMPONENTS: (1) p-Cymene; $C_{10}H_{14}$; [99-87-5] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of p-cymene in water at 25°C was reported to be 0.04 g(1)/100 mL(2). Assuming a solution density of 1.00, the mass percentage and mole fraction, x_1, calculated by the compilers are 0.04 g(1)/100 g sln and 5 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Stoppered Babcock tubes with neck graduated from 0 to 1.6 mL in steps of 0.02 mL were used. A known volume of (2) (generally 50 mL) was added to the tube in a constant-temperature water bath and weighed quantities of (1) were added to this solution. The mixture was then shaken for 5 minutes, returned to the bath for a minimum of 10 minutes and then centrifuged for 5 minutes. After this treatment, the volume of residue was determined directly.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP or highest commercial grade; used as received.

(2) distilled.

ESTIMATED ERROR:

soly. ± 0.1 mL(1)/100 mL(2).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) p-Cymene; $C_{10}H_{14}$; [99-87-6] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES:	**PREPARED BY:**
Temperature: 10-30°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in p-Cymene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0223	1.66
20	0.0305	2.27
30	0.0415	3.08

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) *p*-Cymene; $C_{10}H_{14}$; [99-87-5]

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

ORIGINAL MEASUREMENTS:

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

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

VARIABLES:

One temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *p*-cymene in water was reported to be 1.74 x 10^{-4} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1, solubilities, calculated by the compiler, are 2.34 x 10^{-3} g(1)/100 g sln and 3.13 x 10^{-6} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of *p*-cymene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by GC after exhaustive extraction with hexane. A HP 5370A (FID) instrument and a 3% OV-1 on Chromosorb W column was used. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; purity not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.2°C

Solubility: ±3.1% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:

(1) Diethylbenzene; $C_{10}H_{14}$; [25340-17-4]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 0-50°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Diethylbenzene
(isomer not specified)

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
0	0.0159	1.57
10	0.0226	2.23
20	0.0319	3.15
30	0.0431	4.25
40	0.0574	5.65
50	0.0756	7.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia.
A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland

February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the *tert*-butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Solubility Studies of the *tert*-Butylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Englin *et al.* (ref 2)	283-303	(2) in (1)	analytical
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of the above publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF *TERT*-BUTYLBENZENE (1) IN WATER (2)

The two reported solubilities of *tert*-butylbenzene in water are in reasonable agreement (Table 2).

TABLE 2: Tentative Value of the Solubility of *tert*-Butylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value (± σ_n)^a	
	10^3g(1)/100g sln	10^3g(1)/100g sln	10^6 x_1
298	3.4 (ref 1), 2.95 (ref 3)	3.2 ± 0.2	4.3

a Obtained by averaging, σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN *TERT*-BUTYLBENZENE (1)

As only the solubility values of Englin *et al.* (ref 2) are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al.* are generally reliable at T < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) *tert*-Butylbenzene; $C_{10}H_{14}$; [98-06-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences Warszawa, Poland February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Andrews, L.J.; Keefer, T.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.

2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

3. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) tert-Butylbenzene; $C_{10}H_{14}$; [98-06-6] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of tert-butylbenzene in water at 25°C was reported to be 0.0034 g(1)/100 g sln.

The corresponding mole fraction, x_1 calculated by the compilers is 4.6 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 167.8-168.0°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) tert-Butylbenzene; $C_{10}H_{14}$; [98-06-6]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in tert-Butylbenzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0205	2.03
20	0.0292	2.88
30	0.0389	3.83

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) tert-Butylbenzene; $C_{10}H_{14}$; [98-06-5]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of tert-butylbenzene in water at 25°C was reported to be 29.5 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00295 g(1)/100 g sln and 3.95×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.3 (the standard deviation of the mean for six replicates).

REFERENCES:

COMPONENTS:

(1) tert-Butylbenzene; $C_{10}H_{14}$; [98-06-6]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of tert-butylbenzene in artificial seawater is reported to be 21.2 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 2.12 x 10^{-3} g(1)/100 g sln and 2.92 x 10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.3 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:	EVALUATOR:
(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8] (2) Water; H_2O; [7732-18-5]	A. Maczynski Institute of Physical Chemistry of the Polish Academy of Sciences Warszawa, Poland. November 1981

CRITICAL EVALUATION:

The solubility of sec-butylbenzene (1) in water (2) has been reported in three works listed below:

Authors	Method	T/K	g(1)/100 g sln
Andrews and Keefer (ref 1)	spectrophotometric	298.15	0.0309
Sutton and Calder (ref 3)	GLC	298.15	0.00176
Krzyzanowska and Szeliga (ref 4)	GLC	298.15	0.00101

The data of Andrews and Keefer seem to be high. The mean value of the remaining data is tentative.

The solubility of water (2) in sec-butylbenzene (1) has been reported in one work listed below:

Authors	Method	T/K
Englin *et al.* (ref 2)	gasometric	273.15-323.15

Since these data are from one source only, they are regarded as tentative.

SOLUBILITY OF sec-BUTYLBENZENE (1) IN WATER (2)
TENTATIVE VALUE

T/K	g(1)/100 g sln	x_1
298	0.0014	1.9×10^{-6}

SOLUBILITY OF WATER (2) IN sec-BUTYLBENZENE (1)
TENTATIVE VALUES

T/K	g(2)/100 g sln	x_2
283	0.020	0.0020
293	0.029	0.0029
303	0.039	0.0038

REFERENCES

1. Andrews, L.J.; Keefer, R.M. *J. Amer. Chem. Soc.* 1950, *72*, 5034-7.
2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
3. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
4. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* 1978, *12*, 413-7.

COMPONENTS:

(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1950, *72*, 5034-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of sec-butylbenzene in water at 25°C was reported to be 0.0309 g(1)/100 g sln.

The corresponding mole fraction, x_1 calculated by the compilers is 4.15×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 175.0-175.8°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. i Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in sec-butylbenzene

t/°C	g(2)/100 g sln	x_2 (compiler)
10	0.0226	0.00223
20	0.0317	0.00313
30	0.0426	0.00420

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of sec-butylbenzene in water at 25°C was reported to be 17.6 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00176 g(1)/100 g sln and 2.36×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.2 (the standard deviation of the mean for six replicates).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, 1978, *12*, 413-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of sec-butylbenzene in water at 25°C was reported to be 10.1 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00101 g(1)/100 g sln and 1.36 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

soly. 0.3 mg(1)/kg(2) (standard deviation from 7-9 determinations).

REFERENCES:

COMPONENTS:

(1) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2.

VARIABLES:

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of sec-butylbenzene in artificial seawater is reported to be 11.9 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 1.19×10^{-3} g(1)/100 g sln and 1.64×10^{-6} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.2 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:	EVALUATOR:
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the butylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Solubility Studies of the Butylbenzene (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Andrews and Keefer (ref 1)	298	(1) in (2)	spectrophotometric
Klevens (ref 2)	298	(1) in (2)	spectrophotometric
Jones and Monk (ref 3)	298-308	(2) in (1)	radiotracer
Englin *et al.* (ref 4)	283-303	(2) in (1)	analytical
Massaldi and King (ref 5)	298	(1) in (2)	GLC
Sutton and Calder (ref 6)	298	(1) in (2)	GLC

The original data in all of the above publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF BUTYLBENZENE (1) IN WATER (2)

The available data on the solubility of butylbenzene in water, all at 298K, are summarized in Table 2. The agreement is very poor with the reported values differing by almost two orders of magnitude which makes critical evaluation difficult. Fortunately, an independent estimation of the solubility can be made by extrapolation of the solubilities of the lower *n*-alkylbenzenes as a function of side chain length. This extrapolation predicts a value of 1.7 x 10^{-3} g(1)/100g sln. This value is quite close to the experimental values of Massaldi and King (ref 5) and Sutton and Calder (ref 6), the average of which is therefore suggested as the Tentative solubility of butylbenzene in water. The values of Andrews and Keefer (ref 1) and Klevens (ref 2) are correspondingly rejected.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Solubility of Butylbenzene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values ($\pm\ \sigma_n$)[a]	
	10^3g(1)/100g sln	10^3g(1)/100g sln	$10^6\ x_1$
298	0.126[b] (ref 1), 4.9[b] (ref 2) 1.77 (ref 5), 1.18 (ref 6)	1.5 ± 0.3[c]	2.0

a Obtained by averaging but see text; σ_n has no statistical significance.
b Rejected data, see text.
c Tentative value, see text.

2. SOLUBILITY OF WATER (2) IN BUTYLBENZENE (1)

Although two publications report solubility data of water in butylbenzene, that of Jones and Monk (ref 3) is reported in v/v fractions and is thus excluded from consideration. The remaining data of Englin *et al.* (ref 4) cannot therefore be evaluated. However it may be noted that the values of Englin *et al.* are usually reliable at T < 300K but somewhat too high at greater temperatures. The interested user is referred to the relevant data sheet for the experimental values.

REFERENCES

1. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
3. Jones, J.R.; Monk, C.B. *J. Chem. Soc.* 1963, 2633-5.
4. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
5. Massaldi, H.A.; King, C.J. *J. Chem. Eng. Data* 1973, *18*, 393-7.
6. Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1950, *72*, 5034-7.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of butylbenzene in water at 25°C was reported to be 0.000126 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 1.69×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; fractionally distilled; b.p. range 182.0-183.0°C.

(2) not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES: Temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of butylbenzene in water at 25°C was reported to be 0.05 g(1) L^{-1} sln and 0.00037 mol(1) L^{-1} sln. Assuming that 1.00 kg sln = 1.00 L sln the mass percentage and mole fraction x_1 calculated by the compilers are 0.005 g(1)/100 g sln and 6.7 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.	**SOURCE AND PURITY OF MATERIALS:** (1) not specified. (2) not specified. **ESTIMATED ERROR:** not specified. **REFERENCES:**

COMPONENTS:

(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]

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

ORIGINAL MEASUREMENTS:

Jones, J.R.; Monk, C.B.

J. Chem. Soc. 1963, 2633-35.

VARIABLES:

Temperature: 25-35°C

PREPARED BY:

A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of water in butylbenzene

t/°C	10^4 mL(2)/mL(1)
25	3.5
30	4.1
35	4.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a thermostatted glass-stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mc/mL), decanted, a 5-mL aliquot reshaken for 4 hrs. with 5 mL H_2O in a 10-mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quenching effects (due to solvent) on the scintillator.

SOURCE AND PURITY OF MATERIALS:

(1) laboratory grade dried over $CaCl_2$ and fractionally distilled.

(2) not specified.

ESTIMATED ERROR:

soly. ± 5% to ± 1% (average deviation)

REFERENCES:

1. Vogel *Practical Organic Chemistry* Longmans, Green and Co., London, 1956.

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES: Temperature: 10-30°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Butylbenzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0234	1.74
20	0.0331	2.46
30	0.0448	3.33

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	Massaldi, H.A.; King, C.J. *J. Chem. Eng. Data* 1973, *18*, 393-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of butylbenzene in water at 25°C was reported to be 1.32×10^{-4} mol(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00177 g(1)/100 g sln and 2.4×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A technique based on head-space analysis by gas-liquid chromatography was developed to determine solubilities of sparingly soluble organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is versatile enough to allow determinations provided that the pure vapor pressure of the substances is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson Coleman and Bell Co., highest purity; used as received.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.05°C

REFERENCES:

COMPONENTS: (1) Butylbenzene; $C_{10}H_{14}$; [104-51-8] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Sutton, C.; Calder, J.A. *J. Chem. Eng. Data* 1975, *20*, 320-2.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of butylbenzene in water at 25°C was reported to be 11.8 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00118 g(1)/100 g sln and 1.58×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The concentration of (1) in (2) was determined by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. 0.1 mg(1)/kg(2)
(the standard deviation of the mean for six replicates)

REFERENCES:

COMPONENTS:

(1) Butylbenzene; $C_{10}H_{14}$; [104-51-8]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, *20*, 320-2

VARIABLES:

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of butylbenzene in artificial seawater is reported to be 7.09 mg(1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 7.09×10^{-4} g(1)/kg sln and 9.76×10^{-7} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.

(2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 0.07 (std. dev.)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) (+)-(R)-P-Mentha-1,8-diene (d-Limonene); $C_{10}H_{16}$; [5989-27-5]

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

ORIGINAL MEASUREMENTS:

Massaldi, H.A.; King, C.J.

J. Chem. Eng. Data 1973, *18*, 393-7.

VARIABLES:

Temperature: 0-25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of d-limonene in water

t/°C	mg(1) L sln	10^4 mol(1) L sln	10^3g(1)/100g sln (compiler)	$10^6 x_1$
0	9.7	0.708	0.97	1.3
5	10.4	0.767	1.04	1.4
25	13.8	1.013	1.38	1.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A technique based on head-space analysis by gas-liquid chromatography was developed to determine solubilities of sparingly soluble organics. Saturated solutions need not be prepared in advance whereby phase separation problems are avoided, nor have liquid samples to be analyzed. This method is versatile enough to allow determinations provided that the pure vapor pressure of the substances is known. The gas chromatograph was a Varian Aerograph Model 1740 with a flame ionization detector.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson Coleman and Bell Co., highest purity; kept under N_2 atmosphere at -2°C in a dark container; used as received.

(2) not specified.

ESTIMATED ERROR:

temp. ± 0.05°C

REFERENCES:

COMPONENTS:

(1) Bicyclo[4.4.0]decane (decahydronaphthalene; decalin); $C_{10}H_{18}$; [91-17-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the decalin (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Decalin (1) - Water (2) System

Reference	T/K	Solubility	Method
Booth and Everson (ref 1)	298	(1) in (2)	volumetric
Englin *et al.* (ref 2)	293-313	(2) in (1)	analytical
Price (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DECALIN (1) IN WATER (2)

The solubility of decalin in water has been reported only at 298K (Table 1). However, the datum of Booth and Everson (ref 1) in v/v fraction, is only an order of magnitude result and must thus be excluded. Since this leaves only the single datum of 8.89×10^{-5}g(1)/100g sln ($x_1 = 1.16 \times 10^{-7}$) of Price (ref 3) no Critical Evaluation is possible. Nevertheless, it may be noted that the solubility values reported by Price are usually reliable although for the higher hydrocarbons his results are often about 20% (relative) lower than Recommended values.

2. SOLUBILITY OF WATER (2) IN DECALIN (1)

As only the data of Englin *et al.* (ref 2) over the range 293-313K are available no Critical Evaluation is possible. However, it may be noted that the data of Englin *et al.* are generally reliable when $T < 300$K but are somewhat high at higher temperatures. The interested user is referred to the relevant data sheet for the experimental values.

REFERENCES

1. Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.

2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.

3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

COMPONENTS:

(1) Bicyclo[4.4.0]decane (Decahydronaphthalene); $C_{10}H_{18}$; [91-17-8]

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

ORIGINAL MEASUREMENTS:

Booth, H.S.; Everson, H.

Ind. Eng. Chem. 1948, *4*, 1491-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of bicyclo[4.4.0]decane in water at 25°C was reported to be <0.02 mL(1)/100 mL(2).

A similar result was reported for (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A known volume of water, typically 50 mL, was placed in a stoppered Babcock tube having a neck graduated from 0 to 1.6 mL in steps of 0.03 mL. An excess of solute was added and the mixture allowed to come to equilibrium in a constant temperature bath then centrifuged. The amount of solute dissolved was determined by subtracting the undissolved solute, measured directly in the tube, from the total added.

SOURCE AND PURITY OF MATERIALS:

(1) "Highest grade commercial sample available"; no other details given.

(2) Distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Bicyclo[4.4.0]decane (decahydronaphthalene; decalin) $C_{10}H_{18}$; [91-17-8]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-40°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in Bicyclo[4.4.0]decane

t/°C	g(2)/100 g sln	$10^4\ x_2$ (compiler)
20	0.0063	4.84
30	0.0105	8.06
40	0.0164	12.58

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Bicyclo[4.4.0]decane (decahydronaphthalene; decalin); $C_{10}H_{18}$; [91-17-8]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of bicyclo[4.4.0]decane in water at 25°C and at system pressure was reported to be 0.889 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 8.89×10^{-5} g(1)/100 g sln and 1.16×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.031 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) Pentylcyclopentane; $C_{10}H_{20}$; [3741-00-2]

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

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, *60*, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentylcyclopentane in water at 25°C and at system pressure was reported to be 0.115 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler was 1.15×10^{-5} g(1)/100 g sln and 1.5×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GLC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%.

(2) Distilled.

ESTIMATED ERROR:

Temp. ±1°C

Soly. ±0.011 mg(1)/kg(2)

REFERENCES:

COMPONENTS:

(1) 1-Decene; $C_{10}H_{20}$; [872-05-9]
(2) Water; H_2O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Natarajan, G.S.; Venkatachalam, K.A.
J. Chem. Eng. Data. 1972, *17*, 328-9.

VARIABLES:

Temperature: 15-25°C

PREPARED BY:

M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of 1-decene in 0.001 mol/L HNO_3 sln.

t/°C	10^5 mol/L sln[a] g(1)/100 g sln	10^3 g(1)/100 g sln[b] (compiler)	10^6 x_1 (compiler)
15	8.2	1.1	1.5
20	6.1	0.85	1.1
25	4.1	0.57	0.73

[a] Uncertainties stated to be "standard deviations from mean".
[b] Assuming a solution density of 1.00 g mL^{-1} at all temperatures.

Compilers' note:
Although the data have not been measured in pure water the low concentration of the added acid is unlikely to cause the olefin solubility to differ markedly from that in pure water. Further solubility data are given in the paper for 0.05 and 0.1 mol/L HCℓ.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostatted glass burette. After settling (judged) visually), 5 mL of the aqueous layer was withdrawn and the olefin content determined by titration with bromine using standard procedures.

SOURCE AND PURITY OF MATERIALS:

(1) BDH: 99%

(2) Not specified.

ESTIMATED ERROR:

Temp. ±0.05 K

Soly. see Table above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,7-Dimethyloctane; $C_{10}H_{22}$; [1072-16-8] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
VARIABLES:	**PREPARED BY:**
Temperature: 10-30°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in 2,7-Dimethyloctane

t/°C	g(2)/100 g sln	$10^4\ x_2$ (compiler)
10	0.0048	3.79
20	0.0087	6.87
30	0.0152	12.00

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

EVALUATOR:

M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION:

Quantitative solubility data for the decane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Decane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Baker (ref 1,2)	298	(1) in (2)	radiotracer
Schatzberg (ref 3)	298,313	(2) in (1)	Karl Fischer
Franks (ref 4)	298	(1) in (2)	GLC
McAuliffe (ref 5)	298	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 7)	298	(1) in (2)	GLC
Mackay *et al.* (ref 8)	-[a]	(1) in (2)	GLC
Namiot *et al.* (ref 9)	423-583[b]	(2) in (1)	vap.-liq. equil.
Skripka (ref 10)	398-563[b]	(2) in (1)	vap.-liq. equil.
Becke and Quitzsch (ref 11)	293	mutual	refractometric

a Not specified but probably 298.15K.
b Pressure also varied 1-78 MPa.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition, Roof (ref 6) has reported a three phase critical point of unknown composition at 569K and 9.6 MPa. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DECANE (1) IN WATER (2)

The available data on the solubility of decane in water are summarized in Table 2 with the following exceptions. The value of Baker in ref 2 is quoted in v/v terms and is therefore excluded from consideration (however it is equivalent to that reported by the same author in ref 1). The values of Mackay *et al.* (ref 8) are rejected not only because the measurement temperature was unspecified but also because the authors themselves regard their solubility values below 2 x 10^{-3}g(1)/100g sln as potentially unreliable because of emulsion or colloid formation. The value of McAuliffe (ref 5) is also rejected because it is very much higher than all other reported values.

Agreement among the remaining values (Table 2) is not good enough to enable any of the "Best" values to be Recommended.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Decane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values ($\pm \sigma_n$)^a	
	10^6g(1)/100g sln	10^6g(1)/100g sln	$10^9\ x_1$
293	1.98 (ref 11)	2	2.5
298	1.6 (ref 1), 1.98 (ref 4), 0.87 (ref 7)	1.5 ± 0.5	1.9

a Obtained by averaging; σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN DECANE (1)

At atmospheric pressure the only available values of the solubility of water in decane are those of Schatzberg (ref 3) and Becke and Quitzsch (ref 11). These data are listed in Table 3 but are in poor agreement and can only be regarded as order of magnitude values.

At higher temperatures and pressure only the data of Skripka and co-workers (ref 9,10) are available and so no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for the experimental values.

TABLE 3: Approximate Solubility Values of Water (2) in Decane (1)

T/K	Reported values^a	
	10^2g(2)/100g sln	$10^3\ x_2$
293	2.92 (ref 11)	2.3
298	0.72 (ref 3)	0.6
313	1.36 (ref 3)	1.1

a Values considered as order-of-magnitude data only, see text.

REFERENCES

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints* 1958, *3*, No.4, C61-8.
2. Baker, E.G. *Science* 1959, *129*, 871-4.
3. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

CRITICAL EVALUATION: (continued)

REFERENCES (continued)

4. Franks, F. *Nature* 1966, *210*, 87-8.
5. McAuliffe, C. *Science* 1969, *163*, 478-9.
6. Roof, J.G. *J. Chem. Eng. Data* 1970, *15*, 301-3.
7. Krasnoshchekova, P.Y.; Gubergrits, M.Y. *Neftekhimiya* 1973, *13*, 885-7.
8. Mackay, D.; Shiu, M.W.; Wolkoff, A.W. Water Quality Parameters, ASTM STP 573, 1975, 251-8.
9. Namiot, A.Y.; Skripka, V.G.; Lotler, Y.G. *Zh. Fiz. Khim.* 1976, *50*, 2718; Deposited doc. 1976; VINITI 1213-76.
10. Skripka, V.G. *Tr. Vses. Neftegazov. Nauch-Issled. Inst.* 1976, *61*, 139-51.
11. Becke, A.; Quitzsch, G. *Chem. Techn.* 1977, *29*, 49-51.

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

ORIGINAL MEASUREMENTS:

Baker, E.G.

Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, *3*, N°4, C61-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of decane-1-C^{14} in water at 25°C was reported to be 16 x 10^{-9} g(1)/g(2).

The corresponding mole fraction, calculated by the compiler, is $x_1 = 2.0 \times 10^{-9}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Carbon-14 labeled (1) was used as radioactive tracer.
The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

SOURCE AND PURITY OF MATERIALS:

(1) Nuclear Instrument and Chemical Corporation; used as received.

(2) distilled.

ESTIMATED ERROR:

soly. 20% (standard deviation from 17 replicate runs).

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia* 1956, *1*, N°2, 5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	Baker, E.G. *Science* 1959, *129*, 871-4.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	F. Kapuku

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be 22×10^{-7} mL(1)/100 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
not specified.	not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS: (1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
VARIABLES: Temperature: 25-40°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in decane

t/°C	mg(2)/kg sln	x_2
25	72[a]	5.7×10^{-4}
40	136[b]	10.7×10^{-4}

[a,b] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; research grade; 99.43 mole%; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	Franks, F. *Nature (London)* 1966, *210*, 87-8.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	F. Kapuku

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be in mole fraction $x_1 = 2.5 \times 10^{-9}$.
The corresponding mass percent calculated by the compiler is 1.98×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 ml of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; purum grade; purity > 97% (chromatographic analysis).

(2) not specified.

ESTIMATED ERROR:

soly. ± 12%

REFERENCES:

COMPONENTS: (1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** McAuliffe, C. *Science* 1969, *163*, 478-9.
VARIABLES: One temperature: 25°C	**PREPARED BY:** F. Kapuku

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be 0.052 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5.2×10^{-6} g(1)/100 g sln and 6.58×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: (1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	**SOURCE AND PURITY OF MATERIALS:** (1) not specified. (2) distilled. **ESTIMATED ERROR:** soly. ± 0.0043 mg(1)/kg(2) **REFERENCES:**

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

ORIGINAL MEASUREMENTS:

Krasnoshchekova, P.Ya.;
Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of decane in water at 25°C was reported to be $x_1 = 1.1 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 8.7×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; purity not specified.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.J.; Wolkoff, A.W.

"Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u>, *573*, 251-8.

VARIABLES:

not specified

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported two different values for the solubility of decane in water: 0.182 and 1.22 mg(1)dm^{-3} sln. With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percents calculated by the compiler, are 0.0000182 and 0.000122 g(1)/100 g sln and the corresponding mole fractions, x_1, are 2.3 x 10^{-8} and 1.6 x 10^{-7} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it is possible to calculate the amount of (1) in the original sample.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not estimated.

REFERENCES:

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

ORIGINAL MEASUREMENTS:

Namiot, A.Yu.; Skripka, V.G.;
Lotter, Yu.G.

Zh. Fiz. Khim. 1976, *50*, 2718
Deposited doc. 1976,
VINITI 1213-76.

VARIABLES:

Temperature: 150-310°C
Pressure: 0.52-8.44 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in decane

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
150	5.3	0.52	0.028	0.36
200	18.2	1.79	0.095	1.31
225	30	2.9	0.162	2.39
250	47.2	4.63	0.248	4.01
275	73.2	7.18	0.403	7.87
285	83.9	8.23	0.504	11.4
290	95.4	9.36	0.606	16.3
310	20	2.0	0.029	0.38
310	30	2.9	0.069	0.93
310	40	3.0	0.114	1.60
310	50	4.9	0.171	2.54
310	60	5.9	0.239	3.82
310	70	6.9	0.313	5.45
310	80	7.8	0.407	7.99
310	86.1	8.44	0.520	12.06

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The static method for vapor-liquid equilibrium described in ref 1 was used.
No more details were reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, Yu.A. *Zh. Fiz. Khim.* 1976, *46*, 2170.

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

ORIGINAL MEASUREMENTS:

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

VARIABLES:

Temperature: 225-290°C
Pressure: 2.9-78.5 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in decane

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
225	30	2.9	0.162	2.39
	50	4.9	0.157	2.30
	70	6.9	0.153	2.28
	100	9.8	0.148	2.15
	150	14.7	0.138	1.99
	200	19.6	0.132	1.89
	250	24.5	0.124	1.76
	300	29.4	0.118	1.67
	400	39.2	0.108	1.51
	500	49.0	0.102	1.42
	600	58.8	0.098	1.36
	700	68.6	0.095	1.31
	800	78.5	0.094	1.30
250	50	4.9	0.255	4.15
	70	6.9	0.248	4.01
	100	9.8	0.240	3.84
	150	14.7	0.226	3.56
	200	19.6	0.213	3.31
	250	24.5	0.200	3.07
	300	29.4	0.190	2.88
	400	39.2	0.168	2.49
	500	49.0	0.158	2.32
	600	58.8	0.153	2.24
	700	68.6	0.151	2.20
	800	78.5	0.148	2.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, chemical reagent grade; purity not specified; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Gazov. Prom.* 1971, *4*, 6.

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
275	70	6.9	0.404	7.90
	100	9.8	0.385	7.34
	150	14.7	0.353	6.46
	200	19.6	0.320	5.62
	250	24.5	0.293	4.98
	300	29.4	0.272	4.52
	400	39.2	0.246	3.97
	500	49.0	0.231	3.66
	600	58.8	0.217	3.39
	700	68.6	0.204	3.14
	800	78.5	0.197	3.08
290	100	9.8	0.580	14.88
	150	14.7	0.417	8.30
	200	19.6	0.392	7.54
	250	24.5	0.371	6.95
	300	29.4	0.350	6.38
	400	39.2	0.318	5.57
	500	49.0	0.291	4.94
	600	58.8	0.270	4.47
	700	68.6	0.253	4.11
	800	78.5	0.243	3.90

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

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

ORIGINAL MEASUREMENTS:

Becke, A.; Quitzsch, G.

Chem. Techn. 1977, *29*, 49-51.

VARIABLES:

One temperature: 20°C

PREPARED BY:

P.L. Huyskens and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of decane in water at 20°C was reported to be in mole fraction, $x_1 = 2.5 \times 10^{-9}$. The corresponding mass percent, calculated by the compiler, is 1.976×10^{-6} g(1)/100 g sln. The solubility of water in decane at 20°C was reported to be in mole fraction, $x_2 = 2.3 \times 10^{-3}$. The corresponding mass percent, calculated by the compiler, is 0.0292 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The refractometric and the Karl-Fischer dead-stop titration methods were used.
No more details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

not specified.

ESTIMATED ERROR:

soly. 0.05-1% for (1) in (2)
0.3-1.3% for (2) in (1)

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of decane (1) in seawater (2) has been reported in two works:

Authors	Method	T/K	Salinity g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	298	6	8.7×10^{-6}
Freegarde *et al.* (ref 2)	GLC	?	?	1.5×10^{-5}

Because temperature and salinity are not specified, the data of Freegarde *et al.* are rejected. The value of Krasnoshchekova and Gubergrits is considered doubtful since it is greater than the tentative value for the solubility of decane in pure water at 298 K.

SOLUBILITY OF DECANE (1) IN SEAWATER (2)
DOUBTFUL VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	6	8.7×10^{-6}

REFERENCES

1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.

2. Freegarde, M.; Hatchard, C.G.; Parker, C.A. *Lab. Pract.* 1971, *20*, 35-40.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Decane; $C_{10}H_{22}$; [124-18-5] (2) Seawater (composition not specified)	Freegarde, M.; Hatchard, C.G.; Parker, C.A. *Lab Pract.* 1971, *20*, 35-40.
VARIABLES:	**PREPARED BY:**
Temperature, pressure, salinity not given.	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of decane was reported to be 0.15 mg/L. The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 1.5×10^{-5} g(1)/100 g sln and 1.9×10^{-8}, assuming a solution density of 1.02 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	**SOURCE AND PURITY OF MATERIALS:**
None given except that analysis was done using gas chromatography.	not given.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:

(1) Decane; $C_{10}H_{22}$; [124-18-5]

(2) Seawater

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.;
Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-8.

VARIABLES:

One temperature: 25°C
Salinity: 6 g/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of decane in seawater was reported to be 8.7×10^{-6} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 1.1 \times 10^{-8}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

SOURCE AND PURITY OF MATERIALS:

(1) "chemically pure"

(2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the 1-methylnaphthalene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the 1-Methylnaphthalene (1) - Water (2) System

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	273-323	(2) in (1)	analytical
Eganhouse and Calder (ref 2)	298	(1) in (2)	GLC
Mackay and Shiu (ref 3)	298	(1) in (2)	spectrofluorometric
Schwarz and Wasik (ref 4)	283-298	(1) in (2)	spectrofluorometric
Schwarz (ref 5)	282-305	(1) in (2)	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For further convenience further discussion of this system is divided into two parts.

1. SOLUBILITY OF 1-METHYLNAPHTHALENE (1) IN WATER (2)

All the available data on the solubility of 1-methylnaphthalene in water are summarized in Table 1 with the exception of those of Schwarz and Wasik which have been rejected as they are much more scattered than those in the paper by Schwarz (ref 5). There are insufficient data to warrant plotting.

At 298K, the only temperature where comparison is possible, the data are in excellent agreement and the average value can be Recommended. At other temperatures only the data of Schwarz (ref 5) are available and must thus be considered as Tentative only.

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of 1-Methylnaphthalene (1) in Water (2)

T/K	Solubility values			
	Reported values^a		"Best" values (± σ_n)^b	
	10^3g(1)/100g sln		10^3g(1)/100g sln	$10^6 x_1$
283	2.05*	(ref 5)	2.1	2.7
293	2.56*	(ref 5)	2.6	3.3

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) 1-Methylnaphthalene, $C_{11}H_{10}$; [90-12-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility values		
	Reported values[a]	"Best" values ($\pm\ \sigma_n$)[b]	
	10^3g(1)/100g sln	10^3g(1)/100g sln	$10^6 x_1$
298	2.58 (ref 2), 2.85 (ref 3) 2.95* (ref 5)	2.8 ± 0.2 (R)	3.5 (R)
303	3.35* (ref 5)	3.4	4.3

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a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original data.

b Obtained by averaging where relevant; σ_n has no statistical significance.

2. SOLUBILITY OF WATER (2) IN 1-METHYLNAPHTHALENE (1)

As only the data of Englin *et al.* (ref 1) are available on the solubility of water in 1-methylnaphthalene no Critical Evaluation is possible. However, it may be noted that the solubility values of Englin *et al.* are generally reliable for $T < 300$K but are larger than Recommended values at higher temperatures. The interested user is referred to the relevant Data Sheet for experimental values.

REFERENCES

1. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
2. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
3. Mackay, D.; Shui, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
4. Schwarz, F.P.; Wasik, S.P. *J. Chem. Eng. Data* 1977, *22*, 270-3.
5. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

COMPONENTS:

(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 0-50°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in 1-Methylnaphthalene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
0	0.0202	1.59
10	0.0282	2.22
20	0.0377	2.97
30	0.0485	3.82
40	0.0619	4.87
50	0.0760	5.97

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 1-methylnaphthalene in water at 25°C was reported to be 25.8 mg(1)/kg(2) and 1.81×10^{-4} mol(1) L (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.58×10^{-3} g(1)/100 g sln and 3.27×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 1.2 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1-methylnaphthalene in water at 25°C was reported to be 28.5 mg(1) dm^{-3} sln and $x_1 = 3.55 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00285 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.3 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
VARIABLES:	**PREPARED BY:**
Temperature: 8.6-31.7°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 1-methylnaphthalene in water

t/°C	10^4 mol(1) L^{-1}	10^3 g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
8.6	1.40 ± 0.03	1.99	2.52
14.0	1.59 ± 0.03	2.26	2.86
17.1	1.61 ± 0.03	2.29	2.90
20.0	1.78 ± 0.02	2.53	3.21
23.0	1.94 ± 0.02	2.76	3.49
25.0	2.11 ± 0.07	3.00	3.80
26.1	2.14 ± 0.02	3.04	3.85
29.2	2.34 ± 0.05	3.33	4.21
31.7	2.55 ± 0.04	3.27	4.59

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99.9 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:

(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.; Wasik, S.P.

J. Chem. Eng. Data 1977, *22*, 270-3.

VARIABLES:

Temperature: 10-25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 1-methylnaphthalene in water

t/°C	10^4 mol(1) L^{-1}	10^3 g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
10	1.6	2.3	2.9
14	2.0	2.8	3.6
20	2.0	2.8	3.6
25	2.1	3.0	3.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

SOURCE AND PURITY OF MATERIALS:

(1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%.

(2) distilled from $KMnO_4$ and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 2 x 10^{-5} mol(1) dm^{-3}

REFERENCES:

COMPONENTS:

(1) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]

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

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.1-28.5°C

Salinity: 30 g(2)/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of 1-methylnaphthalene in 0.5 mol(2)/L

t/°C	10^4 mol(1)/L sln
8.1	1.23
11.1	1.35
15.5	1.49
17.4	1.53
18.2	1.54
20.7	1.54
23.3	1.63
25.0	1.69
28.5	1.81

The corresponding mass percent and mole fraction, x_1, at 25.0°C calculated by the compilers are 2.34×10^{-3} g(1)/100 g sln and 3.06×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of 1-methylnaphthalene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of 1-methylnaphthalene to an air-tight 1 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostatted water bath and then its fluorescent intensity was measured at 350 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where 1-methylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of 1-methylnaphthalene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

1-Methylnaphthalene: purity > 99%,

Sodium chloride: reagent grade,

Ethanol: reagent grade,

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.

ESTIMATED ERROR:

Solubility ± 3.6% (author)
Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for 2-methylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data appear to have been reported on the solubility of water in 2-methylnaphthalene.

TABLE 1: Quantitative Solubility Studies of 2-Methylnaphthalene (1) in Water (2)

Reference	*T*/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in excellent agreement and thus the mean value can be Recommended.

TABLE 2: Recommended (*R*) Value of the Solubility of 2-Methylnaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value (± σ_n)^a	
	10^3g(1)/100g sln	10^3g(1)/100g sln	10^6 x_1
298	2.46 (ref 1), 2.54 (ref 2)	2.50 ± 0.04 (*R*)	3.2 (*R*)

a Calculated by averaging; σ_n has no statistical significance.

REFERENCES

1. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 2-methylnaphthalene in water at 25°C was reported to be 24.6 mg(1)/kg(2) and 1.72×10^{-4} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.46×10^{-3} g(1)/100 g sln and 3.12×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.5 mg (1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylnaphthalene in water at 25°C was reported to be 25.4 mg(1) dm^{-3} sln and x_1 = 3.22 x 10^{-6}.

The corresponding mass percent calculated by the compiler is 0.00254 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.2 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 2-Ethyl-1,3,5-trimethylbenzene; $C_{11}H_{16}$; [3982-67-0]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-40°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in 2-Ethyl-1,3,5-trimethylbenzene

$t/°C$	g(2)/100 g sln	$10^3\ x_2$ (compiler)
20	0.0259	2.13
30	0.0350	2.87
40	0.0461	3.78

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) tert-Pentylbenzene; $C_{11}H_{16}$; [2049-95-8] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.*, 1950, *72*, 5034-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of tert-pentylbenzene in water at 25°C was reported to be 0.00105 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 1.27×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. white label; fractionally distilled; b.p. range 188.0-189.0°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) 3-Methylbicyclo[4.4.0]decane (2-methyldecalin); $C_{11}H_{20}$; [2958-76-1]

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

ORIGINAL MEASUREMENTS:

Baker, E.G.

Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, *3*, N°4, C61-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methyl-C^{14}decalin in water at 25°C was reported to be 40.6 x 10^{-9} g(1)/g(2).

The corresponding mass percentage and mole fraction, x_1, calculated by the compiler are 4.06 x 10^{-6} g(1)/100 g sln and 4.82 x 10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Carbon-14 labeled (1) was used as tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

SOURCE AND PURITY OF MATERIALS:

(1) Nuclear Instrument and Chemical Corporation; used as received.

(2) distilled.

ESTIMATED ERROR:

soly. 20% (standard deviation from 17 replicate runs).

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia* 1956, *1*, N°2, 5.

COMPONENTS:

(1) Hexylcyclopentane; $C_{11}H_{22}$; [4457-00-5]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in Hexylcyclopentane

t/°C	g(2)/100 g sln	10^4 x_2 (compiler)
10	0.0052	4.45
20	0.0084	7.19
30	0.0141	12.07

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. December 1985.

CRITICAL EVALUATION:

Quantitative solubility data for the system undecane (1) - water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Undecane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
McAuliffe (ref 2)	298	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF UNDECANE (1) IN WATER (2)

The available data for the solubility of undecane in water are listed in Table 2.

TABLE 2: Solubility Values of Undecane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value ($\pm \sigma_n$)	
	10^7g(1)/100g sln	10^7g(1)/100g sln	10^{10} x_1
298	4.4 (ref 2), 3.6 (ref 3)	4.0 ± 0.4^a	4.6^a

a Order of magnitude only, see text; obtained by averaging.

Although the agreement between the two studies (ref 2,3) is very good considering the very low solubility involved, both values are very much lower than expected from an extrapolation of *n*-alkane solubilities. This may be due (ref 2) to micelle formation. The available data must therefore be considered as Doubtful. The extrapolated value of 1.4×10^{-6} g(1)/100g sln ($x_1 = 1.6 \times 10^{-10}$) may be more realistic.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium. December 1985.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN UNDECANE (1)

As only one publication (ref 1) reports solubility data for water in undecane no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg (ref 1) are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
2. McAuliffe, C. *Science* 1969, *163*, 478-9.
3. Krasnoshchekova, P.Y.; Gubergrits, M.Y. *Neftekhimiya* 1973, *13*, 885-7.

COMPONENTS: (1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
VARIABLES: Temperature: 25-40°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in undecane

t/°C	mg(2)/kg sln	x_2
25	69[a]	6.0×10^{-4}
40	130[b]	11.3×10^{-4}

[a,b] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; research grade; 99.33 mole%; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *Science* 1969, *163*, 478-9.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	F. Kapuku

EXPERIMENTAL VALUES:

The solubility of undecane in water at 25°C was reported to be 0.0044 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.4×10^{-7} g(1)/100 g sln and 5.07×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	**SOURCE AND PURITY OF MATERIALS:**
(1) was equilibrated with (2). Glass vials were filled with the saturated aqueous phase. Half of water was then displaced and replaced by air. The vials were then sealed and shaken for 2 minutes. The gas phase was then displaced through the sample loop of a gas chromatograph for analyzing for hydrocarbon content.	(1) not specified. (2) distilled. **ESTIMATED ERROR:** soly. ± 0.0018 mg(1)/kg(2) **REFERENCES:**

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Undecane; $C_{11}H_{24}$; [1120-21-4] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of undecane in water at 25°C was reported to be $x_1 = 4.10 \times 10^{-10}$.

The corresponding mass percent calculated by the compiler is 3.6×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 10 mL (1) and 300 mL (2) was placed in a double-walled bottom-stoppered vessel and vigorously stirred magnetically for 10-12 hr. The phases were allowed to separate; a first sample of the water phase was rejected and next 200 mL of this phase was taken, 20-mL aliquots were introduced into 40-mL hermetic bottles and (1) was allowed to equilibrate with the air, and the (1)-saturated air was analyzed by glc.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; purity not specified.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Undecane; $C_{11}H_{24}$; [1120-21-4]

(2) Seawater

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.;
Gubergrits, M.Ya.

Neftekhimiya 1973, *13*, 885-8.

VARIABLES:

One temperature: 25°C
Salinity: 6 g/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of undecane in seawater was reported to be 1.0×10^{-6} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 1.2 \times 10^{-9}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

SOURCE AND PURITY OF MATERIALS:

(1) "chemically pure"

(2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION:

Quantitative solubility data for acenaphthene (1) in water (2) have been reported in the publications listed in Table 1. No data appear to have been reported for the solubility of water in acenaphthene.

TABLE 1: Quantitative Studies of the Solubility of Acenaphthene (1) in Water (2)

Reference	T/K	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Eganhouse and Calder (ref 2)	298	GLC
Mackay and Shiu (ref 3)	298	spectrofluorometric
Banerjee *et al.* (ref 4)	298	radiotracer
Rossi and Thomas (ref 5)	298	GLC, spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

At 298K, the only temperature where comparison is possible (Table 1), the data of Wauchope and Getzen (ref 1), Eganhouse and Calder (ref 2) and Mackay and Shiu (ref 3) are in excellent agreement. The values of Banerjee *et al.* (ref 4) and Rossi and Thomas (ref 5) are respectively very much higher and lower and are therefore rejected.

At other temperatures only the data of Wauchope and Getzen (ref 1) are available and must therefore be regarded as Tentative values.

The solubility values of acenaphthene in water are summarized in Table 2 and plotted in Figure 1.

TABLE 2: Recommended (R) and Tentative Solubility Values for Acenaphthene (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values ($\pm\ \sigma_n$)[b]	
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10^7\ x_1$
273	1.45 (ref 1)	1.5	1.8
293	3.2* (ref 1)	3.2	3.7
298	3.88 (ref 1), 3.47 (ref 2), 3.93 (ref 3)	3.8 ± 0.2 (R)	4.4(R)

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility values			
	Reported values[a]	"Best" values ($\pm \sigma_n$)[b]		
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10^7\ x_1$	
303	4.80 (ref 1)	4.8	5.6	
313	7.4* (ref 1)	7.4	8.6	
323	9.2 (ref 1)	9.2	10	
333	19.4* (ref 1)	19	22	
343	32.0* (ref 1)	32	37	
348	42.5 (ref 1)	43	50	

[a] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original data.

[b] Obtained by averaging where appropriate; σ_n has no significance.

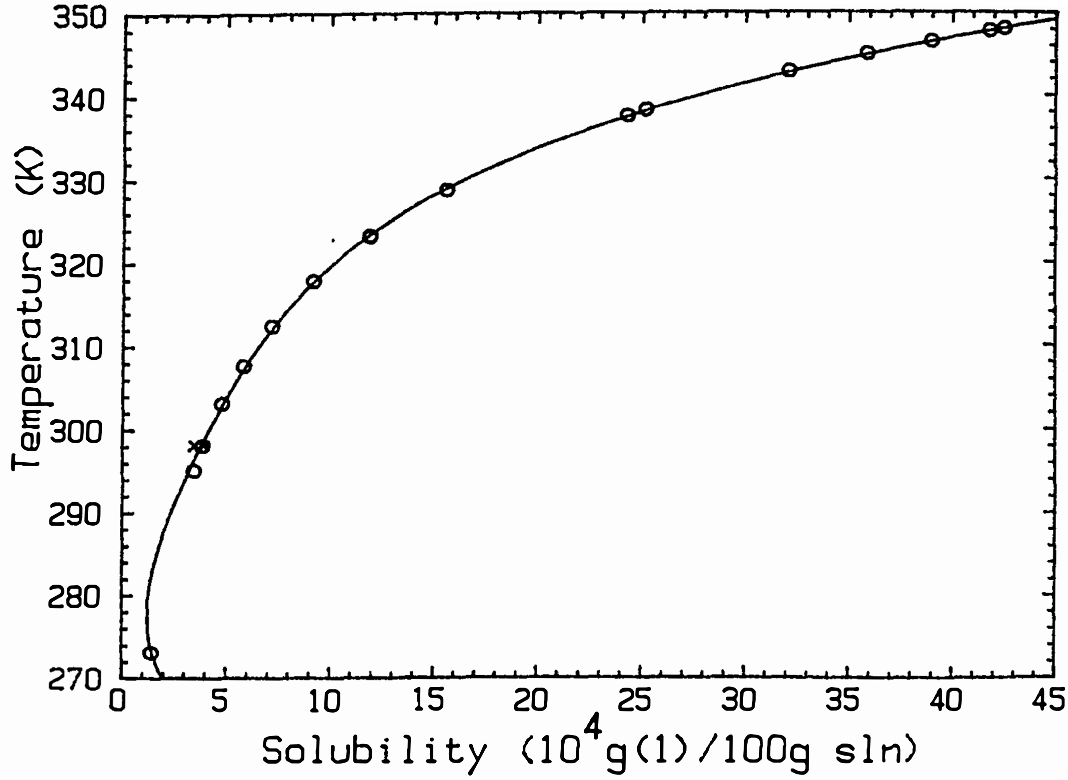

FIGURE 1. Solubility of acenaphthene in water: ref 1 (o); ref 2,3 (x).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. March 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Wauchope, R.D.; Getzen, F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
2. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
4. Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.
5. Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-75°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of acenaphthene in water

t/°C	mg(1)/kg(2) experiment	mg(1)/kg(2) smoothed with (std dev)	10^4 g(1)/100 g sln (compiler)	10^7x_1 (compiler)
0.0		1.45(0.04)	1.45	1.69
22.0	3.57	3.46	3.46	4.04
25.0		3.88(0.07)	3.88	4.53
30.0	4.76, 4.60, 4.72	4.80	4.80	5.61
34.5	6.00, 5.68, 5.73	5.83	5.83	6.81
39.3	6.8, 7.1, 7.0	7.2	7.2	8.4
44.7	9.4, 9.4, 9.3	9.2	9.2	10.7
50.0		11.9(0.1)	11.9	13.9
50.1	12.5, 12.4, 12.4	11.9	11.9	13.9
55.6	15.8, 16.3, 15.9	15.6	15.6	18.2
64.5	25.9, 27.8	24.3	24.3	28.4
65.2	23.7, 23.4, 22.8	25.2	25.2	29.4
69.8	30.1, 34.3, 33.6	32.1	32.1	37.5
71.9	35.2	35.9	35.9	41.9
73.4	39.1, 40.1	39.0	39.0	45.6
74.7	40.8, 39.3	41.8	41.8	48.8
75.0		42.5(0.7)	42.5	49.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction.
Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C

soly. see experimental values above

REFERENCES:

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of acenaphthene in water at 25°C was reported to be 3.47 mg(1)/kg(2) and 2.2×10^{-5} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.47×10^{-4} g(1)/100 g sln and 4.05×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.06 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of acenaphthene in water at 25°C was reported to be 3.93 mg(1) dm^{-3} sln and $x_1 = 4.59 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 3.93×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.014 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS: (1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.
VARIABLES: One temperature: 25°C	**PREPARED BY:** G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acenaphthene in water was reported to be 4.78 x 10^{-5} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction (x_1) solubilities, calculated by the compiler, are 7.37 x 10^{-4} g(1)/100 g sln and 8.60 x 10^{-7} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of acenaphthene was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by liquid scintillation counting. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) ^{14}C-labelled: New England Nuclear, purity not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.2°C

Solubility: ±4.1% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

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

ORIGINAL MEASUREMENTS:

Rossi, S.S.; Thomas, W.H.

Environ. Sci. Technol. 1981, *15*, 715-6.

VARIABLES:

One temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of acenaphthene in distilled water at 25°C was reported to be 2.42 μg/g, corresponding to a mole fraction, x_1, of 1.6×10^{-8}. The corresponding mass per cent calculated by the compiler is 2.42×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Flasks containing 500 mL of water and (1) were placed in a constant temperature (±0.1°C) gyrotary shaker (200 rpm) for at least 24 h. Following a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug into a separatory funnel. Acenaphthene was isolated from solution by triplicate extraction with 10 mL of hexane, which recovered over 99% of hydrocarbon as determined in experiments with spiked solutions. Acenaphthene levels in concentrated extracts were determined on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100 glass column (30 m x 0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally determined by ultraviolet spectrophotometry. Agreement was typically within 2%. Further details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; 99.9% purity; recryst. twice from dist. MeOH.

(2) Doubly distilled in all-glass apparatus; free of trace organics.

ESTIMATED ERROR:

Temperature: ±0.1°C

Solubility: ±0.02 μg/g (std. dev. for 6 determinations)

REFERENCES:

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Seawater; natural

ORIGINAL MEASUREMENTS:

Rossi, S.S.; Thomas, W.H.

Environ. Sci. Technol. 1981, *15*, 715-6.

VARIABLES:

Temperature: 15-25°C

Salinity: 35 g/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

Solubility of Acenaphthene in Seawater

t/°C	μg(1)/g(2)	10^5 Mass %[a] g(1)/100 g sln	10^8 x_1[a]
15	0.214	2.14	2.56
20	0.55	5.5	6.6
25	1.84	18.4	22.0

[a] Calculated by compilers

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solution was prepared by equilibrating seawater with an excess of hydrocarbon for 24 hrs in a constant temperature gyrotary shaker followed by 12 hr stationary period. A 100 mL-aliquot was extracted three times with n-hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the hydrocarbon concentration.

SOURCE AND PURITY OF MATERIALS:

Acenaphthene:	from Aldrich Chemical Co. of 99% purity and doubly distilled from distilled methanol,
n-Hexane:	doubly distilled in glass,
Seawater:	collected off Scripps Pier and was filtered twice through 0.22 μm membrane and twice extracted with n-hexane then its salinity adjusted to 35 ‰.

ESTIMATED ERROR:

Temp. ±0.1°K

Soly. ±2%

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for biphenyl (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in biphenyl.

TABLE 1: Quantitative Solubility Studies of Biphenyl (1) in Water (2)

Reference	*T*/K	Method
Andrews and Keefer (ref 1)	298	spectrophotometric
Bohon and Claussen (ref 2)	274-316	spectrophotometric
Wauchope and Getzen (ref 4)	273-348	spectrophotometric
Ben-Naim *et al.* (ref 5)	283-323[a]	spectrophotometric
Eganhouse and Calder (ref 6)	298	GLC
Mackay and Shiu (ref 7)	298	spectrofluorometric
Banerjee *et al.* (ref 8)	298	HPLC

a Solubility on D_2O also reported.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In addition Bröllos *et al.* (ref 3) have studied the liquid-liquid phase equilibria in the biphenyl-water system at high temperatures and pressures, and Ben-Naim *et al.* (ref 5) have reported free energies of solution of biphenyl in D_2O.

All the available data on the solubility of biphenyl in water are summarized in Table 2 with the exception of the 298K data of Andrews and Keefer (ref 1) and Banerjee *et al.* (ref 8) which are substantially ($>3\sigma_n$) lower than all other values at this temperature (ref 2,4,6,7) and are therefore rejected. The data of Ben-Naim *et al.* (ref 5) expressed as free energies of solution have also been excluded.

In general the remaining data are in excellent agreement enabling values to be Recommended over a wide range of temperature. The data from Table 2 are also plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Values of the Solubility of Biphenyl (1) in Water (2)

T/K	Solubility values Reported values[a] $10^4 g(1)/100g$ sln	"Best" values $(\pm \sigma_n)$[b] $10^4 g(1)/100g$ sln	 $10^7\ x_1$
273	2.80* (ref 2), 2.64 (ref 4)	2.72 ± 0.08 (*R*)	3.2 (*R*)
283	4.06 (ref 2)	4.1	4.8
293	6.25* (ref 2)	6.3	7.4
298	7.48 (ref 2), 7.08 (ref 4), 7.45 (ref 6), 7.0 (ref 7)	7.2 ± 0.2 (*R*)	8.4 (*R*)
303	9.4* (ref 2), 8.8* (ref 4)	9.1 ± 0.3 (*R*)	10.6 (*R*)
313	15.1* (ref 2), 13.7* (ref 4)	14.4 ± 0.7 (*R*)	16.8 (*R*)
323	22.0 (ref 4)	22	26
333	37.1* (ref 4)	37	43

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

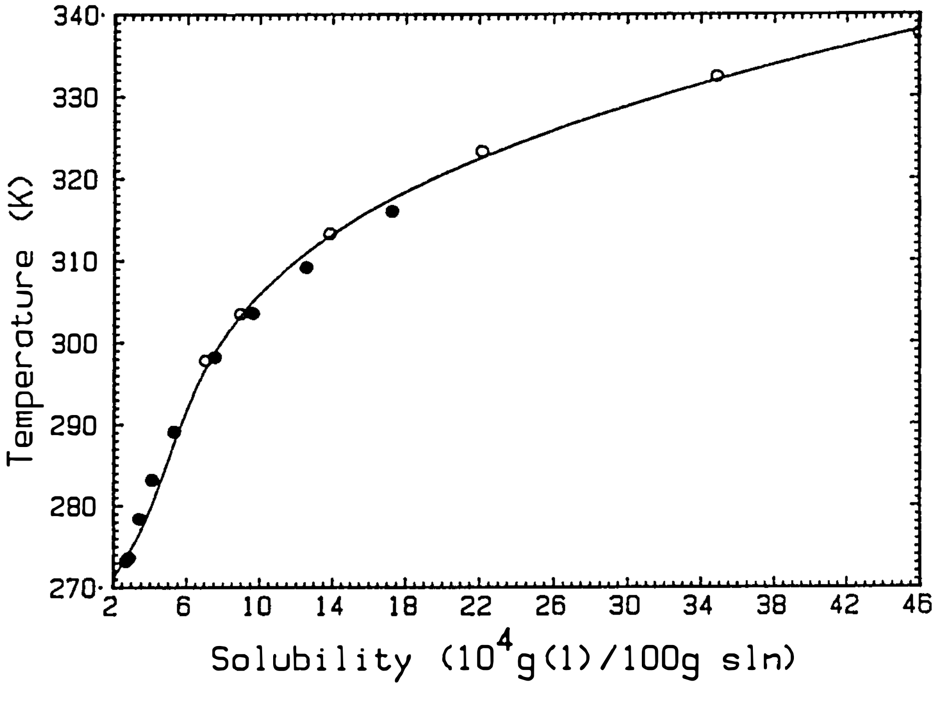

FIGURE 1. Solubility of biphenyl in water, selected data: ref 2(●); ref 4 (o). Solid curve fitted through "Best" values (Table 2).

(continued next page)

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

June 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-7.

2. Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* 1951, *73*, 1571-8.

3. Bröllos, K.; Peter, K.; Schneider, G.M. *Ber. Bunsenges. Phys. Chem.* 1970, *74*, 682-6.

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

5. Ben-Naim, A.; Wilf, J.; Yaacobi, M. *J. Phys. Chem.* 1973, *77*, 95-102.

6. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.

7. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

8. Banerjee, S.; Yalkowski, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-77.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of biphenyl in water at 25°C was reported to be 0.000594 g(1)/100 g sln.

The corresponding mole fraction x_1, calculated by the compilers is 6.9×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co. best grade; m.p. 70.0-70.5°C; used as received.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Bohon, R.L.; Claussen, W.F.

J. Am. Chem. Soc. 1951, *73*, 1571-8.

VARIABLES:

Temperature: 0.4-42.8°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of biphenyl in water

t/°C	$10^4 g(1)/100g\ sln$[a] (compiler)	$10^7 x_1$ (compiler)
0.4	2.83	3.30
2.4	2.97	3.47
5.2	3.38	3.94
7.6	3.64	4.25
10.0	4.06	4.74
12.6	4.58	5.35
14.9	5.11	5.96
15.9	5.27	6.15
25.0	7.48[b]	8.73[b]
25.6	7.78	9.08
30.1	9.64	11.2
30.4	9.58	11.2
33.3	11.0	12.8
34.9	11.9	13.9
36.0	12.5	14.6
42.8	17.2	20.1

[a] Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

[b] Given in the paper as 7.48×10^{-3} g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

(1) Matheson Co., purified by recrystallization from absolute methanol.

(2) Air-free conductivity water, no further details given.

ESTIMATED ERROR:

Temp. ± 0.02°C

Soly. ± 0.5% relative

REFERENCES:

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-64.5°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of biphenyl in water

t/°C	mg(1)/kg(2)		10^4 g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)
	experiment	smoothed with (std dev)		
0.0		2.64(0.07)	2.64	3.08
24.6	7.13, 7.29, 7.35	6.96	6.96	8.13
25.0		7.08(0.09)	7.08	8.27
29.9	8.77, 8.64, 8.95	8.73	8.73	10.2
30.3	8.55, 8.54, 8.48	8.88	8.88	10.4
38.4	13.2, 13.3, 13.5	12.7	12.7	14.8
40.1	13.1, 13.4, 13.4	13.8	13.8	16.1
47.5	18.8, 19.0, 18.7	19.5	19.5	22.8
50.0		22.0(0.2)	22.0	25.7
50.1	20.6, 21.6, 21.8	22.1	22.1	25.8
50.2	20.7, 21.8	22.2	22.2	29.9
54.7	28.3, 28.8, 28.8	27.7	27.7	32.4
59.2	36.4, 36.3, 36.0	34.8	34.8	40.7
60.5	40.4	37.2	37.2	43.5
64.5	43.7, 44.7, 46.6	45.9	45.9	53.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction. Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C

soly. see experimental values above

REFERENCES:

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Ben-Naim, A.; Wilf, J.; Yaacobi, M.

J. Phys. Chem. <u>1973</u>, *77*, 95-102.

VARIABLES:

Temperature: 10-50°C (282-323 K)

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of biphenyl in water is expressed in terms of the standard free energy of solution, $\Delta\mu_s^o$, determined as:

$$\Delta\mu_s^o = \lim_{\rho_s \to 0} [-RT\ \ell n(\rho_s^\ell/\rho_s^g)_{eq}]$$

where $(\rho_s^\ell/\rho_s^g)_{eq}$ is the Ostwald absorption coefficient and ρ_s^ℓ and ρ_s^g are respectively the molar concentrations of the solute s in the liquid and the gas phase at equilibrium.

For the temperature range studied, $\Delta\mu_s$ was fitted to a second degree polynomial of the form:

$$\Delta\mu_s^o = -14740.4 + 52.057\ t - 0.04126\ t^2$$

where t is in °C ($10 < t < 50$°C) and $\Delta\mu_s^o$ is in cal/mol (1 cal = 4.184 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined spectroscopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for *ca.* 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors were measured directly at λ_{max} with a Model 450 Perkin-Elmer spectrophotometer with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three compartment cell, details of which are given in the paper.

SOURCE AND PURITY OF MATERIALS:

1. Fluka; puriss, 99.94%, used as received.
2. Distilled water, further distilled from alk. $KMnO_4$ and acid $K_2Cr_2O_7$; κ, 0.8×10^{-6}S cm^{-1}.

ESTIMATED ERROR:

Temperature: ±0.05°C

Solubility: std. dev. in $\Delta\mu_s^o$, 22.794 cal/mol.

REFERENCES:

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of biphenyl in water at 25°C was reported to be 3.47 mg(1)/kg(2) [illegible]d 4.8×10^{-5} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 7.45×10^{-4} g(1)/100 g sln and 8.70×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.06 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of biphenyl in water at 25°C was reported to be 7.0 mg(1) dm^{-3} sln and $x_1 = 8.15 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 7.0×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.06 mg(1) dm^{-3} sln (maximum deviation from several determinations.)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* 1980, *14*, 1227-9.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of biphenyl in water was reported to be 3.91×10^{-5} mol/L sln. Assuming a solution density of 1.00 kg/L the corresponding mass per cent and mole fraction, x_1, solubilities, calculated by the compiler, are 6.03×10^{-4} g(1)/100 g sln and 7.05×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of biphenyl was added to a tube containing distilled water, and the tube was sealed and allowed to equilibrate at 25 ± 0.2°C with constant or intermittent shaking. Equilibration was generally complete within 1 week. The mixture was then centrifuged at 10,000 rpm for 60 min in a head preequilibrated to 25 ± 0.3°C, following which aliquots of the solution were removed for analysis by high-performance liquid chromatography using a Waters M6000A instrument fitted with a μC_{18} Bondapak column. The mobile phase was a mixture of methanol/water or acenotrile/water. The entire procedure was carried out at least twice for each compound, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; purity not specified.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.2°C

Solubility: ±6.0% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Deuterium oxide (Heavy water); D_2O; [7789-20-0]

ORIGINAL MEASUREMENTS:

Ben-Naim, A.; Wilf, J.; Yaacobi, M.

J. Phys. Chem. 1973, *77*, 95-102.

VARIABLES:

Temperature: 10-50°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of biphenyl in heavy water is expressed in terms of the standard free energy of solution, $\Delta\mu_s^o$, determined as:

$$\Delta\mu_s^o = \lim_{\rho_s \to 0} [-RT \ \ln(\rho_s^\ell/\rho_s^g)_{eq}]$$

where $(\rho_s^\ell/\rho_s^g)_{eq}$ is the Ostwald absorption coefficient and ρ_s^ℓ and ρ_s^g are respectively the molar concentrations of the solute s in the liquid and the gas phase at equilibrium.

For the temperature range studied, $\Delta\mu_s^o$ was fitted to a second degree polynomial of the form:

$$\Delta\mu_s^o = -12827.6 + 39.059\, t - 0.01945\, t^2$$

where t is in °C ($10 < t < 50$°C) and $\Delta\mu_s^o$ is in cal/mol (1 cal = 4.184 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were determined spectroscopically. Saturated solutions were prepared in two ways: (a) direct mixing of benzene and water for *ca.* 48 h, (b) dissolution of benzene through the vapor phase. Absorbances of the solutions and their vapors were measured directly at λ_{max} with a Model 450 Perkin-Elmer spectrophotometer with a thermostatted cell holder. Establishment of equilibrium was checked by use of a special three compartment cell, details of which are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka, puriss, 99.94%, used as received.

(2) Fluka, 99.75%, used as received.

ESTIMATED ERROR:

Temperature: ±0.05°C

Solubility: std. dev. in $\Delta\mu_s^o$, 270.15 cal/mol.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of biphenyl (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10^4 g(1)/100 g sln
Paul (ref 1)	uv spectral	13-64	6.08 - 3.45
Eganhouse and Calder (ref 2)	GLC	35	4.76

The reported data are all from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the recommended value for the solubility of biphenyl in pure water, the data of Paul and of Eganhouse and Calder are adopted as tentative.

SOLUBILITY OF BIPHENYL (1) IN SEAWATER (2)
TENTATIVE VALUE

T/K	g salts/kg sln	10^4 g(1)/100 g sln
298	35	4.76

REFERENCES

1. Paul, M.A. *J. Amer. Chem. Soc.* 1952, *74*, 5274-7.

2. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Sodium chloride; NaCl; [7732-14-5] (3) Water; H_2O; [7647-18-5]	Paul, M.A. *J. Am. Chem. Soc.* 1952, *74*, 5274-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 13-64 g(3)/kg sln	M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

Solubility of Biphenyl and Aqueous Sodium Chloride

mol(2)/L	g(2)/kg sln*	10^5 mol(1)/L	10^4 Mass %*	10^7 x_1*
0.229	13.25	3.98	6.08	7.16
0.458	26.24	3.61	5.46	6.49
0.687	39.05	3.08	4.62	5.55
0.818	46.28	2.79	4.16	5.02
0.916	51.62	2.78	4.13	5.01
1.145	63.97	2.40	3.54	4.32
1.145	63.97	2.34	3.45	4.21

*Calculated by compilers using density and other physical data for NaCl solutions from ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibration flask: 50-mL glass-stoppered flask. The flask was heated in a hot-water bath until the hydrocarbon was melted, then shaken vigorously while cooling until excess hydrocarbon had recrystallized. The flask was then placed into a water bath thermostatically controlled at 25.00 ± 0.05°C for at least 48 hr, and shaken occasionally during that time. Samples were withdrawn with a 10-ml transfer pipet, diluted appropriately and analyzed using a spectrophotometer in the ultra-violet region of the spectrum.

SOURCE AND PURITY OF MATERIALS:

(1) recrystallized from menthanol

(2) reagent grade, dried at 120°C before weighing

(3) redistilled

Sources not specified.

ESTIMATED ERROR:

temp. ± 0.05°C

soly. ± 2.6 %

REFERENCES:

1. Weast, R.C.; *CRC Handbook of Chemistry and Physics*, 59th Edition; CRC Press 1978, pp D299-D300.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25.0°C

Salinity: 35 g/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of biphenyl in seawater is reported to be 4.76 mg/kg. The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 4.76×10^{-4} g(1)/100 g sln and 5.70×10^{-7}.

Graphical results for other salinities are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium flask: 1-dm^3 Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ hr at 215 rpm on a New Brunswick gyrotary shaker; a 24 hr stationary equilibrium period followed. Hydrocarbons were extracted with doubly-distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard.

Analysis: gas chromatography

SOURCE AND PURITY OF MATERIALS:

(1) analytical grade salts for artificial seawater solution, reagent grade.

water: doubly distilled

ESTIMATED ERROR:

temperature: ± 0.5°C

soly: ± 0.293 (95% confidence interval).

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:

(1) 1,3-Dimethylnaphthalene; $C_{12}H_{12}$; [575-41-7]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,3-dimethylnaphthalene in water at 25°C was reported to be 8.0 mg(1) dm^{-3} sln and $x_1 = 9.2 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 8.0×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.5 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Dimethylnaphthalene; $C_{12}H_{12}$; [571-58-4] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,4-dimethylnaphthalene in water at 25°C was reported to be 11.4 mg(1) dm^{-3} sln and $x_1 = 1.31 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00114 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.1 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,5-Dimethylnaphthalene; $C_{12}H_{12}$; [571-61-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 1,5-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1,5-dimethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of 1,5-Dimethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

TABLE 2: Tentative Value of the Solubility of 1,5-Dimethylnaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value ($\pm\ \sigma_n$)^a	
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10^7\ x_1$
298	2.74 (ref 1), 3.38 (ref 2)	3.1 ± 0.3	3.6

^{a} Obtained by averaging; σ_n has no statistical significance.

REFERENCES

1. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.

2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS: (1) 1,5-Dimethylnaphthalene; $C_{12}H_{12}$; [571-61-9] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
VARIABLES: One temperature: 25°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 1,5-dimethylnaphthalene in water at 25°C was reported to be 2.74 mg(1)/kg(2) and 1.8×10^{-5} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.74×10^{-4} g(1)/100 g sln and 8.70×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.1 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:

(1) 1,5-Dimethylnaphthalene;

$C_{12}H_{12}$; [571-61-9]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,5-dimethylnaphthalene in water at 25°C was reported to be 3.38 mg(1) dm^{-3} sln and $x_1 = 3.77 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 3.38×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.04 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 2,3-Dimethylnaphthalene; $C_{12}H_{12}$; [581-40-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 2,3-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2,3-dimethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of 2,3-Dimethylnaphthalene (1) in Water (2)

Reference	*T*/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

TABLE 2: Tentative Value of the Solubility of 2,3-Dimethylnaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value (± σ_n)^a	
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10^7\ x_1$
298	1.99 (ref 1), 3.0 (ref 2)	2.5 ± 0.5	2.9

a Obtained by averaging; σ_n has no statistical significance.

REFERENCES

1. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.

2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylnaphthalene; $C_{12}H_{12}$; [581-40-8] (2) Water; H_2O; [7732-18-5]	Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 2,3-dimethylnaphthalene in water at 25°C was reported to be 1.99 mg(1)/kg(2) and 1.3 x 10^{-5} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.99 x 10^{-4} g(1)/100 g sln and 2.29 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.02 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:

(1) 2,3-Dimethylnaphthalene; $C_{12}H_{12}$; [581-40-8]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3-dimethylnaphthalene in water at 25°C was reported to be 3.0 mg(1) dm^{-3} sln and $x_1 = 3.47 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 3.0×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.01 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 2,6-dimethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2,6-dimethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of 2,6-Dimethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Eganhouse and Calder (ref 1)	298	GLC
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The two values available (Table 1), obtained by different methods, are in reasonable agreement and their mean can be considered as a Tentative value (Table 2).

TABLE 2: Tentative Value of the Solubility of 2,6-Dimethylnaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value ($\pm \sigma_n$)[a]	
	$10^4 g(1)/100g$ sln	$10^4 g(1)/100g$ sln	$10^7 x_1$
298	1.30 (ref 1), 2.0 (ref 2)	1.7 ± 0.4	2.0

[a] Obtained by averaging; σ_n has no statistical significance.

REFERENCES

1. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 2,6-dimethylnaphthalene in water at 25°C was reported to be 1.30 mg(1)/kg(2) and 8.3×10^{-6} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.30×10^{-4} g(1)/100 g sln and 1.50×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.04 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,6-dimethylnaphthalene in water at 25°C was reported to be 2.0 mg(1) dm^{-3} sln and $x_1 = 2.33 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 2.0×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.02 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 1-ethylnaphthalene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 1-ethylnaphthalene.

TABLE 1: Quantitative Solubility Studies of 1-Ethylnaphthalene (1) in Water (2)

Reference	T/K	Method
Mackay and Shiu (ref 1)	298	spectrofluorometric
Schwarz and Wasik (ref 2)	282-305	spectrophotometric
Schwarz (ref 3)	284-298	spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The data available (Table 1) are summarized in Table 2 and plotted in Figure 1. For the purpose of this Evaluation the values of Schwarz (ref 3) are not considered as independent determinations. Nevertheless, the excellent agreement between the data of Schwarz and Wasik (ref 2,3) and Mackay and Shiu (ref 1) at 298K suggests the values of Schwarz and Wasik at other temperatures can be considered as Tentative.

TABLE 2: Recommended (R) and Tentative Solubility Values of 1-Ethylnaphthalene (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values (± σ_n)[b]	
	10^4g(1)/100g sln	10^4g(1)/100g sln	10^7 x_1
283	8.1 (ref 2), 8.1* (ref 3)	8.1	9.4
293	10.0 (ref 2), 8.5* (ref 3)	8.5	9.8
298	10.7 (ref 1), 10.0 (ref 2), 9.5* (ref 3)	10.1 ± 0.5 (R)	11.6 (R)
303	11.0* (ref 3)	11	13

[a] Values marked with an asterisk (*) were obtained by the Evaluators by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. April 1986.

CRITICAL EVALUATION: (continued)

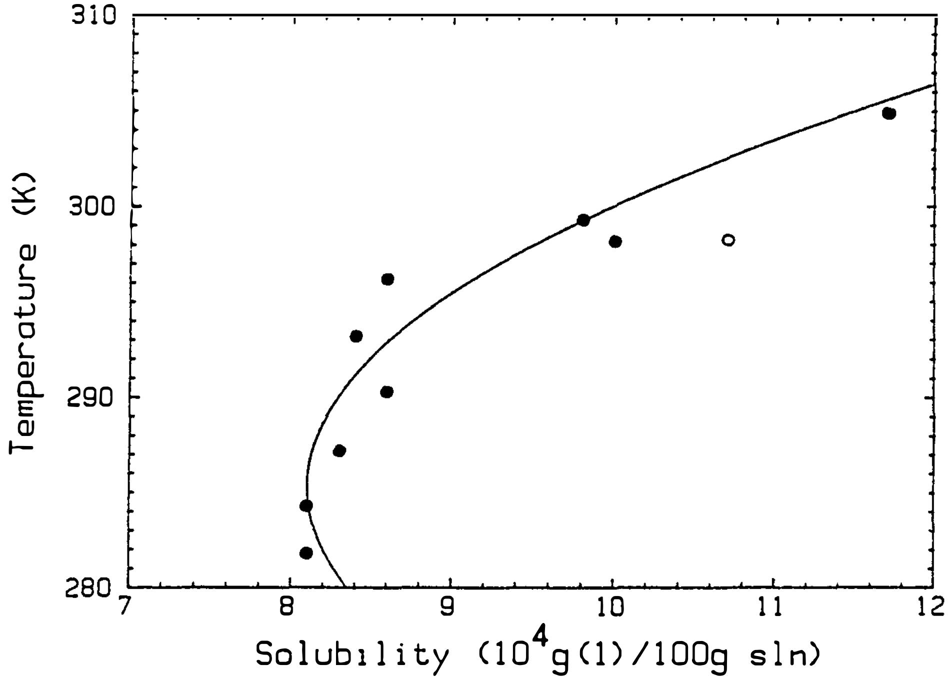

FIGURE 1. Solubility of 1-ethylnaphthalene in water: ref 1(o); ref 2(●). Solid curve is a least squares line of best fit through data of ref 2.

REFERENCES

1. Mackay, C.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
2. Schwarz, F.P.; Wasik, S.P. *J. Chem. Eng. Data* 1977, *22*, 270-3.
3. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

ACKNOWLEDGEMENT

The Evaluators thank Dr Brian Clare for the graphics.

COMPONENTS:

(1) 1-Ethylnaphthalene; $C_{12}H_{12}$;

[1127-76-0]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1-ethylnaphthalene in water at 25°C was reported to be 10.7 mg(1) dm^{-3} sln and $x_1 = 1.24 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.00107 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.3 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.6-31.7°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 1-ethylnaphthalene in water

t/°C	10^5 mol(1) L^{-1}	10^4 g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)
8.6	5.2 ± 0.3	8.1	9.4
11.1	5.2 ± 0.2	8.1	9.4
14.0	5.3 ± 0.1	8.3	9.5
17.1	5.5 ± 0.1	8.6	9.9
20.0	5.4 ± 0.1	8.4	9.7
23.0	5.5 ± 0.1	8.6	9.9
25.0	6.4 ± 0.1	10.0	11.5
26.1	6.3 ± 0.1	9.8	11.3
31.7	7.5 ± 0.2	11.7	13.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99.9 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:

(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.; Wasik, S.P.

J. Chem. Eng. Data 1977, *22*, 270-3.

VARIABLES:

Temperature: 10-25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 1-ethylnaphthalene in water

$t/°C$	10^5 mol(1) L^{-1}	10^4 g(1)/100 g sln (compiler)	10^7x_1 (compiler)
10	5.2 ± 0.2	8.1	9.4
14	5.2 ± 0.1	8.1	9.4
20	6.4 ± 0.1	10.0	11.5
25	6.4 ± 0.1	10.0	11.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined from its absorbance. Since the concentration of (1) in (2) are too low to determine its extinction coefficient accurately, the absorption measurements were performed on measured volumes of the saturated solutions diluted with equal volumes of ethanol.

SOURCE AND PURITY OF MATERIALS:

(1) Chemical Samples Co., Columbus, Ohio; better than 99.9 mole%.

(2) distilled from $KMnO_4$ and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:

(1) 1-Ethylnaphthalene; $C_{12}H_{12}$; [1127-76-0]

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

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.1-28.5°C

Salinity: 30 g(2)/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of 1-ethylnaphthalene in 0.5 mol(2)/L sln

t/°C	10^5 mol(1)/L sln
8.1	3.65
11.1	3.87
17.4	4.23
20.3	4.45
23.3	4.38
25.0	4.67
26.2	4.53
28.5	4.82

The corresponding mass percent and mole fraction x_1, at 25.0°C calculated by the compilers are 7.12×10^{-4} g(1)/100 g sln and 8.44×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of 1-ethylnaphthalene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of 1-ethylnaphthalene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 nm. The Spectrofluorimeter employed a ratio-photon counting mode where 1-ethylnaphthalene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of 1-ethylnaphthalene in ethanol solution therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

1-Ethylnaphthalene: purity >99 mole %

Sodium chloride: reagent grade

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column

Ethanol: reagent grade

ESTIMATED ERROR:

Solubility ± 2.0% (author)

Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:

(1) 2-Ethylnaphthalene; $C_{12}H_{12}$; [939-27-5]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 2-ethylnaphthalene in water at 25°C was reported to be 8.00 mg(1)/kg(2) and 5.1 x 10^{-5} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 8.00 x 10^{-4} g(1)/100 g sln and 9.22 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.1 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:

(1) 2-Allyl-1,3,5-trimethylbenzene; $C_{12}H_{16}$; [4810-05-3]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-40°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in 2-Allyl-1,3,5-trimethylbenzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
20	0.0246	1.15
30	0.0331	1.54
40	0.0438	2.04

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 2-Propyl-1,3,5-trimethylbenzene; $C_{12}H_{18}$; [4810-04-2]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-40°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in 2-Propyl-1,3,5-trimethylbenzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
20	0.0255	2.29
30	0.0343	3.08
40	0.0455	4.09

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 1-Phenylhexane; $C_{12}H_{18}$;
[1077-16-3]

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

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.;
Gubergrits, M.Ya.

Vodnye. Resursy. 1975, *2*, 170-3.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 1-phenylhexane in water at 25°C was reported to be 0.0021 mg(1) cm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00021 g(1)/100 g sln and 2.4×10^{-7}. The assumption that 1.00 L sln = 1.00 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by glc.
A Czech-made Chrom-2 chromatograph was used, equipped with a 5% Apiezon L/Chromosorb G column operated at 90-140°C.

SOURCE AND PURITY OF MATERIALS:

(1) described in ref (1).

(2) distilled.

ESTIMATED ERROR:

temp. ± 1°C

REFERENCES:

1. Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical
and Physical Sciences, Murdoch
University, Perth, W.A., Australia.

April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the system dodecane (1) - water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Dodecane (1) - Water (2) System

Reference	*T*/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF DODECANE (1) IN WATER (2)

The solubility of dodecane in water has been reported in only two publications, both at 298K (Table 1). The agreement between the two studies is very poor with Franks value (ref 2) considerably higher than that reported by Sutton and Calder (ref 3). Support for the lower value comes from extrapolation of the lower *n*-alkane solubilities. However, there is sufficient uncertainty in this extrapolation to preclude rejection of the higher value at this time. The available data are summarized in Table 2.

TABLE 2: Tentative Solubility Values of Dodecane (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value[a]	
	$10^7 g(1)/100g$ sln	$10^7 g(1)/100g$ sln	$10^{10}\ x_1$
298	8.42 (ref 2), 3.7 (ref 3)	3.7	3.9

[a] Datum from ref 3 preferred as Tentative value; see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. April 1986.

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN DODECANE (1)

As only the data of Schatzberg (ref 1) are available no Critical Evaluation is possible. However, it may be noted that the values of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
2. Franks, F. *Nature (London)* 1966, *210*, 87-8.
3. Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.

COMPONENTS: (1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
VARIABLES: Temperature: 25-40°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in dodecane

t/°C	mg(2)/kg sln	x_2
25	65[a]	6.1×10^{-4}
40	127[b]	12.0×10^{-4}

[a] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

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

ORIGINAL MEASUREMENTS:

Franks, F.

Nature (London) **1966**, *210*, 87-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

F. Kapuku

EXPERIMENTAL VALUES:

The solubility of dodecane in water at 25°C was reported to be in mole fraction $x_1 = 8.9 \times 10^{-10}$.
The corresponding mass percent calculated by the compiler is 8.42×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; purum grade; purity > 97% (chromatographic analysis).

(2) not specified.

ESTIMATED ERROR:

soly. ± 12%

REFERENCES:

HWW 2-Z

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

Environ. Sci. Technol. 1974, *8*, 654-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of dodecane in water at 25°C was reported to be 3.7×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1 of 4×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 µm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of dodecane (1) in seawater (2) at 298 K has been reported in three works:

Authors	Method	Salinity g salts/kg sln	10^7 g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	6	5
Sutton and Calder (ref 2)	GLC	35	2.9
Button (ref 3)	isotopic	12	1.74

The reported data are all from different salinities which precludes direct comparison. Since the data are in only fair agreement with each other and with the reported values for the solubility of dodecane in pure water, all three values are adopted as tentative.

SOLUBILITY OF DODECANE (1) IN SEAWATER (2)
TENTATIVE VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	35	2.9×10^{-7}

REFERENCES

1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya*, 1973, *13*, 885-8.

2. Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.

3. Button, D.K. *Geochim. Cosmochim. Acta* 1975, *40*, 435-40.

COMPONENTS: (1) Dodecane; $C_{12}H_{26}$; [112-40-3] (2) Seawater	**ORIGINAL MEASUREMENTS:** Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.
VARIABLES: One temperature: 25°C Salinity: 6 g/kg sln	**PREPARED BY:** M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of dodecane in seawater was reported to be 5×10^{-7} g(1)/100 g sln. and the corresponding mole fraction, $x_1 = 5.0 \times 10^{-10}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution was prepared by vigorously stirring hydrocarbon (1) in seawater (2) for 10-12 hrs. in a flask placed in a temperature controlled bath. A sample of solution was then transferred to a closed flask with head space volume equal to solution volume. Hydrocarbon concentration in the head space was determined by gas chromatography and the corresponding solution concentration calculated.

SOURCE AND PURITY OF MATERIALS:

(1) "chemically pure"

(2) distilled water plus salt mixture.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Seawater

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

Environ. Sci. Technol. 1974, *8*, 654-7.

VARIABLES:

One temperature: 25°C
One salinity: 35 g salts/kg sln

PREPARED BY:

P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of dodecane in seawater was reported to be 2.9×10^{-7} g(1)/100 g sln and $x_1 = 3.1 \times 10^{-10}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES:

COMPONENTS:

(1) Dodecane; $C_{12}H_{26}$; [112-40-3]

(2) Salt mixture (ref 1)

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

ORIGINAL MEASUREMENTS:

Button, D. K.

Geochim. Cosmochim. Acta 1975, *40*, 435-40.

VARIABLES:

One temperature: 25°C
Constant salinity: 12 g(2)/kg sln
Different periods of standing

PREPARED BY:

P. Meyers and D. Shaw

EXPERIMENTAL VALUES:

Dodecene concentration in saline medium after gently stirring for 1 week and then remaining quiescent for the periods shown

Time, Weeks	Dodecane, μg(1)/L(2)
1	2.16 ± 0.03
8	1.80 ± 0.02
16	1.78 ± 0.02

The corresponding mass percent and mole fraction calculated by the compilers for the results at 16 weeks are 1.74×10^{-7} g(1)/100 g sln and 1.89×10^{-10} using the assumption that the solution density is 1.02 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Dodecane solutions were prepared in a chemically defined solution resembling dilute seawater. In addition to the mineral salts and vitamins reported (ref 1), the solution contained 1 mg/L arginine and 10 g/L NaCl. After sterilization (121°C for 30 min), 0·8 μL of ^{14}C-dodecane was sprayed on to the medium surface to form a thin film. Gentle subsurface agitation was induced by a 3 in magnet rotating at 60 rev/min against the inside carboy wall at midlevel. The subsurface dodecane concentration was determined from the radioactivity of samples collected from a port at the bottom of the carboy. The system was stirred for 1 week and then allowed to stand. Equilibrium appeared to have been achieved within 8 weeks.

SOURCE AND PURITY OF MATERIALS:

Amersham Searle Corp. (Arlington Heights, Ill.) supplied the [1-^{14}C] dodecane, 27 μCi/μmol. It was accompanied by a gas chromatogram of the preparation showing a single peak at the appropriate location.

ESTIMATED ERROR:

Experimental error is estimated at ± 1%.

REFERENCES:

1. Button, D. K. *Limnol. Oceanogr.* 1969, *14*, 95-100.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

April 1986.

CRITICAL EVALUATION:

Quantitative solubility data for fluorene (1) in water (2) have been reported in the publications listed in Table 1. No solubility data for water in fluorene have been reported.

TABLE 1: Quantitative Solubility Studies of Fluorene (1) in Water (2)

Reference	T/K	Method
Wauchope and Getzen (ref 1)	273-348	spectrophotometric
Mackay and Shiu (ref 2)	298	spectrofluorometric
May *et al.* (ref 3)	298	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The solubility values are also summarized in Table 2 and plotted in Figure 1.

At 298K, the only temperature where comparison is possible, the available data (ref 1-3) are in good agreement and the average value can be Recommended. At other temperatures only the values of Wauchope and Getzen (ref 1) are available and are therefore regarded as tentative.

TABLE 2: Recommended (R) and Tentative Solubility Values of Fluorene (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values (± σ_n)[b]	
	10^4g(1)/100g sln	10^4g(1)/100g sln	$10^6 x_1$
273	0.66 (ref 1)	0.7	0.8
298	1.90 (ref 1), 1.98 (ref 2), 1.685 (ref 3)	1.9 ± 0.1 (R)	2.1 (R)
303	2.4* (ref 1)	2.4	2.6
313	3.8* (ref 1)	3.8	4.1
323	6.29 (ref 1)	6.3	6.8
333	10.4* (ref 1)	10	11
343	18.5* (ref 1)	19	21

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original values.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Fluorene; $C_{13}H_{10}$; [86-73-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. April 1986.

CRITICAL EVALUATION: (continued)

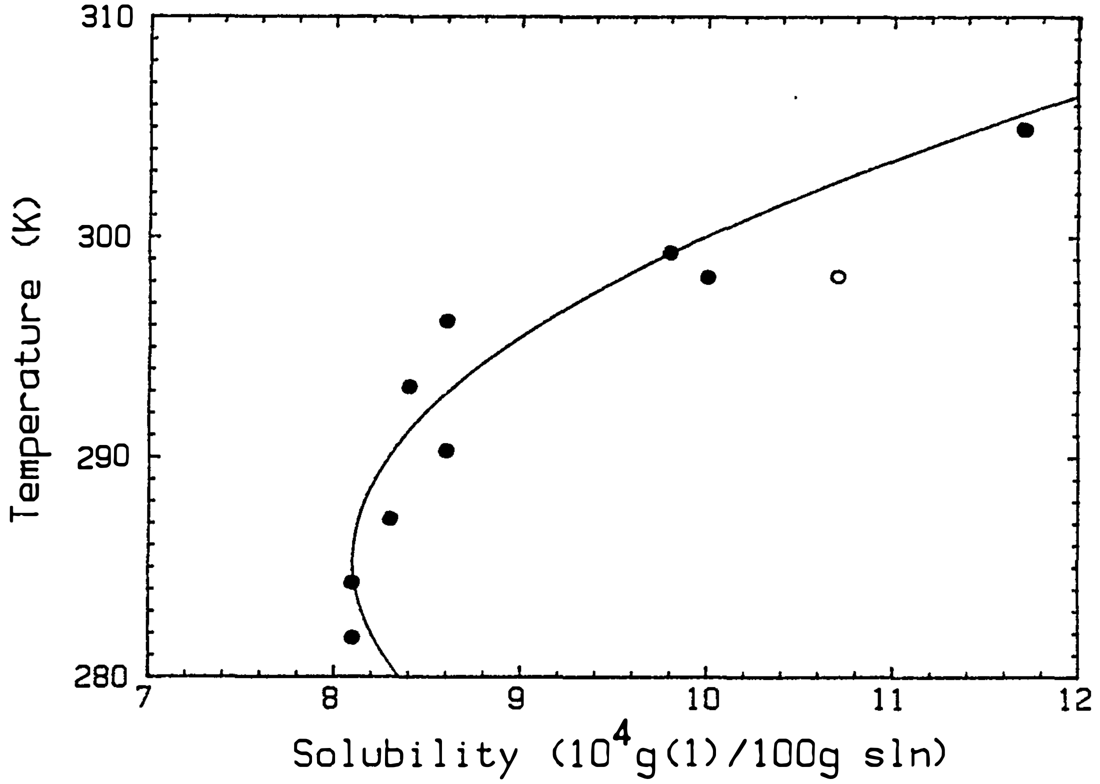

FIGURE 1. Solubility of fluorene in water: ref 1 (o); ref 2,3 (●).

REFERENCES

1. Wauchope, R.D.; Getzen, F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
3. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-75°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of fluorene in water

t/°C	mg(1)/kg(2) experiment	mg(1)/kg(2) smoothed with (std dev)	10^4 g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)
0.0		0.66(0.01)	0.66	7.2
24.6	1.93, 1.87, 1.88	1.86	1.86	20.2
25.0		1.90(0.03)	1.90	20.6
29.9	2.41, 2.33, 2.34	2.37	2.37	25.7
30.3	2.10, 2.25, 2.23	2.41	2.41	26.1
38.4	3.72, 3.73	3.53	3.53	38.2
40.1	3.88, 3.84, 3.85	3.84	3.84	41.6
47.5	5.59, 5.62, 5.68	5.54	5.54	60.0
50.0		6.29(0.05)	6.29	68.2
50.1	6.31, 6.42, 6.54	6.32	6.32	68.5
50.2	6.27	6.35	6.35	68.8
54.7	8.31, 8.41, 8.56	8.02	8.02	86.9
59.2	10.5, 10.5	10.2	10.2	110
60.5	10.7, 11.0, 11.6	10.9	10.9	118
65.1	14.2, 14.1, 14.2	14.1	14.1	153
70.7	18.5, 18.5, 18.9	19.3	19.3	209
71.9	18.8	20.6	20.6	223
73.4	21.5	22.5	22.5	244
75.0		24.7(0.4)	24.7	268

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction.
Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. see experimental values above

REFERENCES:

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of fluorene in water at 25°C was reported to be 1.98 mg(1) dm^{-3} sln and $x_1 = 2.14 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 1.98×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.04 mg(1) dm^{-3} sln (maximum deviation from several determinations.)

REFERENCES:

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of fluorene in water at 25°C was reported to be 1.685 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, values calculated by compiler are 1.685×10^{-4} g(1)/100 g sln and 1.826×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.005 mg(1)/100 kg(2)
(standard deviation)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) Fluorene; $C_{13}H_{10}$; [86-73-7]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of fluorene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_sC_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, K_s = 0.267 with S_o = 1.685.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 1.20×10^{-4} g(1)/100 g sln and 1.30×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

REFERENCES:

COMPONENTS:

(1) Diphenylmethane; $C_{13}H_{12}$; [101-81-5]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1949, *71*, 3644-77.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of diphenylmethane in water at 25°C was reported to be 1.41×10^{-4} g(1)/100 g sln.

The corresponding mole fraction, x_1, value calculated by compiler is 1.51×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co., best grade; purified by fractional freezing; m.p. 25°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) 1,4,5-Trimethylnaphthalene; $C_{13}H_{14}$; [213-41-1]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 1,4,5-trimethylnaphthalene in water at 25°C was reported to be 2.1 mg(1) dm^{-3} sln and $x_1 = 2.15 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 2.1×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.1 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) (2-Ethylcyclopentyl) benzene; $C_{13}H_{18}$; [4810-07-5]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in (2-Ethylcyclopentyl) Benzene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0103	1.00
20	0.0168	1.62
30	0.0273	2.64

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 2-Cyclopentyloctane; $C_{13}H_{26}$; [4810-01-9]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of Water in 2-Cyclopentyloctane

t/°C	g(2)/100 g sln	$10^4\ x_2$ (compiler)
10	0.0048	4.86
20	0.0075	7.59
30	0.0122	12.34

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Tridecane; $C_{13}H_{28}$; [629-50-5]

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

ORIGINAL MEASUREMENTS:

Schatzberg, P.

J. Phys. Chem. 1963, *67*, 776-9.

VARIABLES:

Temperature: 25-40°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in tridecane

t/°C	mg(2)/kg sln	x_2
25	60[a]	6.1×10^{-4}
40	123[b]	12.6×10^{-4}

[a] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; research grade; 99.73 mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in anthracene.

TABLE 1: Quantitative Solubility Studies of Anthracene (1) in Water (2)

Reference	*T*/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Wauchope and Getzen (ref 3)	273-348	spectrophotometric
Mackay and Shiu (ref 4)	298	spectrofluorometric
Schwarz (ref 5)	282-305	spectrophotometric
May *et al.* (ref 6)	278-302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of the 300K datum of Davis *et al.* (ref 1) which is several orders of magnitude lower than all other values, all the available data on the solubility of anthracene in water are summarized in Table 2. Selected data are also plotted in Figure 1.

At 298K the data are clustered around two values (Table 2). A possible explanation for this (ref 6) is that most commercial preparations of anthracene contain about 2% phenanthrene. Although isomeric with anthracene, phenanthrene is about 20 times more soluble which could result in higher observed values for analytical methods such as spectrophotometry which do not distinguish between the two isomers. However, at the present time there are insufficient data to justify rejection of the higher values. Clearly, a careful reinvestigation of this system is justified.

At temperatures lower than 298K the data of Schwarz (ref 5) and May *et al.* (ref 6) are in good agreement. However, in view of the discrepancies at 298K these values are regarded only as Tentative.

At T > 298K only the data of Wauchope and Getzen (ref 3) are available and in view of the disagreement at 298K must also be regarded as very tentative.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Anthracene: $C_{14}H_{10}$; [120-12-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values of the Solubility of Anthracene (1) in Water (2)

T/K	Solubility values		
	Reported values[a]	"Best" values ($\pm\ \sigma_n$)[b]	
	10^6g(1)/100g sln	10^6g(1)/100g sln	$10^8\ x_1$
273	2.2 (ref 3)	2.2	0.22
283	2.38* (ref 5), 1.74* (ref 6)	2.1 ± 0.3	0.21
293	3.48* (ref 5), 3.23* (ref 6)	3.4 ± 0.1	0.34
298	7.5 (ref 2), 7.5 (ref 3) 7.3 (ref 4), 4.46* (ref 5), 4.46 (ref 6)	6.2 ± 1.5[c]	0.62[c]
303	8.0* (ref 3)	8[c]	8[c]
313	16* (ref 3)	16[c]	16[c]
323	28.6 (ref 3)	29[c]	29[c]
333	51* (ref 3)	51[c]	51[c]
343	91 (ref 3)	91[c]	91[c]

[a] Values masked by an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

[c] See text however.

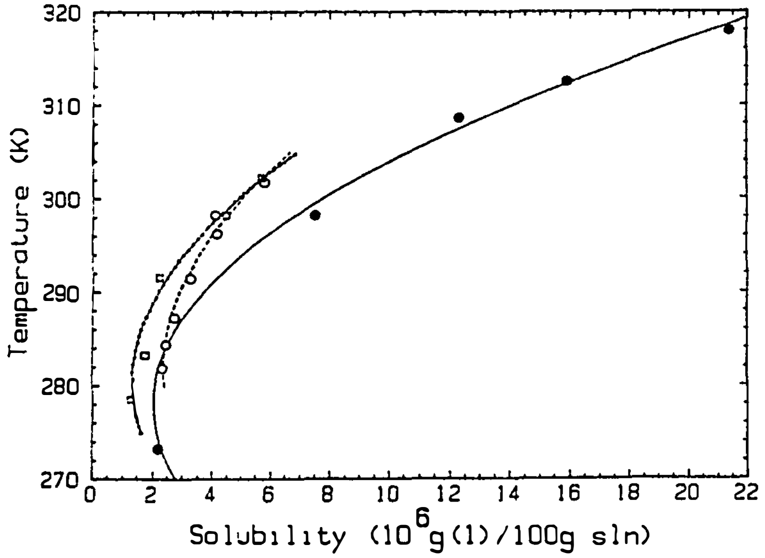

FIGURE 1. Solubility of anthracene in water, selected data: ref 3 (●), solid curve; ref 5 (o), broken curve; ref 6 (□), broken curve.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-298.
3. Wauchope, R.D.; Getzen, F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
4. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
5. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
6. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of anthracene in water

t/°C	10^7 g(1) L^{-1} (2)
27	7.5 ± 0.8
	7.2 ± 0.5
	7.5 ± 0.5

The best value recommended by the authors is 7.5 x 10^{-7} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding values of mass percent and mole fraction, x_1, calculated by the compiler are 7.5 x 10^{-8} g(1)/100 g sln and 7.6 x 10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Company, 450x; m.p. range 215.6-216.5°C; used as received; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above.

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of anthracene in water at 25°C was reported to be 7.5×10^{-5} g(1) dm^{-3} sln and 4.47×10^{-7} mol(1) dm^{-3} sln. Assuming that 1.00 dm^3 sln = 1.00 dm^3 sln the dorresponding mass percent and mole fraction, x_1, calculated by the compiler are 7.5×10^{-6} g(1)/ 100 g sln and 8.07×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-75°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of anthracene in water

t/°C	mg(1)/kg(2) experiment	mg(1)/kg(2) smoothed with (std dev)	10^5 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
0.0		0.022(0.001)	0.22	0.22
25.0		0.075(0.002)	0.75	0.76
35.4	0.125, 0.122, 0.119	0.123	1.23	1.24
39.3	0.152, 0.151, 0.148	0.159	1.59	1.61
44.7	0.208, 0.210, 0.206	0.214	2.14	2.16
47.5	0.279	0.249	2.49	2.52
50.0		0.286(0.003)	2.86	2.89
50.1	0.301, 0.297, 0.302	0.288	2.88	2.91
54.7	0.391, 0.389, 0.402	0.372	3.72	3.76
59.2	0.480, 0.488, 0.525	0.481	4.81	4.86
64.5	0.72, 0.62, 0.64	0.66	6.6	6.7
65.1	0.67, 0.64, 0.67	0.68	6.8	6.9
69.8	0.92	0.90	9.0	9.1
70.7	0.90, 0.97, 0.96	0.95	9.5	9.6
71.9	0.91	1.02	10.2	10.3
74.7	1.19, 1.13, 1.26	1.21	12.1	12.2
75.0		1.23(0.02)	12.3	12.4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane.
In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction.
Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. see experimental values above

REFERENCES:

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of anthracene in water at 25°C was reported to be 0.073 mg(1) dm^{-3} sln and $x_1 = 7.57 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 7.3×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± mg(1) dm^{-3} sln (maximum deviation from several determinations.)

REFERENCES:

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data, 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.6 - 31.3°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of Anthracene in Water

t/°C	10^7 mol(1) L^{-1}	10^6 g(1)/100g sln (compiler)	10^9 x_1 (compiler)
8.6	1.31 ± 0.04	2.33	2.36
11.1	1.37 ± 0.03	2.44	2.47
12.2	1.44 ± 0.03	2.57	2.59
14.0	1.54 ± 0.04	2.74	2.77
15.5	1.66 ± 0.03	2.96	3.00
18.2	1.81 ± 0.03	3.23	3.26
20.3	2.22 ± 0.03	3.96	4.00
23.0	2.34 ± 0.03	4.17	4.21
23.3	2.30 ± 0.04	4.10	4.14
25.0	2.30 ± 0.05	4.10	4.14
26.2	2.67 ± 0.03	4.76	4.81
28.5	3.25 ± 0.06	5.79	5.85
31.3	3.90 ± 0.02	6.95	7.02

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used. At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used. The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 74 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Source not specified; better than 99 mole %, by glc, used as received.

(2) Distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

Temperature: ±0.1°C

Solubility: See above.

REFERENCES:

COMPONENTS: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 175-9 and 997-1000.
VARIABLES: Temperature: 5.2-29.0°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

Solubility of anthracene in water

$t/°C$	µg(1)/kg(2)	10^6 g(1)/100 g sln (compiler)	$10^9 x_1$ (compiler)
5.2	12.7 ± 0.4	1.27	1.28
10.0	17.5 ± 0.3	1.75	1.77
14.1	22.2 ± 0.1	2.22	2.24
18.3	29.1 ± 0.6	2.91	2.94
22.4	37.2 ± 1.1	3.72	3.76
24.6	43.4 ± 0.1	4.34	4.39
25.0	44.6 ± 0.2	4.46	4.51
28.7	55.7 ± 0.7	5.57	5.63
29.0	57.0 ± 3.0	5.7	5.76

$$\mu g(1)/kg(2) = 8.21 + 0.8861\, t + 0.0097\, t^2 + 0.0013\, t^3$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. stand. dev. see above

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:	EVALUATOR:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10^6 g(1)/100 g sln
Schwarz (ref 1)	uv spectral	30	3.55
May *et al.* (ref 2)	HPLC	35.0	3.11

The reported data are from different salinities which precludes direct comparison. Since the data appear consistent with each other and with the tentative value for the solubility of anthracene in pure water, the data of Schwarz, and May *et al.* are adopted as tentative. Schwarz also reports data over the temperature range 281-303 K.

SOLUBILITY OF ANTHRACENE (1) IN SEAWATER (2)
TENTATIVE VALUE

T/K	g salts/kg sln	10^6 g(1)/100 g sln
298	35.0	3.11

REFERENCES

1. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

2. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.2-30.2°C

Salinity: 30 g(2)/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of Anthracene in 0.5 mol(2)/L

t,°C	10^7 mol(1)/L sln
8.2	0.93
8.6	1.01
11.7	1.22
19.2	1.47
21.5	1.68
25.0	2.04
25.3	1.92
27.1	2.02
30.2	2.46

The corresponding mass percent and mole fraction x_1, at 25.0°C calculated by the compilers are 3.55×10^{-6} g(1)/100 g sln and 3.69×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of anthracene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of anthracene to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 258 nm. The Spectrofluorimeter employed a ratio-photon counting mode where anthracene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of anthracene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

Anthracene: purity >99 mole %

Sodium chloride: reagent grade

Ethanol: reagent grade

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.

ESTIMATED ERROR:

Solubility ± 4.3 % (author)

Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 (mol/L) $K_s = 0.238$ with $S_o = 0.0446$.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 3.11×10^{-6} g(1)/kg sln and 3.22×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

K_s ± 0.004

S_o ± 0.0002

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

February 1986.

CRITICAL EVALUATION:

Quantitative solubility data for phenanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported for the solubility of water in phenanthrene.

TABLE 1: Quantitative Solubility Studies of Phenanthrene (1) in Water (2)

Reference	*T*/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Andrews and Keefer (ref 2)	298	spectrophotometric
Klevens (ref 3)	298	spectrophotometric
Wauchope and Getzen (ref 4)	273-348	spectrophotometric
Eganhouse and Calder (ref 5)	298	GLC
Mackay and Shiu (ref 6)	298	spectrofluorometric
Schwarz (ref 7)	282-305	spectrofluorometric
May *et al.* (ref 8)	282-303	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The plethora of values reported (Table 1) at 298K for the solubility of phenanthrene (1) in water (2) enable a particularly critical assessment to be made. Thus the values of Davis *et al.* (ref 1) at 300K and of Klevens (ref 3) have been rejected as they are significantly higher than all other values. The remaining data at 298K are in good agreement enabling the average value to be Recommended.

At other temperatures where comparison is possible the data of May *et al.* (ref 8), Schwarz (ref 7) and Wauchope and Getzen (ref 4) are in excellent agreement enabling the average values to be Recommended over a reasonably wide range. At higher temperatures (> 303K) only the data of Wauchope and Getzen (ref 4) are available and must therefore be regarded as Tentative.

All the available data, except for the rejected values noted above (ref 1, 3), are summarized in Table 2 and plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (*R*) and Tentative Solubility Values of Phenanthrene (1) in Water (2)

T/K	Solubility values Reported values[a] 10^4g(1)/100g sln	"Best" values ($\pm\ \sigma_n$)[b] 10^4g(1)/100g sln	 $10^7\ x_1$
273	0.39 (ref 4)	0.4	0.4
283	0.53* (ref 7), 0.46* (ref 8)	0.50 ± 0.04 (*R*)	0.50 (*R*)
293	0.88* (ref 7), 0.78* (ref 8)	0.85 ± 0.05 (*R*)	0.86 (*R*)
298	0.994 (ref 2), 1.18 (ref 4), 1.07 (ref 5), 1.29 (ref 6), 1.151 (ref 7), 1.002 (ref 8)	1.1 ± 0.1 (*R*)	1.1 (*R*)
303	1.50* (ref 4), 1.46* (ref 7), 1.28* (ref 8)	1.4 ± 0.1 (*R*)	1.4 (*R*)
313	2.45* (ref 4)	2.5	2.5
323	4.14 (ref 4)	4.1	4.1
333	7.2* (ref 4)	7.2	7.2
343	12.8* (ref 4)	13	13
348	17 (ref 4)	17	17

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

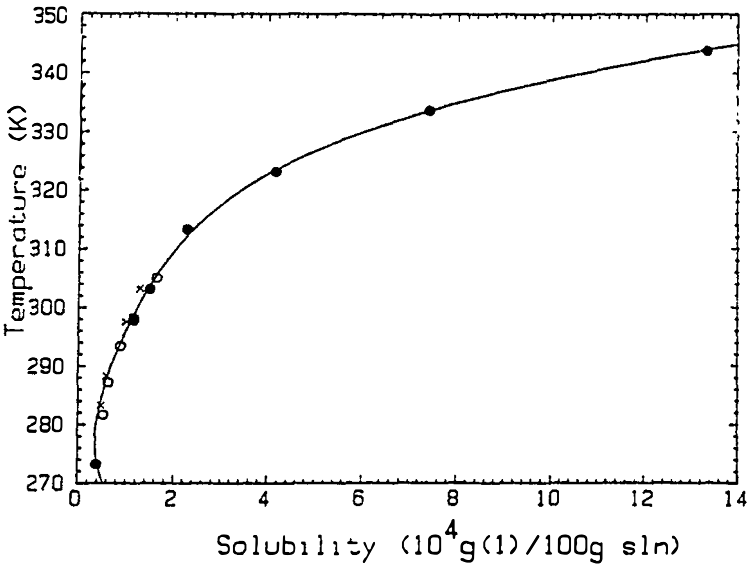

FIGURE 1. Solubility of phenanthrene in water, selected data: ref 4 (●); ref 7 (o); ref 8 (x). Solid curve plotted through "Best" values (Table 2).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. February 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* 1949, *71*, 3644-77.
3. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-298.
4. Wauchope, R.D.; Getzen, F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
5. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
6. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
7. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
8. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Water; H_2O; [7732-18-5]	Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
VARIABLES:	**PREPARED BY:**
One temperature: 27°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of phenanthrene in water

t/°C	10^3 g(1) L^{-1} (2)
27	1.55
	1.62
	1.65

The best value recommended by the authors is 1.60 x 10^{-3} g(1) L^{-1} (2). Assuming that 1.00 L sln = kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.60 x 10^{-4} g(1)/ 100 g sln and 1.62 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Company, 599; m.p. range 100.0-100.9°C; used as received; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.05 x 10^{-3} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1949, *71*, 3644-77.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of phenanthrene in water at 25°C was reported to be 9.94×10^{-5} g(1)/100 g sln.

The corresponding mole fraction, x_1, value calculated by compiler is 1.004×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Co., best grade; recrystallized twice from ethanol; m.p. 101.0°C.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of phenanthrene in water at 25°C was reported to be 0.0016 x 10^{-5} g(1)/L sln and 9.0 x 10^{-6} mole (1)/L sln.
Assuming that 1.00 dm^3 sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.6 x 10^{-4} g(1)/ 100 g sln and 1.62 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-75°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of phenanthrene in water

t/°C	mg(1)/kg(2) experiment	mg(1)/kg(2) smoothed with (std dev)	10^4 g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)
0.0		0.39(0.01)	0.39	0.39
24.6	1.12, 1.11	1.16	1.16	1.17
25.0		1.18(0.02)	1.18	1.19
29.9	1.49, 1.49	1.49	1.49	1.51
30.3	1.47, 1.48	1.52	1.52	1.54
38.4	2.44, 2.45	2.27	2.27	2.29
40.1	2.27, 2.28, 2.25	2.47	2.47	2.50
47.5	3.81, 3.88, 3.87	3.63	3.63	3.67
50.0		4.14(0.04)	4.14	4.18
50.1	4.30, 4.38, 4.32	4.16	4.16	4.20
50.2	4.08, 4.04, 4.11	4.19	4.19	4.23
54.7	5.66, 5.64, 5.63	5.34	5.34	5.40
59.2	7.17, 7.19, 7.21	6.85	6.85	6.92
60.5	7.2, 7.2, 7.6	7.4	7.4	7.5
65.1	9.8, 9.7, 9.8	9.6	9.6	9.7
70.7	12.4, 12.6, 12.4	13.3	13.3	13.4
71.9	12.9	14.2	14.2	14.4
73.4	18.2	15.6	15.6	15.8
75.0		17.2(0.3)	17.2	17.4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction.

Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C

soly. see experimental values above

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

Eganhouse, R.P.; Calder, J.A.

Geochim. Cosmochim. Acta 1976, *40*, 555-61.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of phenanthrene in water at 25°C was reported to be 1.07 mg(1)/kg(2) and 6 x 10^{-6} mol(1) dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.07 x 10^{-4} g(1)/100 g sln and 1.08 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of 500 mL (2) and 0.001 mol (1) was equilibrated in an Erlenmeyer flask for 12 h (agitation) + 24 h (stationary). The saturated solution, 100 mL, was extracted with hexane, concentrated by evaporation under nitrogen and analyzed by glc. A 5700 A Hewlett-Packard instrument equipped with dual compensating columns and flame ionization detectors was employed.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; analytical grade; used as received; no impurities by glc.

(2) doubly distilled; free of trace organics.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. ± 0.01 mg(1)/kg(2)
(from eight determinations)

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of phenanthrene in water at 25°C was reported to be 1.29 mg(1) dm^{-3} sln and $x_1 = 1.3 \times 10^{-7}$.

The corresponding mass percent calculated by the compiler is 1.29×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.07 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.4-31.8°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of phenanthrene in water

t/°C	10^6 mol(1) L^{-1}	10^5 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
8.4	2.81 ± 0.07	5.01	5.06
11.1	3.09 ± 0.07	5.51	5.57
14.0	3.59 ± 0.06	6.40	6.47
17.5	4.40 ± 0.04	7.84	7.92
20.2	4.94 ± 0.09	8.80	8.90
23.3	6.09 ± 0.07	10.85	10.97
25.0	6.46 ± 0.02	11.51	11.63
29.3	7.7 ± 0.2	13.72	13.87
31.8	9.13 ± 0.08	16.27	16.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. <u>1978</u>, *50*, 175-9 and 997-1000.

VARIABLES:

Temperature: 8.5-29.9°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of phenanthrene in water

$t/°C$	µg(1)/kg(2)	10^4 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
8.5	423 ± 4	0.423	0.427
10.0	468 ± 2	0.468	0.473
12.5	512 ± 1	0.512	0.517
15.0	601 ± 7	0.601	0.607
21.0	816 ± 8	0.816	0.825
24.3	995 ± 1	0.995	1.006
25.0	1002 ± 11	1.002	1.013
29.0	1220 ± 13	1.220	1.233
29.9	1277 ± 11	1.277	1.291

$$\mu g(1)/kg(2) = 324.0 + 5.413\ t + 0.8059\ t^2 + 0.0025\ t^3$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. stand. dev. see above

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* <u>1975</u>, *13*, 535.

COMPONENTS:	EVALUATOR:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of phenanthrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Method	Salinity g salts/kg sln	10^5 g(1)/100 g sln
Eganhouse and Calder (ref 1)	GLC	35	7.1
Schwarz (ref 2)	uv spectral	30	9.94
May *et al.* (ref 3)	HPLC	35	6.63
Aquan-Yuen *et al.* (ref 4)	uv spectral	28.6	8.3

At 298 K and a salinity of 35 g salts/kg sln the data of Eganhouse and Calder and of May *et al.* are in very good agreement. Therefore their mean, 6.9 x 10^{-5} g (1)/100 g sln is adopted as the recommended value for the solubility of phenanthrene at the indicated temperature and salinity. The value of Aquan-Yuen *et al.* appears consistent with the data discussed above and with the recommended value for the solubility of phenanthrene in pure water and is adopted at tentative. The value of Schwarz appears slightly high and is considered doubtful.

THE SOLUBILITY OF PHENANTHRENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

T/K	g salts/kg sln	10^5 g(1)/100 g sln
298	35	6.9

REFERENCES

1. Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
2. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
3. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
4. Aquan-Yuen, M.; Mackay, D.; Shui, W.Y. *J. Chem. Eng. Data* 1979, *24*, 30-4.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Artificial seawater (ref. 1)	Eganhouse, R.P.; Calder, J.A. *Geochim. Cosmochim. Acta* 1976, *40*, 555-61.
VARIABLES:	**PREPARED BY:**
One temperature: 25.0°C Salinity: 35 g/kg sln	M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of phenanthrene in seawater is reported to be 0.71 mg/kg the corresponding mass percent and mole fraction, x_1, calculated by the compilers are 7.1×10^{-5} g(1)/100 g sln and 7.4×10^{-8}.

Graphical results for other salinities are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Equilibrium flask: 1-dm^3 Erlenmeyer flask with ground glass stopper and sidearm tap at base plugged with glass wool. The mixtures were agitated 12+ hr at 215 rpm on a New Brunswick gyrotary shaker; a 24 hr stationary equilibrium period followed. Hydrocarbons were extracted with doubly-distilled hexane 3 times; concentrated by evaporation, with losses checked against an internal standard.
Analysis: gas chromatography.

SOURCE AND PURITY OF MATERIALS:

(1) analytical grade salt for artificial seawater solution, reagent grade.
Water: doubly distilled.

ESTIMATED ERROR:

temperature: ± 0.5°C
soly: ± 0.025 (95% confidence interval)

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* 1940, *3*, 135.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
VARIABLES:	**PREPARED BY:**
Temperature: 11.1 - 31.8°C Salinity: 30 g(2)/kg sln	W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of phenanthrene in 0.5 mol(2)/L

t/°C	10^6 mol(1)/L sln
11.1	2.88
14.0	3.2
17.5	4.07
20.2	4.51
23.2	5.75
25.0	5.72
29.3	7.2
31.8	7.9

The corresponding mass percent and mole fraction x_1 at 25.0°C calculated by the compilers are 9.94×10^{-5} g(1)/100 g sln and 1.034×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of phenanthrene was determined by fluorescence and UV absorption measurements. For fluorescence method, an excess amount of phenanthrene was added to an air-tight 1X1 cm quartz fluorescence cell containing 5 mL of salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 365 and 320 nm. The Spectrofluorimeter employed a ratio-photon counting mode where phenanthrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of phenanthrene in ethanol solution and therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

Phenanthrene: purity 99.9%

Sodium chloride: reagent grade

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.

Ethanol: reagent grade

ESTIMATED ERROR:

Solubility ± 8.4% (author)

Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of phenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L,

$K_s = 0.275$ with $S_o = 1.002$.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 6.63×10^{-5} g(1)/100 g sln and 6.78×10^{-8}.

Graphical data for other temperatures are also presented.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

K_s ± 0.010

S_o ± 0.011

REFERENCES:

COMPONENTS:

(1) Phenanthrene; $C_{14}H_{10}$; [85-01-8]

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

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

ORIGINAL MEASUREMENTS:

Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1979, *24*, 30-4.

VARIABLES:

One temperature: 25°C

Salinity: 29-108 g(2)/kg sln

PREPARED BY:

M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

Solubility of phenanthrene in aqueous NaCl

mol(2)/L sln	g(2)/kg sln[a]	mg(1)/L sln	10^5mass%(1)[a]	$10^8 x_1$[a]
0.50	28.6	0.85	8.3	8.6
1.00	56.2	0.67	6.4	6.8
1.50	82.6	0.48	4.5	4.9
2.00	108.2	0.33	3.1	3.3

'a' calculated by compilers using density and other physical data for NaCl solutions from ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solutions were prepared by adding excess (1) to a previously prepared salt solution. The resulting mixture was stirred for 24 hours and then allowed to settle for 48 hours. An aliquot was extracted with cyclohexane which was then analyzed spectrofluorometrically.

SOURCE AND PURITY OF MATERIALS:

(1) fluorescence grade, from Eastman Kodak.

(2) reagent grade, from Fisher Scientific.

ESTIMATED ERROR:

temp ± 0.5°C

soly ± 3 relative %

REFERENCES:

1. Weast, R.C.; *CRC Handbook of Chemistry and Physics*, 59th Edition; 1978; CRC Press pp. D299-D300.

COMPONENTS:

(1) (E)-Stilbene; $C_{14}H_{12}$; [103-30-3]

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

ORIGINAL MEASUREMENTS:

Andrews, L.J.; Keefer, R.M.

J. Am. Chem. Soc. 1950, *72*, 5034-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of (E)-stilbene in water at 25°C was reported to be 2.9×10^{-5} g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 2×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass-stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

(1) from the State University of Iowa;
m.p. 120-121°C;

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) 1,4-Dicyclopentylbutane; $C_{14}H_{26}$; [2980-70-3]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Technol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in 1,4-Dicyclopentylbutane

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0088	0.94
20	0.0139	1.50
30	0.0241	2.59

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) Tetradecane; $C_{14}H_{30}$; [629-59-4]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
June 1986

CRITICAL EVALUATION:

Quantitative solubility data for the tetradecane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Tetradecane (1) - Water (2) System

Reference	*T* /K	Solubility	Method
Schatzberg (ref 1)	313	(2) in (1)	Karl Fischer
Franks (ref 2)	298	(1) in (2)	GLC
Sutton and Calder (ref 3)	298	(1) in (2)	GLC
Mackay *et al.* (ref 4)	- [a]	(1) in (2)	GLC

[a] Not specified but probably close to 298 K.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. SOLUBILITY OF TETRADECANE (1) IN WATER (2)

The solubility of tetradecane in water has been reported only at 298K (Table 1). Unfortunately, the results are in very poor agreement (Table 2). Furthermore, all the reported values are very much higher than the value of ~ 3×10^{-8} g(1)/100 g sln which is predicted by extrapolation of the lower hydrocarbon homologue solubilities. Thus, the values given in Table 2 must be regarded very sceptically and no "Best" value has been calculated.

TABLE 2: Reported Solubility Values of Tetradecane (1) in Water (2)

T/K	Reported solubility values [a] 10^7 g(1)/100 g sln
298	6.94 (ref 2), 2.2 (ref 3), 25.9 [b] (ref 4)

[a] All values may be high. "Best" values not determined because of uncertainties in data, see text.

[b] Assumed to be at 298K for the purpose of comparison.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986

CRITICAL EVALUATION: (continued)

2. SOLUBILITY OF WATER (2) IN TETRADECANE

As only the datum of Schatzberg at 313K is available no Critical Evaluation is possible. However, it may be noted that the data of Schatzberg in well characterized systems are generally reliable. The interested user is referred to the appropriate Data Sheet for the experimental value.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.

2. Franks, F. *Nature (London)* 1966, *210*, 87-8.

3. Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8* , 654-7.

4. Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. 1975, *573* , 251-8.

COMPONENTS:

(1) Tetradecane; $C_{14}H_{30}$; [629-59-4]

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

ORIGINAL MEASUREMENTS:

Schatzberg, P.

J. Phys. Chem. 1963, *67*, 776-9.

VARIABLES:

One temperature: 40°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in tetradecane at 40°C was reported to be 114 mg(2)/kg sln corresponding to a mole fraction, x_2, of 1.26 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Phillips Petroleum Co.; pure grade; 99+ mole %; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:

(1) Tetradecane; $H_{14}H_{30}$; [629-59-4]

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

ORIGINAL MEASUREMENTS:

Franks, F.

Nature (London) 1966, *210*, 87-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

F. Kapuku

EXPERIMENTAL VALUES:

The solubility of tetradecane in water at 25°C was reported to be in mole fraction $x_1 = 6.3 \times 10^{-10}$.
The corresponding mass percent calculated by the compiler is 6.94×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; purum grade;
purity > 97% (chromatographic analysis).

(2) not specified.

ESTIMATED ERROR:

soly. ± 12%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of tetradecane in water at 25°C was reported to be 2.2×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 2×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 μm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS: (1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u>, *573*, 251-8.
VARIABLES: not specified	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported a value of 0.0259 mg(1)dm^{-3} sln for the solubility of tetradecane in water.
With the assumption of a solution density of 1.00 g cm^{-3} the corresponding mass percent, calculated by the compiler, is 2.59 x 10^{-6} g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.4 x 10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) is partially partitioned into the vapor phase by equilibration of the aqueous sample with helium in a gas syringe, the vapor then being transferred to a gas sampling valve and then to the column of a gas chromatograph equipped with a flame ionization detector. By injecting gas samples from repeated equilibrations it is possible to calculate the amount of (1) in the original sample.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not estimated.

REFERENCES:

COMPONENTS: (1) Tetradecane; $C_{14}H_{30}$; [629-59-4] (2) Seawater	**ORIGINAL MEASUREMENTS:** Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES: One temperature: 25°C One salinity: 35 g salts/kg sln	**PREPARED BY:** P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of tetradecane in seawater was reported to be 1.7×10^{-7} g(1)/100 g sln and $x_1 = 1.5 \times 10^{-10}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES:

COMPONENTS:

(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
June 1986

CRITICAL EVALUATION:

Quantitative solubility data for 2-methylanthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in 2-methylanthracene.

TABLE 1: Quantitative Solubility Studies of 2-Methylanthracene (1) in Water (2)

Reference	*T* /K	Method
Mackay and Shiu (ref 1)	298	spectofluorometric
May *et al.* (ref 2)	279-304	chromatographic

The original data in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

At 298K, the only temperature at which comparison is possible, the datum of Mackay and Shiu (ref 1) is in only fair agreement with that of May *et al.* (ref 2). Thus all the available data, which are summarized in Table 2, must be regarded as very tentative.

TABLE 2: Tentative Solubility Values of 2-Methylanthracene (1) in Water (2)

T /K	Solubility values		
	Reported values[a]	"Best values (± σ_n)[b]	
	10^6 g(1)/100 g sln	10^6 g(1) g sln	10^9 x_1
278	0.64* (ref 2)	0.6	0.6
283	0.89* (ref 2)	0.9	0.8
293	1.60* (ref 2)	1.6	1.5
298	3.9 (ref 1), 2.16* (ref 2)	3.0 ± 0.9	2.8
303	2.93 (ref 2)	3.0	2.8

[a] Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

REFERENCES

1. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22* , 399-402.

2. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) 2-Methylanthracene; $C_{15}H_{12}$;
[613-12-7]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylanthracene in water at 25°C was reported to be 0.039 mg(1) dm^{-3} sln and $x_1 = 3.67 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 3.9×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.004 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 175-9 and 997-1000.

VARIABLES:

Temperature: 6.3-31.1°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 2-methylanthracene in water

t/°C	μg(1)/kg(2)	10^6 g(1)/100 g sln (compiler)	$10^9 x_1$ (compiler)
6.3	7.06 ± 0.18	0.706	0.661
9.1	8.48 ± 0.09	0.848	0.794
10.8	9.43 ± 0.37	0.943	0.883
13.9	11.1 ± 0.3	1.11	1.04
18.3	14.5 ± 0.1	1.45	1.36
23.1	19.1 ± 0.6	1.91	1.79
25.0	21.3 ± 0.3	2.13	1.99
27.0	24.2 ± 0.1	2.42	2.27
31.1	32.1 ± 0.3	3.21	3.01

$$\mu g(1)/kg(2) = 2.78 + 0.8180\ t + 0.0306\ t^2 + 0.0011\ t^3$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. stand. dev. see above

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) 2-Methylanthracene; $C_{15}H_{12}$; [613-12-7]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of 2-methylanthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_sC_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7mol/L, K_s = 0.336 with S_o = 0.0213.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 1.29×10^{-6} g(1)/100 g sln and 1.24×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

K_s ± 0.006

S_o ± 0.003

REFERENCES:

COMPONENTS:

(1) 9-Methylanthracene; $C_{15}H_{12}$; [779-02-2]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 9-methylanthracene in water at 25°C was reported to be 0.261 mg(1) dm^{-3} sln and $x_1 = 2.44 \times 10^{-8}$.

The corresponding mass percent calculated by the compiler is 2.61×10^{-5} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.002 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Methylphenanthrene; $C_{15}H_{12}$; [832-69-6] (2) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 175-9 and 997-1000.
VARIABLES:	**PREPARED BY:**
Temperature: 6.6-29.9°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 1-methylphenanthrene in water

t/°C	μg(1)/kg(2)	10^5 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
6.6	95.2 ± 0.2	0.952	0.892
8.9	114.0 ± 4.0	1.14	1.07
14.0	147.0 ± 1.0	1.47	1.38
19.2	193.0 ± 1.0	1.93	1.81
24.1	255.0 ± 5.0	2.55	2.39
25.0	269.0 ± 3.0	2.69	2.69
26.9	304.0 ± 1.0	3.04	2.85
29.9	355.0 ± 2.0	3.55	3.32

$$\mu g(1)/kg(2) = 55.42 + 6.8016\,t + 0.1301\,t^2 + 0.0080\,t^3$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. stand. dev. see above

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) 1-Methylphenanthrene; $C_{15}H_{12}$; [832-69-9]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of 1-methylphenanthrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_sC_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, $K_s = 0.211$ with $S_o = 0.269$.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 1.95×10^{-5} g(1)/100 g sln and 1.87×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

K_s ± 0.018

S_o ± 0.003

REFERENCES:

COMPONENTS:

(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]
(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for fluoranthene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in fluoranthene.

TABLE 1. Quantitative Solubility Studies of Fluoranthene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May *et al.* (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. They are also summarized in Table 2. The values at 298 K are in reasonable agreement given the low solubility and the average value is Recommended. The remaining data are regarded as Tentative only.

TABLE 2. Recommended (R) and Tentative Solubility Values of Fluoranthene (1) in Water (2)

T /K	Solubility values		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	10^5 g(1)/100 g sln	10^5 g(1)/100 g sln	10^8 x_1
298	2.65 (ref 2), 2.6 (ref 3), 2.06 (ref 4)	2.4 ± 0.3 (R)	2.1 (R)
300	2.40 (ref 1)	2.4	2.1
302	2.64 (ref 4)	2.6	2.3

a Obtained by averaging where appropriate; σ_n has no statistical significance.

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
4. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of fluoranthene in water

t/°C	10^4 g(1) L^{-1} (2)
27	2.40 ± 0.20
	2.25 ± 0.20
	2.40 ± 0.20

The best value recommended by the authors is 2.40 x 10^{-4} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction are 2.40 x 10^{-5} g(1)/100 g sln and 2.15 x 10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 110.0-110.7°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of fluoranthene in water at 25°C was reported to be 2.65×10^{-4} g(1) L^{-1} and 1.32×10^{-6} mole/L^{-1}. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.65×10^{-5} g(1)/100 g sln and 2.37×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:

(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of fluoranthene in water at 25°C was reported to be 0.26 mg(1) dm^{-3} sln and $x_1 = 2.28 \times 10^{-8}$.

The corresponding mass percent calculated by the compiler is 2.6×10^{-5} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.002 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

Temperature: 25 and 29°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of fluoranthene in water

t/°C	mg(1)/kg(2)	10^5 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
25	0.206	2.06	1.83
29	0.264	2.64	2.35

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.002 mg(1)/kg(2)
(standard deviation)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) Fluoranthene; $C_{16}H_{10}$; [206-44-0]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of fluoranthene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, $K_s = 0.339$ with $S_o = 0.206$.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are $1.24 \text{ g} \times 10^{-5}$ g(1)/100 g sln and 1.14×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

K_s ± 0.010

S_o ± 0.002

REFERENCES:

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]
(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in pyrene.

TABLE 1. Quantitative Solubility Studies of Pyrene (1) in Water (2)

Reference	*T*/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Wauchope and Getzen (ref 3)	273-348	spectrophotometric
Mackay and Shiu (ref 4)	298	spectrofluorometric
Schwarz (ref 5)	285-304	spectrofluorometric
May *et al.* (ref 6)	298-302	chromatographic
Rossi and Thomas (ref 7)	298	GLC, spectrophotometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. At 298 K the values of Mackay and Shiu (ref 4), Schwarz (ref 5), May *et al.* (ref 6) and Rossi and Thomas (ref 7) are in excellent agreement and their average is Recommended. The values of Wauchope and Getzen (ref 3) and especially Klevens (ref 2) are signifigantly higher ($>3\sigma_n$) than the other studies and are thus rejected. At 303 K the values of Wauchope and Getzen (ref 3) are in good agreement with those of Schwarz (ref 5) and May *et al.* (ref 6). At other temperatures the data are mainly those of Wauchope and Getzen and must therefore be regarded as Tentative.

With the exception of the rejected values noted above and the 300 K datum of Davis *et al.* (ref 1) which is omitted for representational convenience, all the available data are summarized in Table 2. Selected data are also plotted in Figure 1.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

(continued)

TABLE 2. Recommended (*R*) and Tentative Solubility Values of Pyrene (1) in Water (2)

T/K	Solubility values Reported values[a] 10^5 g(1)/100 g sln	"Best" values $(\pm\sigma_n)$[b] 10^5 g(1)/100 g sln	10^8 x_1
273	0.49 (ref 3)	0.5	0.4
293	0.91* (ref 5)	0.9	0.8
298	1.35 (ref 4), 1.295 (ref 5), 1.32 (ref 6), 1.3 (ref 7)	1.32 ± 0.02(*R*)	1.17(*R*)
303	1.80* (ref 3), 1.76* (ref 5), 1.70* (ref 6)	1.75 ± 0.04(*R*)	1.56(*R*)
313	3.30* (ref 3)	3	3
323	5.32 (ref 3)	5	4
333	9.4* (ref 3)	9	8
343	16.9 (ref 3)	17	15
348	23.1 (ref 3)	23	20

[a] Values marked with an asterisk (*) were obtained by the Evaluator by graphical interpolation of the authors' original data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

(continued)

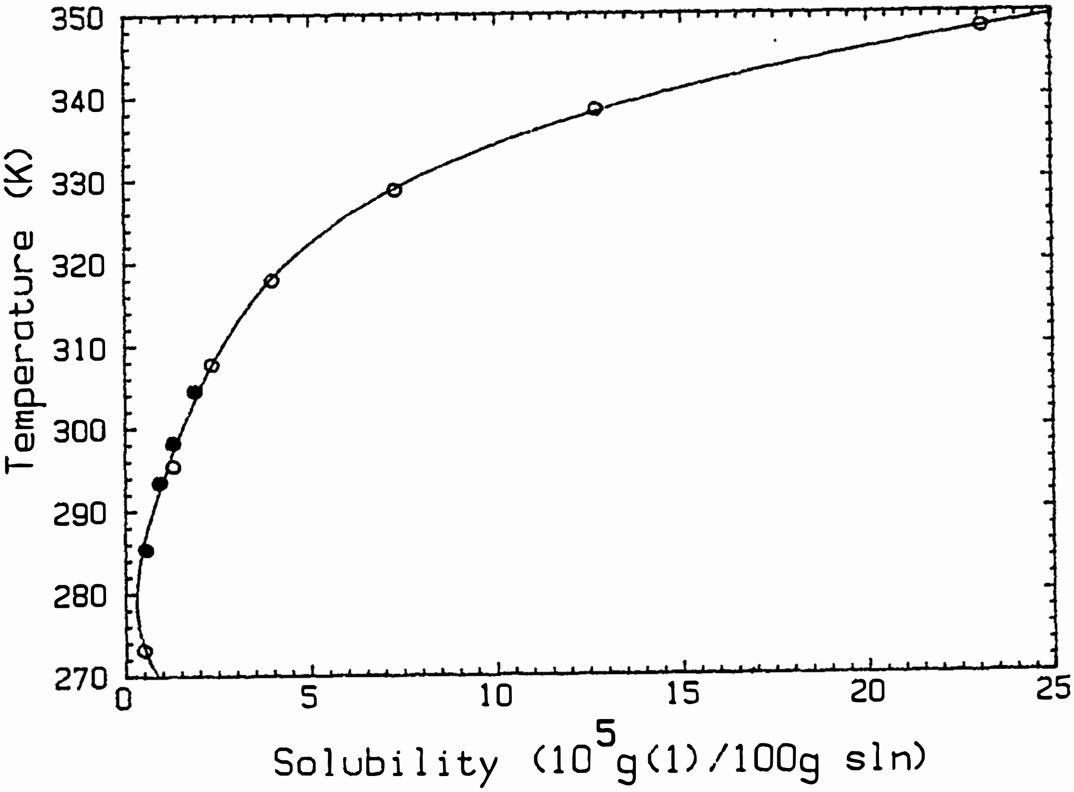

FIGURE 1. Solubility of pyrene in water, selected data: ref 3 (o); ref 5 (●).

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54* , 283-98.
3. Wauchope, R.D.; Getzen,F.W. *J. Chem. Eng. Data* 1972, *17*, 38-41.
4. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
5. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.
6. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
7. Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.

ACKNOWLEDGEMENT

The Evaluator thanks Dr Brian Clare for the graphics.

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pyrene in water

t/°C	10^4 g(1) L^{-1} (2)
27	1.60 ± 0.10
	1.65 ± 0.05

The best value recommended by the authors is 1.65 x 10^{-4} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.65 x 10^{-5} g(1)/100 g sln and 1.45 x 10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 149.6-150.5°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C

soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pyrene in water at 25°C was reported to be 1.75×10^{-4} g(1) L^{-1} sln and 7.7×10^{-7} mol(1) L^{-1} sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.75×10^{-5} g(1)/ 100 g sln and 1.39×10^{-8}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.	(1) not specified. (2) not specified. **ESTIMATED ERROR:** not specified. **REFERENCES:**

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

ORIGINAL MEASUREMENTS:

Wauchope, R.D.; Getzen, F.W.

J. Chem. Eng. Data 1972, *17*, 38-41.

VARIABLES:

Temperature: 0-75°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of pyrene in water

t/°C	mg(1)/kg(2) experiment	mg(1)/kg(2) smoothed with (std dev)	10^5 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
0.0		0.049(0.001)	0.49	0.44
22.2	0.129, 0.128, 0.124	0.130	1.30	1.15
25.0		0.148(0.002)	1.48	1.32
34.5	0.228, 0.235	0.235	2.35	2.09
44.7	0.397, 0.395, 0.405	0.399	3.99	3.55
50.0		0.532(0.004)	5.32	4.74
50.1	0.558, 0.576, 0.556	0.534	5.34	4.75
55.6	0.75, 0.75, 0.77	0.73	7.3	6.5
56.0	0.74	0.74	7.4	6.6
60.7	0.96, 0.95, 0.90	0.97	9.7	8.6
65.2	1.27, 1.29	1.27	12.7	11.3
71.9	1.83, 1.86, 1.89	1.90	19.0	16.9
74.7	2.21	2.26	22.6	20.1
75.0		2.31(0.03)	23.1	20.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 20 g of (1) was placed in each of three 250-mL glass-stoppered flasks with (2). The flasks were suspended in an open water bath and shaken gently from one to three weeks between measurements. Samples of the replicate were extracted with cyclohexane. In all cases, spectra taken of second extracts or of the aqueous layer after extraction indicated complete extraction.
Standard solutions were prepared either by direct weighing using a Cahn electrobalance, or by weighing 0.1-0.2 g of samples followed by serial dilution in calibrated glassware.

SOURCE AND PURITY OF MATERIALS:

(1) Baker reagent; recrystallized three times from ether; vacuum-sublimed twice; purity not specified.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.5°C
soly. see experimental values above

REFERENCES:

COMPONENTS: (1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pyrene in water at 25°C was reported to be 0.135 mg(1) dm^{-3} sln and $x_1 = 1.2 \times 10^{-8}$.

The corresponding mass percent calculated by the compiler is 0.0000135 g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.005 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 12.2-31.3°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of pyrene in water

t/°C	10^7 mol(1) L^{-1}	10^6 g(1)/100 g sln (compiler)	$10^9 x_1$ (compiler)
12.2	2.70 ± 0.03	5.46	4.86
15.5	3.39 ± 0.03	6.86	6.11
17.4	3.91 ± 0.05	7.91	7.04
20.3	4.57 ± 0.04	9.25	8.23
23.0	5.78 ± 0.06	11.69	10.41
23.3	5.82 ± 0.03	11.77	10.48
25.0	6.40 ± 0.05	12.95	11.53
26.2	7.13 ± 0.07	14.42	12.84
26.7	7.18 ± 0.04	14.53	12.93
28.5	8.09 ± 0.08	16.37	16.90
31.3	9.3 ± 0.1	18.81	16.75

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. see above

REFERENCES:

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

Temperature: 25 and 29°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of pyrene in water

t/°C	mg(1)/kg(2)	10^5 g(1)/100 g sln (compiler)	$10^8 x_1$ (compiler)
25	0.132	1.32	1.18
29	0.162	1.62	1.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.01 mg(1)/kg(2)
(standard deviation)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

ORIGINAL MEASUREMENTS:

Rossi, S.S.; Thomas W.H.

Environ. Sci. Technol. 1981, *15*, 715-6.

VARIABLES:

One temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of pyrene in distilled water at 25°C was reported to be 0.13 μg/g, corresponding to a mole fraction, x_1, of 6.4×10^{-10}. The corresponding mass per cent calculated by the compiler is 1.3×10^{-5} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

500 mL of water and an excess of (1) were equilibrated for at least 24 h in a 1 L Erlenmeyer flask placed in a constant temperature (±0.1°C) gyrotary shaker (200 rpm). After a 12 h stationary equilibration period, 100 mL of saturated solution was drained through a glass-wool plug into a calibrated separatory funnel. Pyrene was isolated from solution by triplicate extraction with 10 mL of hexane (recovery >99%) and determined on a Hewlett-Packard Model 5840A gas chromatograph using a WCOTSP-2100 glass column (30 m x 0.25 mm i.d.). Hydrocarbon concentrations in extracts were additionally determined by UV spectrophotometry (Beckman ACTA MVI). Agreement between GC and UV analyses was typically within 2%. Further details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich; purified by derivatization with 2,4,6-trinitrophenol

(2) Doubly distilled in all-glass apparatus; free of trace organics.

ESTIMATED ERROR:

Temperature: ±0.1°C

Solubility: ±0.01 μg/g (std. dev. for 6 determinations)

REFERENCES:

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Seawater

EVALUATOR:

D.G. Shaw
Institute of Marine Science
University of Alaska
Fairbanks, Alaska USA

December 1982

CRITICAL EVALUATION:

The solubility of pyrene (1) in seawater (2) at 298 K has been reported in four works:

Authors	Methods	Salinity g salts/kg sln	10^6 g(1)100 g sln
Krasnoshchekova *et al.* (ref 1)	spectral	6	7.705
Schwarz (ref 2)	uv spectral	30	9.48
May *et al.* (ref 3)	HPLC	35	8.60
Rossi and Thomas (ref 4)	GLC	35	8.9

At 298 K and a salinity of 35 g salts/kg sln the data of May *et al.* and Rossi and Thomas are in very good agreement. Since the value reported by May *et al.* is more precise and derived from several measurements using the Setschenow equation, it is adopted as the recommended value for the solubility of pyrene in seawater at the temperature and salinity indicated. Rossi and Thomas and Schwarz each report data over a range of temperatures.

SOLUBILITY OF PYRENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

T/K	g salts/kg sln	10^6 g(1)/100 g sln
298	35	8.60

REFERENCES

1. Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.

2. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

3. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

4. Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* 1981, *15*, 715-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Salt Water	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of pyrene in salt water was reported to be 78.9 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 7.705×10^{-6} g(1)/100 g sln and 7.02×10^{-9} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

Not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 2.93
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

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

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.6-31.1°C

Salinity: 30 g(2)/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of pyrene in 0.5 g-mol(2)/dm^3

t/°C	10^7 mol(1)/L sln
8.6	2.00
12.2	2.50
15.5	2.85
18.2	3.22
20.7	3.57
23.0	3.90
25.0	4.41
28.1	5.19
31.1	5.96

The corresponding mass percent and mole fraction, x_1, at 25.0°C calculated by the compilers are 9.48×10^{-6} g(1)/100 g sln and 7.97×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of pyrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of pyrene to an air-tight 1 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 395 nm. The Spectrofluorimeter employed a ratio-photon counting mode where pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of pyrene in ethanol therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

Pyrene: purity > 99 mole %,

Sodium chloride: reagent grade,

Ethanol: reagent grade,

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column.

ESTIMATED ERROR:

Solubility ± 1.6% (author)

Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Pyrene; $C_{16}H_{10}$; [129-00-0] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of pyrene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_sC_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, K_s = 0.286 with S_o = 0.132.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 8.60×10^{-6} g(1)/100 g sln and 7.84×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	**SOURCE AND PURITY OF MATERIALS:**
A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.	(1) greater than 97% pure. (2) reagent grade. (3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.
	ESTIMATED ERROR: temp ± 0.05°C K_s ± 0.003 S_o ± 0.001
	REFERENCES:

COMPONENTS:

(1) Pyrene; $C_{16}H_{10}$; [129-00-0]

(2) Seawater; natural

ORIGINAL MEASUREMENTS:

Rossi, S.S.; Thomas, W.H.

Environ. Sci. Technol. 1981, *15*, 715-6.

VARIABLES:

Temperature: 15 - 25°C

Salinity: 35 g/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of pyrene in seawater

t/°C	μg(1)/g(2)	10^6Mass%[a] g(1)/100 g sln	10^9 x_1[a]
15	0.056	5.6	5.1
20	0.071	7.1	6.5
25	0.089	8.9	8.1

[a] calculated by compilers

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Saturated solution was prepared by equilibrating seawater with an excess of pyrene for at least 24 hr. in a constant-temperature gyrotary shaker followed by a 12 hr stationary equilibration period. A 100 mL aliquot was extracted three times with n-hexane. The concentrated hexane extract was analyzed by a gas chromatograph equipped with a flame ionization detector to determine the pyrene concentration.

SOURCE AND PURITY OF MATERIALS:

Pyrene: from Aldrich Chemical Co. and purified with 2,4,6-trinitrophenol.

n-Hexane: doubly distilled in glass.

Seawater: collected off Scripps Pier and was filtered twice through 0.22 μm membrane and twice extracted with n-hexane then its salinity was adjusted to 35%.

ESTIMATED ERROR:

Solubility ± 11%

Temperature ± 0.1°C

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 9,10-Dimethylanthracene; $C_{16}H_{14}$; [781-43-1] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 9,10-dimethylanthracene in water at 25°C was reported to be 0.056 mg(1) dm^{-3} sln and $x_1 = 4.90 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 5.6×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.0005 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 2,4,6-Trimethyl-2-phenylheptene; $C_{16}H_{26}$; [4810-06-4]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 10-30°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in 2,4,6-Trimethyl-2-phenylheptene

t/°C	g(2)/100 g sln	$10^3\ x_2$ (compiler)
10	0.0096	1.16
20	0.0154	1.87
30	0.0252	3.05

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified.

(2) Not specified.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:

(1) 7,8-Dimethyltetradecane; $C_{16}H_{34}$; [2801-86-7]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-50°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 7,8-dimethyltetradecane

t/°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
20	0.0077	9.67
30	0.0134	16.83
40	0.0219	27.48
50	0.0344	43.09

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the hexadecane (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1. Quantitative Solubility Studies of the Hexadecane (1) - Water (2) System

Reference	T/K	Solubility	Method
Schatzberg (ref 1)	298,313	(2) in (1)	Karl Fischer
Englin *et al.* (ref 2)	293-323	(2) in (1)	analytical
Franks (ref 3)	298	(1) in (2)	GLC
Yoshida and Yamane (ref 4)	-[a]	(1) in (2)	GLC
Skripka and Namiot (ref 5)	598[b]	(2) in (1)	-[a]
Sutton and Calder (ref 6)	298	(1) in (2)	GLC
Skripka and Sultanov (ref 7,8)	523-598[b]	(2) in (1)	-[a]

a Not specified.
b Pressure also varied.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. For convenience further discussion of this system will be divided into two parts.

1. THE SOLUBILITY OF HEXADECANE (1) IN WATER (2)

All data on the solubility of hexadecane in water have probably been obtained at 298 K (Table 1, although Yoshida and Yamane (ref 4) did not specify their temperature). However the values are in poor agreement and no "best" value has been calculated. It may also be noted that all values are higher than the value of ~2 x 10^{-9} g(1)/100 g sln predicted by extrapolation of lower hydrocarbon solubilities (although whether this extrapolation remains valid for very long chain hydrocarbons is not known).

TABLE 2. Reported Solubility Values of Hexadecane (1) in Water (2)

T/K	Reported values[a] 10^7 g(1)/100 g sln
298	6.3 (ref 3), 5.57[b] (ref 4), 0.9 (ref 6)

a No "best" value calculated due to uncertainties in data, see text.
b Temperature not specified.

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]
(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

June 1986

CRITICAL EVALUATION:

(continued)

2. THE SOLUBILITY OF WATER (2) IN HEXADECANE (1)

The solubility of water in hexadecane at atmospheric pressure have been reported by Schatzberg (ref 1) and Englin *et al.* (ref 2) over a range of temperatures. However, agreement is poor (Table 3) and the data must be considered as very Tentative.

TABLE 3. Tentative Solubility Values of Water (2) in Hexadecane (1)

T/K	Solubility values		
	Reported values	"Best" values ($\pm\sigma_n$)[b]	
	10^3 g(2)/100 g sln	10^3 g(2)/100 g sln	10^3 x_2
293	6.9 (ref 2)	7	0.9
298	5.4 (ref 1), 9.6[a] (ref 2)	8 ± 2	1.0
303	12.3 (ref 2)	12	1.5
313	10.4 (ref 1), 20.9 (ref 2)	16 ± 5	2.0
323	33.2	33	4.2

[a] Obtained by the Evaluator by graphical interpolation of the authors' data.

[b] Obtained by averaging where appropriate; σ_n has no statistical significance.

At higher pressures the solubility of water in hexadecane has been reported over the range 523-598 K and 1.7-78.5 MPa by Skripka *et al.* (ref 5, 7, 8). As these are the only data available under these conditions no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheet for the experimental values.

REFERENCES

1. Schatzberg, P. *J. Phys. Chem.* 1963, *67*, 776-9.
2. Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* 1965, *10*, 42-6.
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5. Skripka, V.G.; Namiot, A.Yu. *Zh. Fiz. Khim.* 1974, *48*, 782.
6. Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
7. Skripka, V.G.; *Tr. Vses. Neftegazov Nauch Issled. Inst.* 1976, *61*, 139-51.
8. Sultanov, R.G.; Skripka, V.G. *Zh. Fiz. Khim.* 1973, *47*, 1035.

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]

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

ORIGINAL MEASUREMENTS:

Schatzberg, P.

J. Phys. Chem. 1963, *67*, 776-9.

VARIABLES:

Temperature: 25-40°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in hexadecane

t/°C	mg(2)/kg sln	x_2
25	54[a]	6.8×10^{-4}
40	104[b]	13.1×10^{-4}

[a,b] See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) was saturated by storing over a layer of (2) in a brown glass bottle without any agitation. The bottle was sealed with serum cap and completely submerged in the water-bath for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe. Stabilized Karl Fischer reagent diluted to a titer of 1.0-1.3 mg(2)/mL was used to titrate (2) in (1) directly in the presence of methanol to a "dead-stop" end-point using a Beckman KF3 automatic titrimeter.

SOURCE AND PURITY OF MATERIALS:

(1) Humphrey-Wilkinson, Inc.; ASIM normal cetane; passed repeatedly through a column of silica gel until no absorption occurred in the 220 to 340 nm spectral range.

(2) distilled and deionized.

ESTIMATED ERROR:

temp. ± 0.02°C
soly. a) 0-6%; b) 0-2% (deviations from the mean)

REFERENCES:

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]

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

ORIGINAL MEASUREMENTS:

Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.

Khim. Tekhnol. Topl. Masel 1965, *10*, 42-6.

VARIABLES:

Temperature: 20-50°C

PREPARED BY:

A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in hexadecane

t/°C	g(2)/100 g sln	10^4x_2 (compiler)
20	0.0069	8.67
30	0.0123	15.45
40	0.0209	26.22
50	0.0332	41.59

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hours with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS: (1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Franks, F. *Nature (London)* <u>1966</u>, *210*, 87-8.
VARIABLES: One temperature: 25°C	**PREPARED BY:** F. Kapuku

EXPERIMENTAL VALUES:

The solubility of hexadecane in water at 25°C was reported to be in mole fraction $x_1 = 5 \times 10^{-10}$.
The corresponding mass percent calculated by the compiler is 6.3×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analysis was performed by gas liquid chromatography. After equilibrating the (1)/(2) mixtures in a thermostat, up to 0.5 mL of the aqueous phase was injected into the fractionator fitted to the chromatographic column, and (2) was removed by "Drierite". The (1) concentrations were obtained from the peak areas, after initial calibrations.

SOURCE AND PURITY OF MATERIALS:

(1) Fluka; purum grade; purity > 97% (chromatographic analysis).

(2) not specified.

ESTIMATED ERROR:

soly. ± 12%

REFERENCES:

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]

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

ORIGINAL MEASUREMENTS:

Yoshida, F.; Yamane, T.

Biotechnol. Bioeng. 1971, *13*, 691-6.

VARIABLES:

One temperature: not specified

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexadecane in water was reported to be 5.57 x 10^{-9} g(1) cm^{-3} sln.

With the assumption that a solution density of 1.00 g/cm, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5.57 x 10^{-7} g(1)/100 g sln and 4.45 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The analytical method was used. 10 mL of (1) and 1200 mL of (2) were placed in a stoppered flask and agitated with a magnetic stirrer at a speed of 200 rpm for 9 to 24 hrs. (1) was extracted from 1000 ml of (2) with 2 mL of heptane and its concentration determined by gas chromatography using a Shimadzu equipped with hydrogen flame detectors.

SOURCE AND PURITY OF MATERIALS:

not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-3]

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

ORIGINAL MEASUREMENTS:

Skripka, V.G.; Namiot, A.Yu.

Zh. Fiz. Khim. 1974, *48*, 782.

VARIABLES:

One temperature: 325°C
Pressure: 1.7-13.18 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in hexadecane at 325°C

p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
17.3	1.7	0.083	0.71
41.5	4.07	0.232	2.34
62.5	6.13	0.352	4.14
94.2	9.24	0.517	7.85
134.4	13.18	0.712	16.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Method was described in refs 1 and 2. Nothing more was reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; CP reagent; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Neft. Khoz.* 1972, *2*, 57.
2. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Gazov. Delo* 1972, *10*, 43.

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$ [544-76-3]

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

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

Environ. Sci. Technol. 1974, *8*, 654-7.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexadecane in water at 25°C was reported to be 0.9×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 0.7×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 μm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS:

(1) Hexadecane; $C_{16}H_{34}$; [544-76-5]

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

ORIGINAL MEASUREMENTS:

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

VARIABLES:

Temperature: 250-325°C
Pressure: 3.9-78.5 MPa

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES: Solubility of water in hexadecane

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
250	40	3.9	0.230	2.32
	53	5.2	0.227	2.28
	93	9.1	0.217	2.16
	100	9.8	0.216	2.14
	134	13.1	0.212	2.10
	150	14.7	0.211	2.08
	200	19.6	0.208	2.05
	300	29.4	0.197	1.91
	400	39.2	0.193	1.87
	500	49.0	0.190	1.83
	600	58.8	0.186	1.78
	700	68.6	0.182	1.74
	800	78.5	0.178	1.69
275	53	5.2	0.355	4.19
	93	9.1	0.345	4.02
	100	9.8	0.343	3.99
	134	13.1	0.336	3.87
	150	14.7	0.333	3.82
	200	19.6	0.325	3.69
	300	29.4	0.308	3.42
	400	39.2	0.290	3.15
	500	49.0	0.273	2.90
	600	58.8	0.260	2.72
	700	68.6	0.250	2.58
	800	78.5	0.244	2.50

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The experimental technique was described in ref 1. No details reported in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified, chemical reagent grade; purity not specified; used as received.

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Sultanov, R.G.; Skripka, V.G.; Namiot, A.Yu. *Gazov. Prom.* 1971, *4*, 6.

(1) Hexadecane; $C_{16}H_{34}$; [544-76-5]

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

Skripka, V.G.
Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1976, *61*, 139-51.

Sultanov, R.G.; Skripka, V.G.
Zh. Fiz. Khim. 1973, *47*, 1035.

t/°C	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
300	93	9.1	0.517	7.84
	100	9.8	0.505	7.51
	134	13.1	0.480	6.84
	150	14.7	0.469	6.56
	200	19.6	0.441	5.90
	300	29.4	0.404	5.11
	400	39.2	0.384	4.72
	500	49.0	0.366	4.39
	600	58.8	0.348	4.07
	700	68.6	0.329	3.75
	800	78.5	0.310	3.45
325	134	13.1	0.712	16.43
	150	14.7	0.643	12.53
	200	19.6	0.571	9.57
	300	29.4	0.509	7.62
	400	39.2	0.480	6.84
	500	49.0	0.466	6.49
	600	58.8	0.450	6.11
	700	68.6	0.435	5.77
	800	78.5	0.414	5.32

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexadecane; $C_{16}H_{34}$; [544-76-3] (2) Seawater	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of hexadecane in seawater was reported to be 4×10^{-8} g(1)/100 g sln and $x_1 = 3 \times 10^{-11}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]fluorene; $C_{17}H_{12}$; [238-84-3] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of Benzo[a]fluorene in water at 25°C was reported to be 0.045 mg(1) dm^{-3} sln and x_1 = 3.75 x 10^{-9}.

The corresponding mass percent calculated by the compiler is 4.5 x 10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.0012 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[b]fluorene; $C_{17}H_{12}$; [243-17-4] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzo[b]fluorene in water at 25°C was reported to be 0.0020 mg(1) dm^{-3} sln and $x_1 = 9.56 \times 10^{-10}$.

The corresponding mass percent calculated by the compiler is 2.0×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 3 x 10^{-5} mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for benz[a]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in bena[a]anthracene.

TABLE 1. Quantitative Solubility Studies of Benz[a]anthracene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May *et al.* (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. In general the available data are in good agreement given the very low solubility of benz[a]anthracene in water. Although the data of Mackay and Shiu is somewhat higher than all other values there are at the present time insufficient grounds for its rejection. The available data are summarized in Table 2 and may be regarded as Tentative.

TABLE 2. Tentative Solubility Values of Benz[a]anthracene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	10^6 g(1)/100 g sln	10^6 g(1)/100 g sln	10^{10} x_1
298	0.983 (ref 2), 1.4 (ref 3), 0.94 (ref 4)	1.1 ± 0.2	9
300	1.1 (ref 1)	1.1	9
302	1.22 (ref 4)	1.2	9

a Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

(continued)

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
4. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of benz[a]anthracene in water

t/°C	10^5 g(1) L^{-1} (2)
27	1.1
	1.1
	1.2

The best value recommended by the authors is 1.1 x 10^{-5} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction calculated by the compiler are 1.1 x 10^{-6} g(1)/100 g sln and 8.7 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 161.4-161.8°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.1 x 10^{-5} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benz[a]anthracene in water at 25°C was reported to be 10^{-5} g(1) L^{-1} sln and 4.31 x 10^{-8} mol(1) L^{-1} sln. Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 9.83 x 10^{-7} g(1)/ 100 g sln and 7.78 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benz[a]anthracene in water at 25°C was reported to be 0.014 mg(1) dm^{-3} sln and $x_1 = 1.1 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 1.4×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.0002 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

Temperature: 25 and 29°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benz[a]anthracene in water

t/°C	mg(1)/kg(2)	10^6 g(1)/100 g sln (compiler)	$10^{10}x_1$ (compiler)
25	0.0094	0.94	7.4
29	0.0122	1.22	9.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Haas, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.001 mg(1)/kg(2) (stand. dev.)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$; [55-56-3]

(2) Seawater

EVALUATOR:

D.G. Shaw
Institute of Marine Science
University of Alaska
Fairbanks, Alaska USA

December 1982

CRITICAL EVALUATION:

The solubility of benz[a]anthracene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10^7 g(1)/100 g sln
Krasnoshchekova *et al.* (ref 1)	spectral	6	0.62
May *et al.* (ref 2)	HPLC	35	5.6

The value reported by May *et al.* was derived from several measurements using the Setschenow equation and is consistent with the recommended value for the solubility of benz[a]anthracene in pure water. Therefore their value is adopted as tentative. The value of Krasnoshchekova *et al.* appears slightly low and is considered doubtful.

SOLUBILITY OF BENZ[A]ANTHRACENE (1) IN SEAWATER (2)
TENTATIVE VALUE

T/K	g salts/kg sln	10^7 g(1)/100 g sln
298	35	5.6

REFERENCES

1. Krasnoshchekova, R.Ya.; Pakpill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.

2. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

(2) Salt Water

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.

Khim. Tverd. Topl. 1977, *11*(2), 133-6.

VARIABLES:

One temperature: 25°C

Salinity: 6 g/kg sln (ref. 1)

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of benz[a] anthracene in salt water was reported to be 0.63 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 6.2×10^{-8} g(1)/100 g sln and 5.2×10^{-11} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

Not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.075
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3] (2) Sodium Chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 0-40 g(2)/kg sln	W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of benz[a]anthracene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, $K_s = 0.354$ with $S_o = 0.0094$.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 5.6×10^{-7} g(1)/100 g sln and 4.5×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C
K_s ± 0.002
S_o ± 0.001

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Chrysene; $C_{18}H_{12}$; [218-01-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for chrysene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in chrysene.

TABLE 1. Quantitative Solubility Studies of Chrysene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric
May *et al.* (ref 4)	298,302	chromatographic

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of Klevens (ref 2) value at 298K, which is very much higher than other studies (ref 3,4) and is therefore rejected, all the available data are summarized in Table 2 below. The solubilities are in reasonable agreement although their limited number and temperature range suggests a Tentative classification at this stage.

TABLE 2. Tentative Solubility Values for Chrysene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values $(\pm\sigma_n)^a$	
	10^7 g(1)/100 g sln	10^7 g(1)/100 g sln	10^{10} x_1
298	2.0 (ref 3), 1.8 (ref 4)	1.9 ± 0.1	1.5
300	1.5 (ref 1)	1.5	1.2
302	2.2 (ref 4)	2.2	1.7

a Obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
A. Maczynski, Institute of Physical Chemistry of the Polish Academy of Sciences, Warszawa, Poland.

June 1986.

CRITICAL EVALUATION: (continued)

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
4. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* 1978, *50*, 997-1000.

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of chrysene in water

t/°C	10^6 g(1) L^{-1} (2)
27	1.5 ± 0.5
	1.5 ± 0.2

The best value recommended by the authors is 1.5 x 10^{-6} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.5 x 10^{-7} g(1)/100 g sln and 1.2 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 253.2-253.8°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

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

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of chrysene in water at 25°C was reported to be 6×10^{-6} g(1) L^{-1} sln and 2.76×10^{-8} mol(1) L^{-1} sln.
Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 6.29×10^{-7} g(1)/100 g sln and 4.98×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of chrysene in water at 25°C was reported to be 0.0020 mg(1) dm^{-3} sln and $x_1 = 1.58 \times 10^{-10}$.

The corresponding mass percent calculated by the compiler is 2.0×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.00017 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

Temperature: 25 and 29°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of chrysene in water

t/°C	mg(1)/kg(2)	10^7 g(1)/100 g sln (compiler)	$10^{10}x_1$ (compiler)
25	0.0018	1.8	1.4
29	0.0022	2.2	1.7

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The dynamic coupled column liquid chromatography (DCCLC) method was based on generating saturated solutions by pumping water through a column packed with glass beads that have been coated with the component (1) (generator column). The concentration of (1) in the effluent of the generator column was measured by a modification of the coupled column liquid chromatographic process that has been described in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) commercial product; less than 3% impurities.

(2) distilled over $KMnO_4$ and NaOH and passed through a column packed with XAD-2 (Rohm and Hass, Philadelphia, Pa).

ESTIMATED ERROR:

temp. ± 0.05°C
soly. ± 0.001 mg(1)/kg(2)
(standard deviation)

REFERENCES:

1. May, W.; Chesler, S.; Cram, S.; Gump, B.; Hertz, H.; Enagonio, D.; Dyszel, S. *J. Chromatogr. Sci.* 1975, *13*, 535.

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

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

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

ORIGINAL MEASUREMENTS:

May, W.E.; Wasik, S.P.; Freeman, D.H.

Anal. Chem. 1978, *50*, 997-1000.

VARIABLES:

One temperature: 25°C

Salinity: 0-40 g(2)/kg sln

PREPARED BY:

W.Y. Shiu and D. Mackay

EXPERIMENTAL VALUES:

The solubility of chrysene in aqueous sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_o/S) = K_s C_s$$

where;

S_o is the solubility of (1) in water (mg/L)

S is the solubility of (1) in saline solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s in the concentration of sodium chloride (mol/L)

evaluating the equation for S over the range of C_s 0-0.7 mol/L, $K_s = 0.336$ with $S_o = 0.0018$.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 1.1×10^{-7} g(1)/100 g sln and 8.8×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) was prepared by pumping salt water through a "generation column" which was packed with glass beads coated with 1% by weight of (1). The saturated solution was extracted with an "extractor column" packed with a superficially porous bonded C_{18} stationary phase, then a water-acetonitrile solvent was passed through for extraction. The extract was introduced into a liquid chromatograph and the concentration of (1) was measured with a UV detector.

SOURCE AND PURITY OF MATERIALS:

(1) greater than 97% pure.

(2) reagent grade.

(3) distilled from potassium permanganate-sodium hydroxide and passed through an XAD-2 column.

ESTIMATED ERROR:

temp ± 0.05°C

K_s ± 0.010

S_o ± 0.0001

REFERENCES:

COMPONENTS:

(1) Naphthacene; $C_{18}H_{12}$; [92-24-0]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
A. Maczynski, Institute of Physical Sciences, Warszawa, Poland.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for naphthacene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in naphthacene.

TABLE 1. Quantitative Solubility Studies of Naphthacene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

The data are also summarized in Table 2 below. The reported values are in poor agreement. The value of Mackay and Shiu (ref 3) being lower than the other reported values (ref 1,2) is preferred as the Tentative solubility at 298K.

TABLE 2. Tentative Solubility Value of Naphthacene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value	
	10^8 g(1)/100 g sln	10^8 g(1)/100 g sln	10^{11} x_1
298	15^a (ref 2), 5.7 (ref 3)	6	5
300	10^a (ref 1)		

a Values probably high.

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) Naphthacene; $C_{18}H_{12}$; [92-24-0]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.;
Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*,
108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of naphthacene in water

t/°C	10^6 g(1) L^{-1} (2)
27	1.0 ± 0.5
	1.0 ± 0.2

The best value recommended by the authors is 1.0 x 10^{-6} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.-0 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.0 x 10^{-7} g(1)/ 100 g sln and 7.9 x 10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 341.5-343.0°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of naphthacene in water at 25°C was reported to be 6.6×10^{-9} mol(1) L^{-1} sln.

Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction calculated by the compiler are 1.5×10^{-7} g(1)/100 g sln and 1.2×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Naphthacene; $C_{18}H_{12}$; [92-24-0] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of naphthacene in water at 25°C was reported to be 0.00057 mg(1) dm^{-3} sln and $x_1 = 3.7 \times 10^{-11}$.

The corresponding mass percent calculated by the compiler is 5.7×10^{-8} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.00003 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. A. Maczynski, Institute of Physical Sciences, Warszawa, Poland. June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for triphenylene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in triphenylene.

TABLE 1. Quantitative Solubility Studies of Triphenylene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The reported data which are summarized in Table 2 are in excellent agreement. However the solubility values are not sufficiently well characterized, at this stage, to justify Recommending the average value.

TABLE 2. Tentative Solubility Value of Triphenylene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" value	
	10^6 g(1)/100 g sln	10^6 g(1)/100 g sln	10^9 x_1
298	4.28 (ref 2), 4.3 (ref 3)	4.3	3.4
300	3.8[a] (ref 1)	-	-

[a] Datum not sufficiently well characterized to justify inclusion in "best" values.

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
3. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of triphenylene in water

t/°C	10^5 g(1) L^{-1} (2)
27	3.8 ± 0.8
	3.6 ± 0.4
	4.0 ± 0.4

The best value recommended by the authors is 3.8 x 10^{-5} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.8 x 10^{-6} g(1)/ 100 g sln and 3.0 x 10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 197.5-197.9°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Triphenylene; $C_{18}H_{12}$; [217-59-4] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.
VARIABLES:	**PREPARED BY:**
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of triphenylene in water at 25°C was reported to be 4.3×10^{-5} g(1) L^{-1} sln and 1.88×10^{-7} mol(1) L^{-1} sln. Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.28×10^{-6} g(1)/100 g sln and 3.39×10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	**SOURCE AND PURITY OF MATERIALS:**
The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	not specified.
	REFERENCES:

COMPONENTS:

(1) Triphenylene; $C_{18}H_{12}$; [217-59-4]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of triphenylene in water at 25°C was reported to be 0.043 mg(1) dm^{-3} sln and $x_1 = 3.39 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 4.3×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.00017 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Octadecane; $C_{18}H_{38}$; [593-45-3]
(2) Water; H_2O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for octadecane (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in octadecane.

TABLE 1. Quantitative Solubility Studies of Octadecane (1) in Water (2)

Reference	T/K	Method
Baker (ref 1)	298-353	radiotracer
Baker (ref 2)	298	radiotracer
Baker (ref 3)	298	not specified
Sutton and Calder (ref 4)	298	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

With the exception of the graphical (ref 1) and v/v data (ref 3) reported by Baker which have been excluded from consideration, all the available data (ref 2,4) are summarized in Table 2 below. The reported values are in poor agreement and both are several orders of magnitude higher than would be predicted by an extrapolation of the lower n-alkane solubilities, *viz.* ~ 10^{-10} g(1)/100 g sln, although the validity of this extrapolation is unknown. Nevertheless it must be recognized that the reported values *may* be substantially in error and no "best" value has been suggested.

TABLE 2. Reported Values of the Solubility of Octadecane (1) in Water (2)

T/K	Reported values[a]	
	10^7 g(1)/100 g sln	10^{10} x_1
298	6 (ref 2), 2.1 (ref 4)	4.2 (ref 2), 1.5 (ref 4)

[a] No "best" values suggested because of possible errors in data; see text.

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water ; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

CRITICAL EVALUATION:

(continued)

REFERENCES

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints - Symposia* 1956, *1*, No.2, 5-17.
2. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints* 1958, *3*, No.4, C61-8.
3. Baker, E.G. *Science* 1959, *129*, 871-4.
4. Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]	Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia* 1956, *1*, N°2, 5-17.
VARIABLES:	**PREPARED BY:**
Temperature: 5-80°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported that the solubility of octadecane in water increases from about 55 ppb by weight at room temperature to twice this amount at 80°C. A graph reporting the mole fraction x_1 a function of the reciprocal absolute temperature is given.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Tritio-octadecane was used as radioactive tracer. 0.01 of active (1) was shaken with (2); the mixture was filtered through a 0.05 μm filter; 0.01 mL of filtrate was vaporized in hot oxygen and passed over CuO at 600°C; the H_2O-T_2O derived from the vaporized solvent as well as from the combusted (1) was trapped at -78°C; the melted ice was reduced by Zn and the gas was counted. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) tritio-octadecane prepared by hydrogenating octadecene-1 with tritium; 100 curies of tritium were introduced per mole of (1).

(2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Octadecane; $C_{18}H_{38}$; [593-45-3]

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

ORIGINAL MEASUREMENTS:

Baker, E.G.

Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, *3*, N°4, C61-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of octadecane-1,2-H^3 in water at 25°C was reported to be 6 x 10^{-9} g(1)/g(2) and that of octadecane-1-C^{14} 5.7 x 10^{-9} g(1)/g(2).
The corresponding mass fraction and mole fraction, x_1, calculated by the compiler are 6 x 10^{-7} g(1)/100 g sln and 4 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Tritiated or carbon-14 labeled (1) was used as tracer. The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1. A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

SOURCE AND PURITY OF MATERIALS:

(1) Octadecane-1,2-H^3 from Tracer Lab.; percolated through silica gel.
Octadecane-1-C^{14} from Nuclear Instrument and Chemical Corporation; used as received.

(2) distilled.

ESTIMATED ERROR:

soly. 20% (standard deviation from 17 replicate runs).

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc., Div. Petrol. Chem., Preprints-Symposia* 1956, *1*, N°2, 5.

COMPONENTS: (1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Baker, E.G. *Science* 1959, *129*, 871-4.
VARIABLES: One temperature: 25°C	**PREPARED BY:** F. Kapuku

EXPERIMENTAL VALUES:

The solubility of octadecane in water at 25°C was reported to be 7.75×10^{-7} mL(1)/100 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: not specified.	**SOURCE AND PURITY OF MATERIALS:** not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Water; H_2O; [7732-18-5]	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of octadecane in water at 25°C was reported to be 2.1×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 1.5×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 μm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS: (1) Octadecane; $C_{18}H_{38}$; [593-45-3] (2) Seawater	**ORIGINAL MEASUREMENTS:** Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES: One temperature: 25°C One salinity: 35 g salts/kg sln	**PREPARED BY:** P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of octadecane in seawater was reported to be 8×10^{-8} g(1)/100 g sln and $x_1 = 5 \times 10^{-11}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES:

COMPONENTS:

(1) 1-Methylbenz[a]anthracene; $C_{19}H_{14}$; [2498-77-3]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 1-methylbenz[a]anthracene in water

t/°C	10^5 g(1) L^{-1} (2)
27	5.5 ± 0.2
	5.4 ± 0.4
	5.5 ± 0.2

The best value recommended by the authors is 5.5×10^{-5} g(1) L^{-1} (2). Assuming that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5.5×10^{-6} g(1)/100 g sln and 4.1×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 138.5-139.0°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc* 1940, *62*, 3086.

COMPONENTS:

(1) 9-Methylbenz[a]anthracene; $C_{19}H_{14}$; [2381-16-0]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 9-methylbenz[a]anthracene in water at 27°C was reported to be 6.6×10^{-5} g(1) L^{-1} (2).
(Two identical results have been obtained)
With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 6.6×10^{-6} g(1)/100 g sln and 4.5×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 138.0-138.8°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.3×10^{-5} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 10-Methylbenz[a]anthracene; $C_{19}H_{14}$; [2381-15-9]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 10-methylbenz[a]anthracene in water at 27°C was reported to be 5.5×10^{-5} g(1) L^{-1} (2).
(Four identical results have been obtained)
With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5.5×10^{-6} g(1)/100 g sln and 4.1×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 140.0-140.5°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.5×10^{-5} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 5-Methylchrysene; $C_{19}H_{14}$; [3697-24-3]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 5-methylchrysene in water

t/°C	10^5 g(1) L^{-1} (2)
27	6.5 ± 0.5
	6.5 ± 0.5
	5.8 ± 0.5
	5.5 ± 0.5
	6.1 ± 0.3
	6.2 ± 0.3

The best value recommended by the authors is 6.2 x 10^{-5} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 6.2 x 10^{-6} g(1)/100 g sln and 4.6 x 10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at the Ohio State University; m.p. range 117.3-117.7°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, 1940, *62*, 3086.

COMPONENTS:

(1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
A. Maczynski, Institute of Physical Sciences, Warszawa, Poland.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for benzo[a]pyrene (1) in water (2) have been reported in the publications listed in Table 1. No data have been reported on the solubility of water in benzo[a]pyrene.

TABLE 1. Quantitative Solubility Studies of Benzo[a]pyrene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Mackay and Shiu (ref 2)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. It can be seen from Table 2 that the reported solubility values are in good agreement, given that they have been measured at slightly different temperatures. However, further studies are required before any data can be Recommended.

TABLE 2. Tentative Solubility Values of Benzo[a]pyrene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values	
	10^7 g(1)/100 g sln	10^7 g(1)/100 sln	10^{10} x_1
298	3.8 (ref 2)	3.8	2.7
300	4.0 (ref 1)	4.0	2.9

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of benzo[a]pyrene in water

t/°C	10^6 g(1) L^{-1} (2)
27	3.0 ± 0.5
	4.5 ± 0.5
	4.0 ± 0.1
	4.0 ± 0.5
	3.5 ± 0.5

The best value recommended by the authors is 4.0 x 10^{-6} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction calculated by the compiler are 4.0 x 10^{-7} g(1)/100 g sln and 2.9 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Hoffman La-Roche; used as received; m.p. range 176.3-177.0°C, (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzo[a]pyrene in water at 25°C was reported to be 0.0038 mg(1) dm^{-3} sln and $x_1 = 2.73 \times 10^{-10}$.

The corresponding mass percent calculated by the compiler is 3.8×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.00031 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8]

(2) Salt Water

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.

Khim. Tverd. Topl. 1977, *11*, 133-6.

VARIABLES:

One temperature: 25°C

Salinity: 6 g/kg sln (ref. 1)

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of benzo[a]pyrene in salt water was reported to be 0.13 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 1.3×10^{-8} g(1)/100 g sln and 9.5×10^{-12} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

Not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.008
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973,

COMPONENTS:

(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2]

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.6-31.7°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzo[e]pyrene in water

t/°C	10^8 mol(1) L	10^7 g(1)/100 g sln (compiler)	$10^{10}x_1$ (compiler)
8.6	1.29 ± 0.07	3.25	2.32
14.0	1.42 ± 0.05	3.58	2.56
17.0	1.76 ± 0.13	4.44	3.17
17.5	1.56 ± 0.08	3.94	2.81
20.0	1.82 ± 0.09	4.59	3.28
20.2	1.90 ± 0.14	4.79	3.42
23.0	2.01 ± 0.20	5.07	3.62
23.2	2.12 ± 0.10	5.35	3.82
29.2	2.55 ± 0.02	6.43	4.59
31.7	2.70 ± 0.15	6.81	4.86

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Two methods were used.

At 25°C the solubility of (1) in (2) was determined from UV absorption measurements and was used as a standard at other temperatures. At other temperatures the spectrofluorimetry method was used.

The sealed fluorescence cells contained 5 mL of the aqueous solution and an excess of (1) were rotated at least 72 h in a water bath, then removed, quickly wiped dry and placed in the fluorimeter.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; better than 99 mole%, by glc; used as received.

(2) distilled over $KMnO_4$ and NaOH and passed through a Sephadex column.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. see above

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of benzo[e]pyrene (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	10^7 g(1)/100 g sln
Krasnoshchekova *et al.* (ref 1)	spectral	6	1.79
Schwarz (ref 2)	uv spectral	30	3.32

The two reported values are in fair agreement and therefore both are adopted as tentative at their respective salinities. Schwarz also provides data over the temperature range 282-303 K.

SOLUBILITY OF BENZO[E]PYRENE (1) IN SEAWATER (2)
TENTATIVE VALUES

T/K	g salts/kg sln	10^7 g(1)/100 g sln
298	6	1.79
298	30	3.32

REFERENCES

1. Krasnoshchekova, R.Ya.; Pakpill, Yu.A; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.
2. Schwarz, F.P. *J. Chem. Eng. Data* 1977, *22*, 273-7.

COMPONENTS:

(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2]

(2) Salt Water

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.

Khim. Tverd. Topl. 1977, *11*, 133-6.

VARIABLES:

One temperature: 25°C

Salinity: 6 g/kg sln (ref. 1)

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of Benzo[e]pyrene in salt water was reported to be 1.83 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 1.79×10^{-7} g(1)/100 g sln and 1.34×10^{-10} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

Not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.111
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Benzo[e]pyrene; $C_{20}H_{12}$; [192-97-2]

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

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

ORIGINAL MEASUREMENTS:

Schwarz, F.P.

J. Chem. Eng. Data 1977, *22*, 273-7.

VARIABLES:

Temperature: 8.9-30.2°C

Salinity: 30 g(2)/kg sln

PREPARED BY:

W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of benzo[e]pyrene in 0.5 mol(2)/L

t/°C	10^8 mol(1)/L sln
8.9	0.82
10.8	0.88
15.6	1.01
17.0	1.01
19.2	1.04
21.7	1.13
25.3	1.35
27.1	1.42
30.2	1.66

The corresponding mass percent and mole fraction, x_1, at 25.3°C calculated by the compilers are 3.32×10^{-7} g(1)/100 g sln and 2.44×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of benzo[e]pyrene in NaCl solution was determined by fluorescence and UV absorption measurements. In the fluorescence method, saturated solution was prepared by adding excess amount of benzo[e]pyrene to an air-tight 1 x 1 cm quartz fluorescence cell containing 5 mL salt solution. The cell was rotated at 20 rpm for at least 72 hr in a thermostated water bath and then its fluorescent intensity was measured at 410 and 265 nm. The Spectrofluorimeter employed a ratio-photon counting mode where benzo[e]-pyrene concentration was linearly related to the fluorescence signal. The UV method was used to obtain the absorptivity of benzo[e]pyrene in cyclohexane therefore provide an absolute solubility scale for the fluorescence method.

SOURCE AND PURITY OF MATERIALS:

Benzo[e]pyrene: purity > 99 mole %,

Sodium chloride: reagent grade,

Water: distilled over a $KMnO_4$ - NaOH solution and passed through a Sephadex column,

Cyclohexane: reagent grade.

ESTIMATED ERROR:

Solubility ± 19.5% (author)

Temperature ± 0.1°C (author)

REFERENCES:

COMPONENTS:

(1) Perylene; $C_{20}H_{12}$; [198-55-0]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of perylene in water at 25°C was reported to be 0.0004 mg(1) dm^{-3} sln and $x_1 = 2.83 \times 10^{-11}$.

The corresponding mass percent calculated by the compiler is 4×10^{-8} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 2×10^{-5} mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Cholanthrene; $C_{20}H_{14}$; [479-23-2]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cholanthrene in water at 27°C was reported to be 3.5×10^{-6} g(1) L^{-1} (2). (Two identical results were obtained). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 3.5×10^{-7} g(1)/100 g sln and 2.5×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 170.1-170.6°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.5×10^{-6} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 7,12-Dimethylbenz[a]anthracene; $C_{20}H_{16}$; [57-97-6]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 7,12-dimethylbenz[a]anthracene in water at 25°C was reported to be 0.061 mg(1) dm^{-3} sln and $x_1 = 4.26 \times 10^{-9}$.

The corresponding mass percent calculated by the compiler is 6.1×10^{-6} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.0006 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) 9,10-Dimethylbenz[a]anthracene; $C_{20}H_{16}$; [56-56-4]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 9,10-dimethylbenz[a]anthracene in water

t/°C	10^5 g(1) L^{-1} (2)
27	4.3 ± 0.2
	4.5 ± 0.4
	4.5 ± 0.1
	4.3 ± 0.3
	3.9 ± 0.4

The best value recommended by the authors is 4.3 x 10^{-5} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.3 x 10^{-6} g(1)/100 g sln and 3.0 x 10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 122.6-122.9°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 10-Ethylbenz[a]anthracene; $C_{20}H_{16}$; [14854-08-1]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 10-ethylbenz[a]anthracene in water

t/°C	10^5 g(1) L^{-1} (2)
27	4.5 ± 0.5
	4.5 ± 0.5
	3.5 ± 0.5
	4.5 ± 0.3
	4.5 ± 0.5
	4.0 ± 0.5
	4.0 ± 0.8

The best value recommended by the authors is 4.5 x 10^{-5} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.5 x 10^{-6} g(1)/100 g sln and 3.2 x 10^{-9}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 112.4-112.8°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Eicosane; $C_{20}H_{42}$; [112-95-8] (2) Water; H_2O; [7732-18-5]	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of eicosane in water at 25°C was reported to be 1.9×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 1.1×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 μm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Eicosane; $C_{20}H_{42}$; [112-95-8] (2) Seawater	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C One salinity: 35 g salts/kg sln	P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of eicosane in seawater was reported to be 8×10^{-8} g(1)/100 g sln and $x_1 = 5 \times 10^{-11}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 μm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES:

COMPONENTS:

(1) 5-Methylbenzo[a]pyrene; $C_{21}H_{14}$; [2319-96-2]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 5-methylbenzo[a]pyrene in water

t/°C	10^7 g(1) L^{-1} (2)
27	8 ± 2
	10 ± 4
	8 ± 2

The best value recommended by the authors is 8 x 10^{-7} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 8 x 10^{-8} g(1)/100 g sln and 6 x 10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 216.6-217.3°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 3-Methylcholanthrene; $C_{21}H_{16}$; [56-49-5]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
A. Maczynski, Institute of Physical Sciences, Warszawa, Poland.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for 3-methylcholanthrene (1) in water (2) have been reported in the publications listed in Table 1. No data are available on the solubility of water in 3-methylcholanthrene.

TABLE 1. Quantitative Solubility Studies of 3-Methylcholanthrene (1) in Water (2)

Reference	T/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Mackay and Shiu (ref 3)	298	spectrofluorometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. Unfortunately, the available data, obtained at slightly different temperatures are in poor agreement. Although the values of Mackay and Shiu (ref 2) are generlly more reliable than those of Davis *et al.* (ref 1) the system is not sufficiently well-characterized to justify a preference at this stage and no "best" values have been nominated.

TABLE 2. Reported Solubility Values of 3-Methylcholanthrene (1) in Water (2)

T/K	Reported values^a	
	10^7 g(1)/100 g sln	10^{10} x_1
298	2.9 (ref 2)	1.9 (ref 2)
300	1.5 (ref 1)	1.0 (ref 1)

a No "best" values nominated because of uncertainties in the available data, see text.

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.

COMPONENTS:

(1) 3-Methylcholanthrene; $C_{21}H_{16}$; [56-49-5]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 3-methylcholanthrene in water

$t/°C$	10^6 g(1) L^{-1} (2)
27	1.3
	1.8
	1.8

The best value recommended by the authors is 1.5 x 10^{-6} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.5 x 10^{-7} g(1)/100 g sln and 1.0 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Hoffman La-Roche; used as received; m.p. range 175.3-177.1°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 0.3 x 10^{-6} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylcholanthrene; $C_{21}H_{16}$; [56-49-5] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylcholanthrene in water at 25°C was reported to be 0.0029 mg(1) dm^{-3} sln and $x_1 = 1.92 \times 10^{-10}$.

The corresponding mass percent calculated by the compiler is 2.9×10^{-7} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 0.000021 mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2]

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

ORIGINAL MEASUREMENTS:

Mackay, D.; Shiu, W.Y.

J. Chem. Eng. Data 1977, *22*, 399-402.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzo[ghi]perylene in water at 25 °C was reported to be 0.00026 mg(1) dm^{-3} sln and $x_1 = 1.73 \times 10^{-11}$.

The corresponding mass percent calculated by the compiler is 2.6×10^{-8} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 10^{-5} mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:

(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2]

(2) Salt Water

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.

Khim. Tverd. Topl. 1977, *11*, 133-6.

VARIABLES:

One temperature: 25°C

Salinity: 6 g/kg sln (ref. 1)

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of benzo[ghi]perylene in salt water was reported to be 0.21 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 2.1×10^{-8} g(1)/100 g sln and 1.4×10^{-11} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

Not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 0.048
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Benzo[b]triphenylene; $C_{22}H_{14}$; [215-58-7]

(2) Salt Water

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.

Khim. Tverd. Topl. 1977, *11*, 133-6.

VARIABLES:

One temperature: 25°C

Salinity: 6 g/kg sln (ref. 1)

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of benzo[b]triphenylene in salt water was reported to be 27.84 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 2.719×10^{-6} g(1)/100 g sln and 1.841×10^{-9} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

not given.

ESTIMATED ERROR:

temp. ± 1°C

soly. ± 1.48

type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [58-70-3]

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

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

June 1986.

CRITICAL EVALUATION:

Quantitative solubility data for dibenz[a,h]anthracene (1) in water (2) have been reported in the publications listed in Table 1. No data are available for the solubility of water in dibenz[a,h]anthracene.

TABLE 1. Quantitative Solubility Studies of Dibenz[a,h]anthracene (1) in Water (2)

Reference	*T*/K	Method
Davis *et al.* (ref 1)	300	nephelometric
Klevens (ref 2)	298	spectrophotometric

The original data and related information in both of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. The data are also summarized in Table 2 below. The two reported values, although obtained at slightly different temperatures, are in excellent agreement. Nevertheless there are insufficient data and the system is insufficiently well-characterized to justify a higher than Tentative classification.

TABLE 2. Tentative Solubility Values of Dibenz[a,h]anthracene (1) in Water (2)

T/K	Solubility values		
	Reported values	"Best" values	
	10^8 g(1)/100 g sln	10^8 g(1)/100 g sln	10^{11} x_1
298	5.84 (ref 2)	6	4
300	5 (ref 1)	5	3

REFERENCES

1. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1942, *64*, 108-10.
2. Klevens, H.B. *J. Phys. Chem.* 1950, *54*, 283-98.

COMPONENTS:

(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [58-70-3]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of dibenz[a,h]anthracene in water at 27°C was reported to be 5×10^{-7} g(1) L^{-1} (2).

(Two identical results have been obtained)

With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5×10^{-8} g(1)/100 g sln and 3×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed.
Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) Eastman Kodak Company; purified; m.p. range 266.6-266.9°C or Hoffman La Roche; m.p. range 262.7-264°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. ± 10^{-7} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [58-70-3]

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

ORIGINAL MEASUREMENTS:

Klevens, H.B.

J. Phys. Chem. 1950, *54*, 283-98.

VARIABLES:

Temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of dibenz[a,h]anthracene in water at 25°C was reported to be 2.15×10^{-9} mol(1) L^{-1} sln.
With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5.84×10^{-8} g(1)/100 g sln and 3.88×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long as three months. Aliquots were removed and concentrations determined by spectra.

SOURCE AND PURITY OF MATERIALS:

(1) not specified.

(2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

COMPONENTS:

(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [53-70-3]

(2) Salt Water

ORIGINAL MEASUREMENTS:

Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya.

Khim. Tverd. Topl. 1977, *11*, 133-6.

VARIABLES:

One temperature: 25°C

Salinity: 6 g/kg sln (ref. 1)

PREPARED BY:

M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of dibenz[a,h]anthracene in salt water was reported to be 21.13 μg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 2.064×10^{-6} g(1)/100 g sln and 1.397×10^{-9} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

Not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 1.14
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*,

COMPONENTS:

(1) Dibenz[a,j]anthracene; $C_{22}H_{14}$; [224-41-9]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of dibenz[a,j]anthracene in water

t/°C	10^5 g(1) L^{-1} (2)
27	1.1 ± 0.1
	1.0 ± 0.2
	1.3 ± 0.2

The best value recommended by the authors is 1.2 x 10^{-5} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.2 x 10^{-6} g(1)/100 g sln and 7.8 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2).
A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at the Ohio State University; m.p. range 198.0-198.4°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dibenz[a,j]anthracene; $C_{22}H_{14}$; [224-41-9] (2) Salt Water	Krasnoshchekova, R.Ya.; Pakhapill, Yu.A.; Gubergrits, M.Ya. *Khim. Tverd. Topl.* 1977, *11*, 133-6.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C Salinity: 6 g/kg sln (ref. 1)	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of dibenz[a,j]anthracene in salt water was reported to be 10.544 µg/L.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 1.029×10^{-6} g(1)/100 g sln and 6.970×10^{-10} assuming a solution density of 1.004 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

1 L of a 0.5 g/L solution of the hydrocarbon in acetone was distributed over the inside surface of a 1-L round-bottomed flask; the acetone was evaporated with gentle heating. 0.5 L water [or salt water] was added to the dried residue, and the solution was stirred for 6 hr and allowed to settle for 16-18 hr. The upper layer (about 0.3 L) was taken for analysis. The solution was centrifuged twice at 7000 g to remove suspended particles. The hydrocarbon was extracted with benzene and concentrated by evaporation, then purified using thin-layer chromatography. Spectrometric analysis of an octane solution of the hydrocarbon was done using the quasilinear luminescence spectra.

SOURCE AND PURITY OF MATERIALS:

not given.

ESTIMATED ERROR:

temp. ± 1°C
soly. ± 1.05
type of error not specified

REFERENCES:

1. Krasnoshchekova, R.Ya; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885.

COMPONENTS:

(1) Picene; $C_{22}H_{14}$; [213-46-7]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of picene in water at 27°C was reported to be 2.5×10^{-6} g(1) L^{-1} (2).

With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.5×10^{-7} g(1)/100 g sln and 1.6×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at the Ohio State University; m.p. range 363.5-364.5°C; (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C

soly. ± 0.5×10^{-6} g(1) dm^{-3}(2)

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 10-Butylbenz[a]anthracene; $C_{22}H_{20}$; [31632-63-0]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 10-butylbenz[a]anthracene in water

t/°C	10^6 g(1) L^{-1} (2)
27	7 ± 0.7
	7 ± 0.7
	7 ± 0.7
	8 ± 1
	8 ± 1

The best value recommended by the authors is 8.0 x 10^{-6} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 8.0 x 10^{-7} g(1)/100 g sln and 5.1 x 10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 96.4-96.7°C.

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc.* 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc.* 1940, *62*, 3086.

COMPONENTS:

(1) 7-Pentylbenz[a]anthracene; $C_{23}H_{22}$; [63019-00-1]

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

ORIGINAL MEASUREMENTS:

Davis, W.W.; Krahl, M.E.; Cloves, G.H.A.

J. Am. Chem. Soc. 1942, *64*, 108-10.

VARIABLES:

One temperature: 27°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 10-penthylbenz[a]anthracene in water

t/°C	10^7 g(1) L^{-1} (2)
27	9 ± 1
	8 ± 3
	8 ± 2

The best value recommended by the authors is 8 x 10^{-7} g(1) L^{-1} (2). With the assumption that 1.00 L sln = 1.00 kg sln, the corresponding mass percent and mole fraction, x_1, calculated by the compiler are 8 x 10^{-8} g(1)/100 g sln and 5 x 10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The method consisted of preparing serial dilutions of a suspension of (1) in (2) and determining nephelometrically the amount of (1) per unit volume beyond which further dilution caused no reduction in light scattering, which remained equal to that of pure (2). A Bausch and Lomb Dubosque colorimeter model 100-mm was employed. Many details are reported in ref 1.

SOURCE AND PURITY OF MATERIALS:

(1) prepared at Harvard University; m.p. range 82.6-83.3°C (cf. ref 2).

(2) dust-free.

ESTIMATED ERROR:

temp. ± 3°C
soly. see above

REFERENCES:

1. Davis, W.W.; Parker, Jr., T.V. *J. Am. Chem. Soc*. 1942, *64*, 101.
2. Davis, W.W.; Krahl, M.E.; Cloves, G.H.A. *J. Am. Chem. Soc*. 1940, *62*, 3086.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Coronene; $C_{24}H_{12}$; [191-07-1] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* 1977, *22*, 399-402.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of coronene in water at 25°C was reported to be 0.00014 mg(1) dm^{-3} sln and $x_1 = 8.56 \times 10^{-12}$.

The corresponding mass percent calculated by the compiler is 1.4×10^{-8} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A saturated solution of (1) in (2) was vigorously stirred in a 250 mL flask for 24 hrs. and subsequently settled at 25°C for at least 48 hrs. Then the saturated solution was decanted and filtered and 50-100 mL extracted with approximately 5 mL of cyclohexane in a separatory funnel. After shaking for 2 hrs. the cyclohexane extract was removed for analysis. An Aminco-Browman spectrophotofluorometer (American Instruments Ltd.) was used for analysis. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Aldrich Chemicals, Eastman Kodak, or K and K Laboratories, commercial highest grade; used as received.

(2) doubly distilled.

ESTIMATED ERROR:

soly. ± 2×10^{-5} mg(1) dm^{-3} sln (maximum deviation from several determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexacosane; $C_{26}H_{54}$; [110-82-7] (2) Water; H_2O; [7732-18-5]	Sutton, C.; Calder, J.A. *Environ. Sci. Technol.* 1974, *8*, 654-7.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexacosane in water at 25°C was reported to be 1.7×10^{-7} g(1)/100 g(2) corresponding to a mole fraction x_1, of 0.8×10^{-10}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

175 mg (1) were equilibrated with 700 mL (2) in closed flasks by shaking on a constant temperature bath for 12 hours. The flasks were then allowed to stand for 24 hours. Aliquots of 100 mL were removed, filtered through a 0.45 μm Millipore filter, then extracted three times with 10-mL portions of hexane containing an internal standard. The concentration of (1) was determined by injection of the hexane extract into a dual column gas chromatograph equipped with flame ionization detectors.

SOURCE AND PURITY OF MATERIALS:

(1) Analabs Inc., 99+%.

(2) doubly distilled.

ESTIMATED ERROR:

temp. ± 0.1°C
soly. ± 16%

REFERENCES:

COMPONENTS:

(1) Hexacosane; $C_{26}H_{54}$; [630-01-3]

(2) Seawater

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

Environ. Sci. Technol. 1974, *8*, 654-7.

VARIABLES:

One temperature: 25°C
One salinity: 35 g salts/kg sln

PREPARED BY:

P.A. Meyers and D. Shaw

EXPERIMENTAL VALUES:

The solubility of hexacosane in seawater was reported to be 1×10^{-8} g(1)/100 g sln and $x_1 = 6 \times 10^{-12}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

(1) and (2) were placed in a glass stoppered flask fitted with a Teflon stopcock near the bottom. The components were equilibrated by gentle shaking for 12 hrs at 25.0 ± 0.1°C The mixture was then allowed to stand for 24 hrs. Samples removed via the stopcock were filtered with suction through 0.45 µm membrane filters to remove any hydrocarbon droplets. The filtrate was extracted three times with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

Analabs, Inc., North Haven, Conn. 99 + % pure hydrocarbons.

Seawater collected from 25 m depth in Gulf of Mexico, poisoned with $HgCl_2$ sln to prevent bacterial growth, and filtered through Gelman glass fiber filter. Natural n-alkane levels too low to cause interference.

ESTIMATED ERROR: Eight replications were made. The average of the deviations of the mean gave an experimental error of ± 16%, yet some accommodation may have occurred due to presence of natural dissolved organic matter.

REFERENCES:

COMPONENTS:

(1) Hexatriacontane; $C_{36}H_{74}$; [630-06-8]

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

ORIGINAL MEASUREMENTS:

Baker, E.G.

Am. Chem. Soc., Div. Petrol. Chem., Preprints 1958, *3*, N°4, C61-8.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexatriacontane-18,19-C^{14} in water at 25°C was reported to be 1.7×10^{-9} g(1)/g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 1.7×10^{-7} g(1)/100 g sln and 6.1×10^{-11}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Carbon-14 labeled (1) was used as tracer.
The technique of preparing a saturated aqueous solution of (1) by ultrafiltration of a (1)-(2) dispersion has been described in ref 1.
A Packard Tri-Carb Liquid Scintillation Spectrometer was used to detect the radioactive (1) dissolved in (2).

SOURCE AND PURITY OF MATERIALS:

(1) New England Nuclear Corporation; used as received.

(2) distilled.

ESTIMATED ERROR:

soly. 20% (standard deviation from 17 replicate runs).

REFERENCES:

1. Baker, E.G. *Am. Chem. Soc. Div. Petrol. Chem., Preprints-Symposia* 1956, *1*, N°2, 5.

COMPONENTS: (1) Hexatriacontane; $C_{36}H_{74}$; [630-06-8] (2) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Baker, E.G. *Science* 1959, *129*, 871-4.
VARIABLES: One temperature: 25°C	**PREPARED BY:** F. Kapuku

EXPERIMENTAL VALUES:

The solubility of hexatriacontane in water at 25°C was reported to be 2.09 x 10^{-7} mL (1)/100 mL (2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE: not specified.	**SOURCE AND PURITY OF MATERIALS:** not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

SYSTEM INDEX

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

REGISTRY NUMBER INDEX

Pages preceded by E refer to evaluation texts whereas those not preceded by E refer to compiled tables.

AUTHOR INDEX

Page numbers preceded by E refer to evaluation text whereas those not preceded by E refer to compiled tables.

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