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SOLUBILITY DATA SERIES

Volume 37

HYDROCARBONS WITH WATER AND SEAWATER

Part I: *Hydrocarbons C₅ to C₇*

SOLUBILITY DATA SERIES

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HYDROCARBONS WITH WATER AND SEAWATER

Part I: *Hydrocarbons C$_5$ to C$_7$*

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FOREWORD

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

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

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

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

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

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

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 5, 6 or 7 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 528. 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 deter-
mine 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 approxi-
mately 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 pro-
posed. 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

<u>Mole fraction</u> of component 1, x_1 or $x(1)$:

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

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.

<u>Mole per cent</u> of component 1 is $100x_1$.

<u>Mass fraction</u> of component 1, w_1

$$w_1 = m_1/\underset{i}{\Sigma}m_i$$

where m_i is the mass of component i.

<u>Mass percent</u> 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, cyclo-
       alkane, 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 dis-cussed 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 evalua-tion. However, the authors's units are expressed according to IUPAC re-commendations (ref 3,4) as far as possible.

In addition, compiler-calculated values of mole fractions and/or mass per-cent are included if the original data do not use these units. 1975 or 1977 atomic weights (ref 5) are used in such calculations. When appro-priate, 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 pos-sible 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 signifi-cant 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.
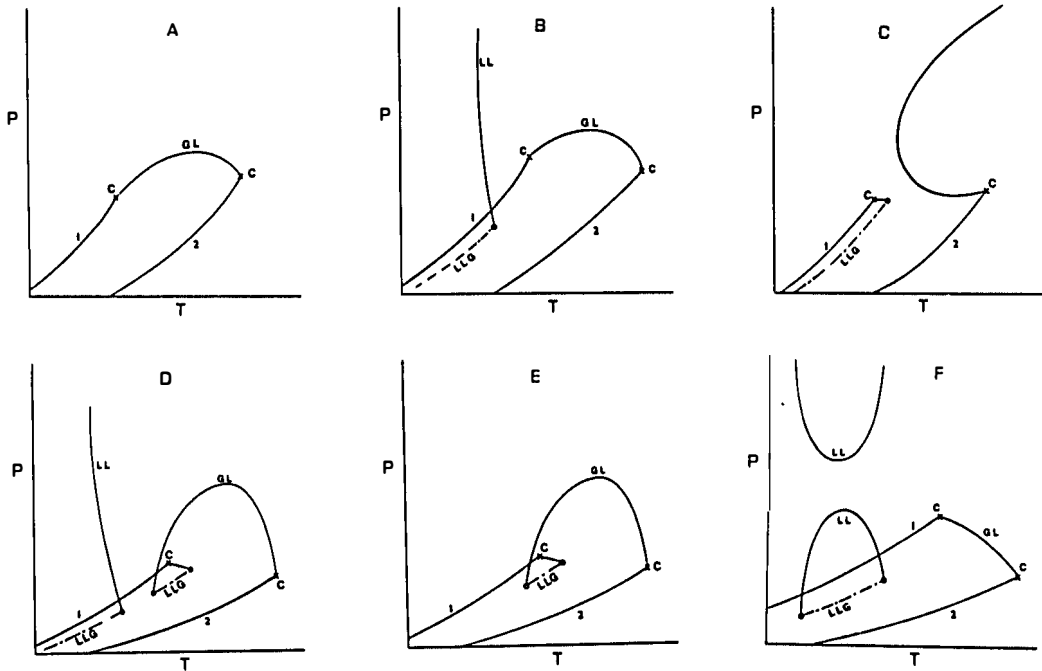
Fig. 1. Pressure-temperature projections for the six types of phase equili-
bria in binary mixtures. A - Type I; B - Type II; C - Type III; D - Type
IV; E - Type V; F - Type VI. Lines labelled 1 and 2 are the vapor pressure
of the two components; lines labelled LLG, GL and LL are three phase lines,
gas-liquid critical loci and liquid-liquid critical loci respectively;
points denoted C are critical points of the pure components.
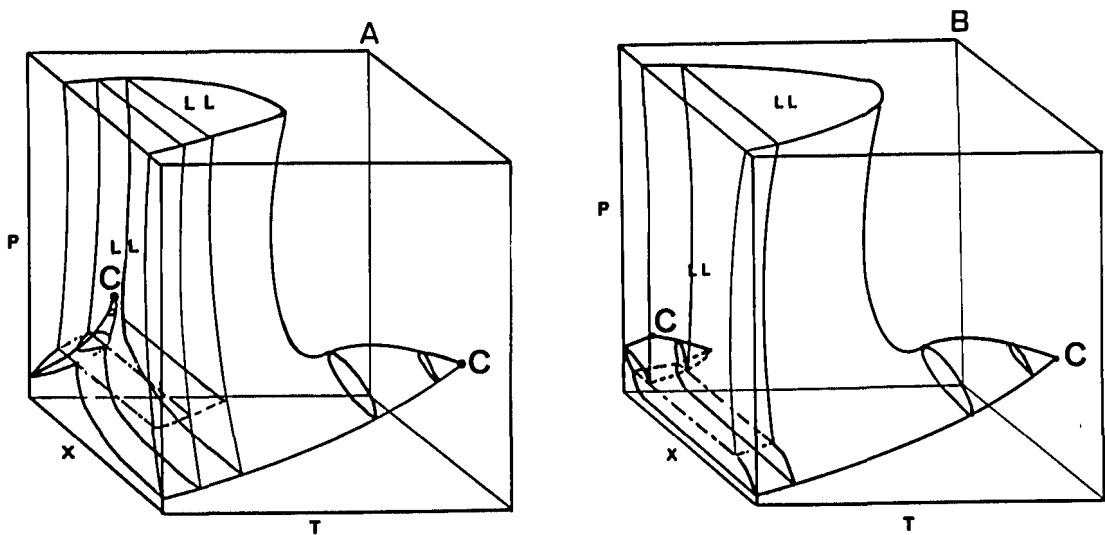
Fig. 2. Pressure-temperature-composition diagrams for two Type III systems.
The three phase line is denoted -.-.-.- . The region in which two liquids
coexist is denoted LL.
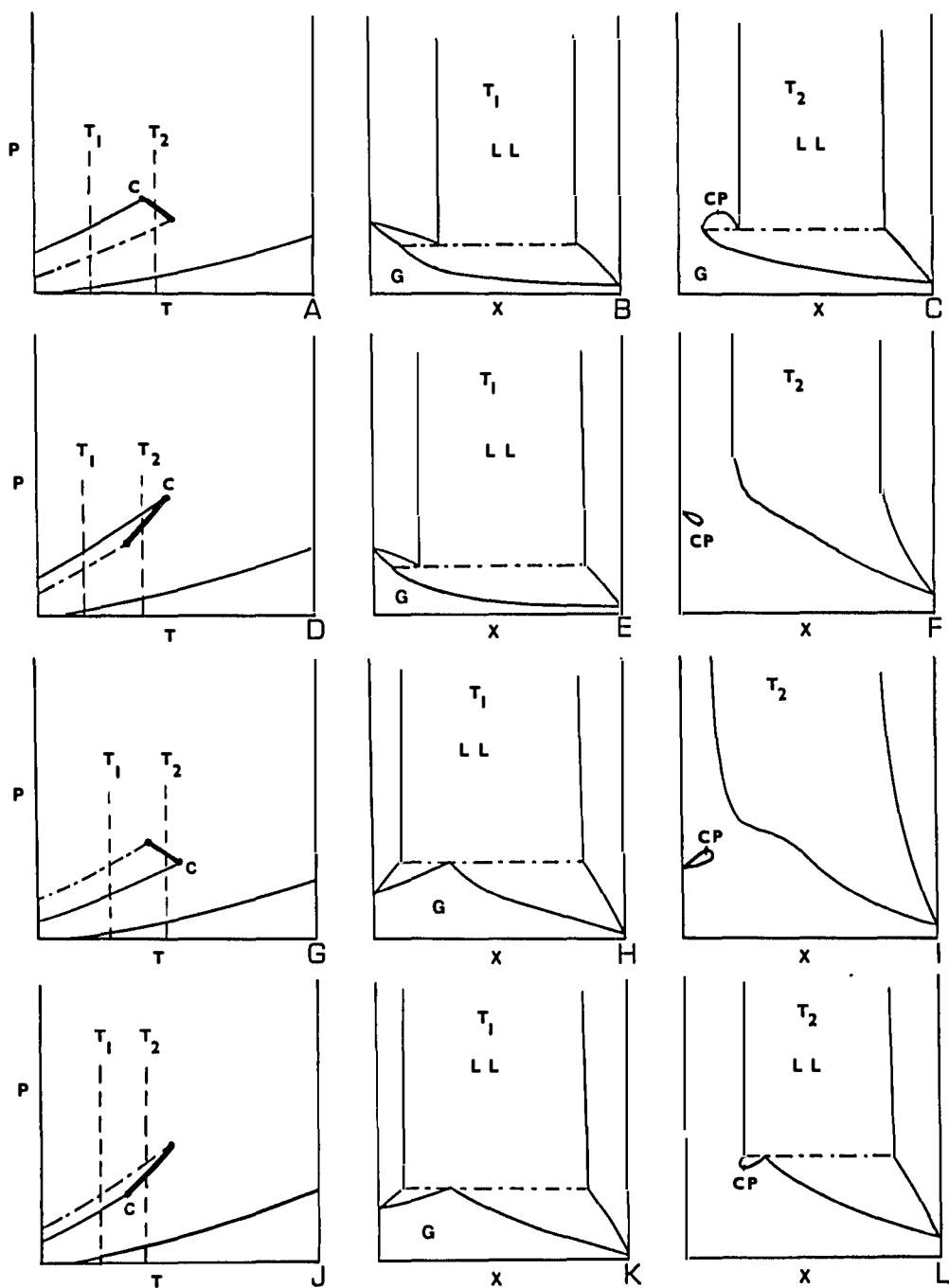
Fig. 3. The four possibilities for the relative position of the three phase line and vapor pressure curves of pure components for type III phase behavior. Figures A, D, G and J are pressure-temperature projections of the four classes. Figures B, E, H and K are the constant temperature, T_1, sections 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 coexist-
ing phases dependings on the overall composition. At some compositions only
one phase will be present.
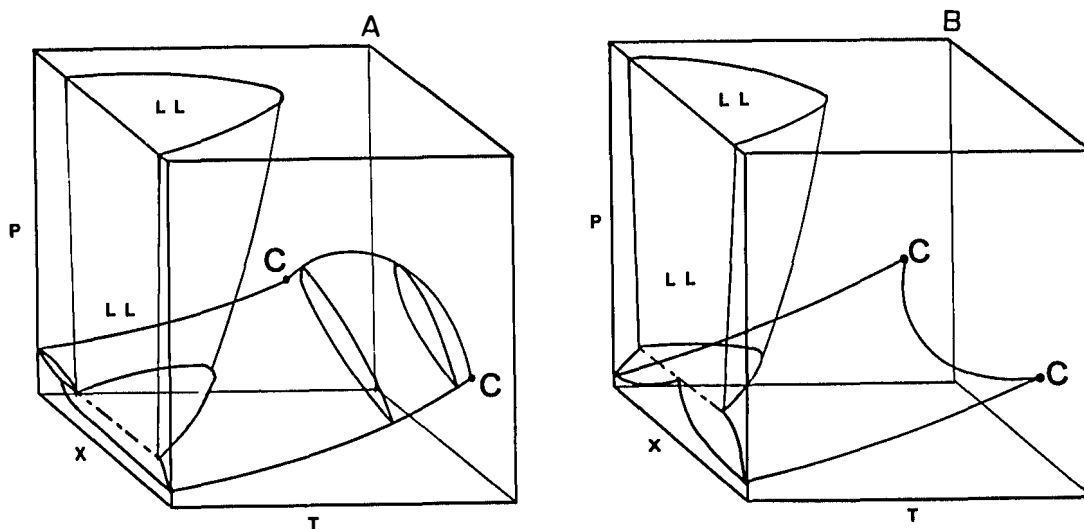
Fig. 4. Pressure, temperature, composition diagrams for two Type II
systems. The three phase line is denoted -.-.-.- . The region in which two
liquids coexist is denoted LL.

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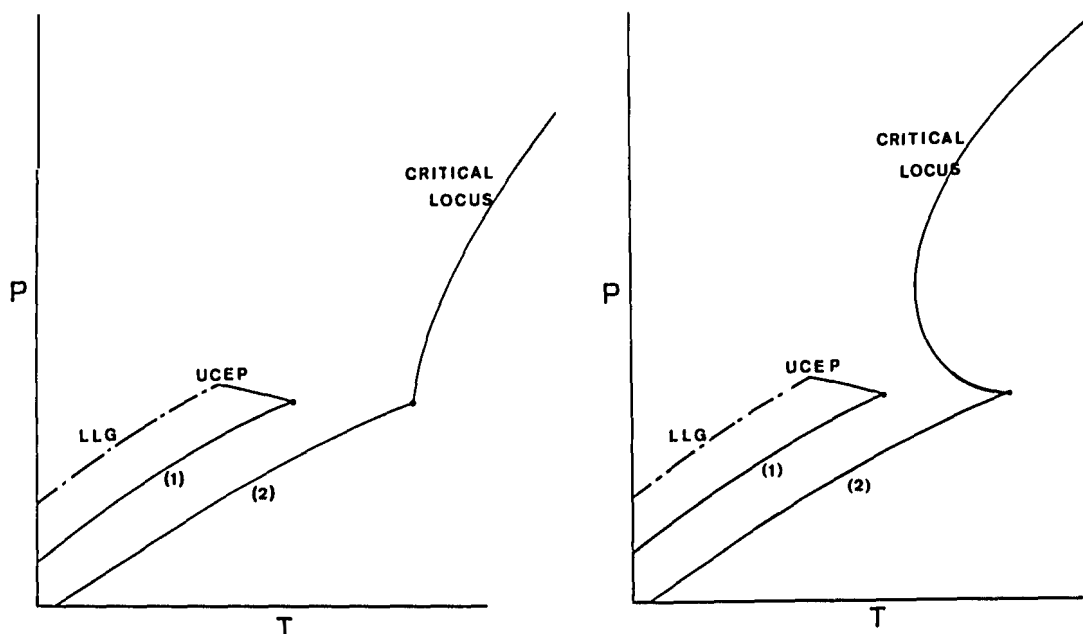
Fig. 5. Pressure, temperature projections for systems exhibiting gas-gas immiscibility. Figure 5A - immiscibility of the first kind. Figure 5B - immiscibility of the second kind.

References.

1. Scott, R. L.; van Konynenburg, P. H.; *Phil. Trans. Roy. Soc.*, *London* 1980, *A298*, 495.
2. Hicks, C. P.; Young, C. L.; *Chem. Rev.* 1975, *75*, 119.
3. Gubbins, K. E.; Shing, K. S.; Streett, W. B.; *J. Phys. Chem.* 1983, *87*, 4573.
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7. De Loos, Th. W.; Penders, W. G.; Lichtenthaler, R. N.; *J. Chem. Thermodyn.* 1982, *14*, 83.
8. Tsiklis, D. S.; Rott, L. A.; *Russ. Chem. Rev.* 1967, *36*, 351.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3 Cyclopentadiene; C_5H_6; [542-92-7] (2) Water; H_2O; [7732-18-5]	Streitweiser, A.; Nebenzahl, L.L. *J. Am. Chem. Soc.* 1976, *98*, 2188-90.

VARIABLES:	PREPARED BY:
Room Temperature	M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclopentadiene in water at room temperature was reported to be 0.0103 mol L^{-1}.[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 0.068 g(1)/100 g sln and 1.8×10^{-4} respectively.

[a] According to a footnote in the paper the experimental data were apparently obtained by J. Cambray (presumably *unpublished observations*) but experimental details are given in the paper.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Water was saturated by shaking with excess (1) and then centrifuged. The saturated solution so obtained was then diluted and analysed by UV spectrophotometry assuming the absorptivity to be the same as in ethanol.	(1) Aldrich; distilled onto molecular sieves and used within 1h; analysed by GC. (2) Distilled; purity not specified.
	ESTIMATED ERROR: Not given.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Cyclopentene; C_5H_8; [142-24-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia. November 1984.

CRITICAL EVALUATION:

Quantitative solubility data for the solubility of cyclopentene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of
Cyclopentene (1) in Water (2)

Reference	T/K	Method
McAuliffe (ref 1)	298	GLC
Pierotti and Liabastre (ref 2)	298,308	GLC

Solubilities of cyclopentene have also been reported in various aqueous salt solutions (ref 3) but will not be considered in this Evaluation. No solubility data appear to have been reported for the solubility of (2) in (1).

The reported solubilities of (1) in (2) are listed in Table 2. The results are in poor agreement, those of Pierotti and Liabastre (ref 2) being about three times higher than those of McAuliffe (ref 1). These results are typical of a wide variety of hydrocarbon-water systems investigated by these authors. In general the results of McAuliffe are in good agreement with other literature values in well-investigated systems (e.g. benzene in H_2O) whereas those of Pierotti and Liabastre are substantially higher. This situation is discussed in greater detail in the Critical Evaluation of the cyclopentane-water system. For the present system, in the absence of confirmatory studies, the data of Pierotti and Liabastre are not rejected but they should be regarded as order-of-magnitude values only. The datum of McAuliffe may be considered as "Tentative".

TABLE 2: Solubility Values of Cyclopentene (1) in Water (2)

T/K	Solubility values		
	Reported values g(1)/100g sln	"Best" value[a] g(1)/100g sln	$10^4 x_1$
298	0.0535 (ref 1), 0.165 (ref 2)	0.054	1.4
308	0.175 (ref 2)		

a See text.

COMPONENTS:	EVALUATOR:
(1) Cyclopentene; C_5H_8; [142-24-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia. November 1984.

CRITICAL EVALUATION: (continued)

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

2. Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water solutions.* U.S. Nat. Tech. Inform. Serv., PB Rep. <u>1972</u>, No. 21163, 113 pp.

3. Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

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

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0535 g(1)/100 g sln and 1.41 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 chromato-graphed in conjunction with a flame-ionization detector.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 20 g(1)/10^6 g(2)
        (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclopentene in water was reported to be 8.978×10^{-3} 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 0.0611 g(1)/100 g sln and 1.62×10^{-4}.

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:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Prepared by dehydration of cyclopentanol and then washed, dried, and fractionated. Purity (not specified) was determined by chromatography. (2) Not specified.
	ESTIMATED ERROR: Temp. ± 0.05 K Soly. not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentene; C_5H_8; [142-29-0] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., <u>1972</u>, No. 21163, 113 p.

VARIABLES:	PREPARED BY:
Temperature: 298.26-308.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclopentene in water

T/K	g(1)/100 g sln	$10^3 x_1$
298.26	0.1645 ± 0.0049	0.4350
308.36	0.1748 ± 0.0044	0.4623

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) K & K Laboratories, Inc.; 95-99%; used as received. (2) laboratory distilled water.
	ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-1,3-butadiene; C_5H_8; [78-79-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia.
(2) Water; H_2O; [7732-18-5]	November 1984.

CRITICAL EVALUATION:

Quantitative solubility data for the system 2-methyl-1,3-butadiene (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the
2-Methyl-1,3-butadiene (1) - Water (2) System

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
Pavlova *et al*. (ref 2)	293-533	mutual	GLC, Karl Fischer

As only one study of the solubility of (2) in (1) has been reported (ref 2), no Critical Evaluation of those data can be made. The interested user is referred to the relevant data sheet for experimental values.

The reported values of the solubility of (1) in (2) are listed in Table 2 and plotted in Figure 1. The agreement at 298 K between the value of McAuliffe (ref 1) and the interpolated value of Pavlova *et al*. (ref 2) is reasonable so the "Best" values in Table 2 may be considered "Tentative", subject to further studies.

TABLE 2: Tentative Values of the Solubility of
2-Methyl-1,3-butadiene (1) in Water (2)

T/K	Reported values g(1)/100g sln	"Best" values ($\pm \sigma_n$) g(1)/100g sln	$10^4 x_1$
293	0.0545 (ref 2)	0.054	1.44
298	0.0642 (ref 1), 0.0572[a] (ref 2)	0.061 ± 0.004[b]	1.61 [b]
313	0.0665 (ref 2)	0.066	1.76
323	0.0761 (ref 2)	0.076	2.01
333	0.0867 (ref 2)	0.087	2.29

[a] Graphically interpolated by the Evaluator.
[b] "Best" value obtained by averaging; σ_n has no statistical significance.

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CRITICAL EVALUATION: (continued)

FIGURE 1. Solubility of 2-methyl-1,3-butadiene (1) in water: ref 1 (x); ref 2 (o).

REFERENCES

1.   McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

2.   Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. *Promyshlennost. Sinteticheskogo Kauchuka* 1966, *3*, 18-20.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1,3-butadiene; C_5H_8; [78-79-5] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 2-methyl-1,3-butadiene in water at 25°C was
reported to be 642 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0642 g(1)/100 g sln and 1.70 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5K soly. 10 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1,3-butadiene; C_5H_8; [78-79-5]	Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S.
(2) Water; H_2O; [7732-18-5]	*Promyshlennost. Sinteticheskogo Kauchuka* <u>1966</u>, *3*, 18-20.

VARIABLES:	PREPARED BY:
Temperature: 20-60°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 2-methyl-1,3-butadiene in water

$t/°C$	$10^4 x_1$	g(1)/100 g sln (compiler)
20	1.441	0.05448
40	1.758	0.06646
50	2.013	0.07609
60	2.294	0.08671

Solubility of water in 2-methyl-1,3-butadiene

$t/°C$	$10^3 x_2$	g(2)/100 g sln (compiler)
20	2.26	0.0598
40	3.58	0.0949
60	5.53	0.1468

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) source not specified; better than 99.7 wt%. (2) doubly distilled.

	ESTIMATED ERROR:
	temp. ± 0.1K

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Pentadiene; C_5H_8; [591-93-5]	McAuliffe, C.
(2) Water; H_2O; [7732-18-5]	*J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,4-pentadiene in water at 25°C was reported to be 558 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0558 g(1)/100 g sln and 1.48×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.

ESTIMATED ERROR:

temp. ± 1.5K
soly. 27 g(1)/10^6 g(2)
          (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Pentyne; C_5H_8; [627-19-0] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-pentyne in water at 25°C was reported
to be 1570 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.1570 g(1)/100 g sln and 4.15×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5K soly. 33 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia September 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system cyclopentane (1) and water (2) have been reported in the references listed in Table 1.

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

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	326-472	(1) in (2)	synthetic
Englin *et al.* (ref 2)	273-313	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Pierotti and Liabastre (ref 4)	278-318	(1) in (2)	GLC
Price (ref 5)	298-426	(1) in (2)	GLC

The original data in all of these publications, along with the datum of Krzyzanowska and Szeliga (ref 6) are compiled in the Data Sheets immediately following this Critical Evaluation. However, the latter have not been included in this Evaluation as they do not appear to be independent of those of Price (ref 5). For convenience, further discussion of this system will be divided into two parts.

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

The various solubility data for cyclopentane in water are listed in Table 2. Because of the large discrepancies amongst the data and the small data base it is not possible at this stage for the Evaluator to decide on "Tentative" solubility values. The data are further discussed on the next page.

TABLE 2: Solubility of Cyclopentane (1) in Water (2)^a

T/K	Reported solubilities, g(1)/100 g sln
278	0.0339 (ref 4)
288	0.0342 (ref 4)
298	0.0156 (ref 3), 0.0342 (ref 4), 0.0160 (ref 5)
303	0.0160 (ref 5)
313	0.035* (ref 4), 0.0163*(ref 5)
333	0.050* (ref 1), 0.0185*(ref 5)
353	0.075* (ref 1), 0.0230*(ref 5)
373	0.110* (ref 1), 0.029* (ref 5)
393	0.160* (ref 1), 0.040* (ref 5)
413	0.260* (ref 1), 0.062* (ref 5)
433	0.385* (ref 1)
453	0.67* (ref 1)
473	1.4* (ref 1)

a Values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original measurements in the Data Sheets.

COMPONENTS:	EVALUATOR:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1984.

CRITICAL EVALUATION: (continued)

The solubilities in Table 2 fall into two markedly differing groups with the data of Guseva and Parnov (ref 1) and Pierotti and Liabastre (ref 4) approximately twice as high as those of McAuliffe (ref 3) and Price (ref 5). Interestingly, in spite of the disagreement, the two data sets show a similar temperature dependence (Figure 1). Application of the van't Hoff equation to these data gives ΔH^{∞}_{sln} = -2.5 (ref 4) and -2.8 (ref 5) kJ mol^{-1} which is typical for hydrocarbons in water (ref 7). However, the corresponding $\Delta C^{\infty}_{p,sln}$ values (~ -10 J K^{-1} mol^{-1}) are too negative by about 300 J K^{-1} mol^{-1} (ref 7).

Pierotti and Liabastre (ref 4) have previously noted inconsistency between their solubilities and those of McAuliffe (ref 3) for a variety of hydro-carbons. They claimed that lower solubilities are obtained by using, as McAuliffe did, a pre-absorbing column on the GLC to remove water. However, Price's GLC values (ref 5) tend to support McAuliffe's data and it should be noted that Pierotti and Liabastre's results have been found to differ markedly from "Recommended" values in a number of well-characterised systems (e.g. the benzene-water system). On the other hand, the only non-GLC data available (ref 1) are in reasonable agreement with Pierotti and Liabastre's results. This system clearly requires thorough re-investigation to resolve existing anomalies.
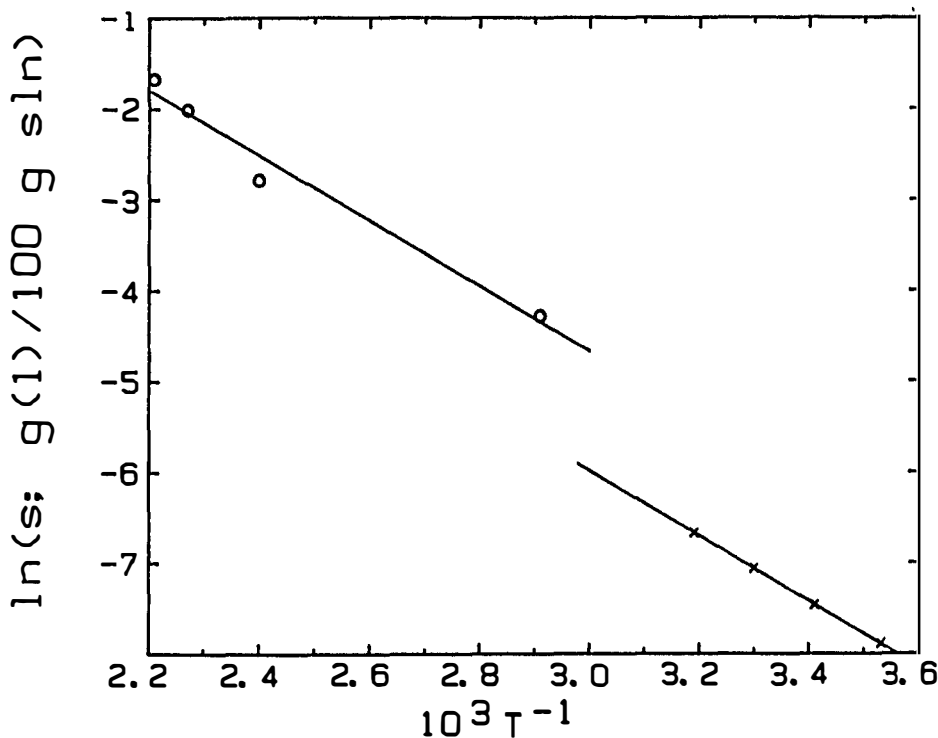
FIGURE 1. Solubility of cyclopentane (1) in water as a function of temperature: Ref 4 (X); Ref 5 (O). Data plotted as $\ln s$ vs. T^{-1} for representational convenience. (continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1984.

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN CYCLOPENTANE

The solubility of water in cyclopentane has been reported in only one publication: Englin *et al.* (ref 2), and thus no Critical Evaluation can be made. The interested user is referred to the appropriate data sheet following this Critical Evaluation. However, it should be noted that in a number of well-characterised systems where comparison is possible (e.g. the benzene-water system) the data of Englin *et al.* are generally reliable at low temperatures but are usually much higher than "Recommended" values above 300 K.

REFERENCES

1. Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ., Khim.* <u>1964</u>, *19*, 77-8.

2. Englin, B.A.; Plate, A.F.; Tugolikov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 42-6.

3. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

4. Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water solutions*. U.S. Nat. Tech. Inform. Serv., PB Rep. <u>1972</u>, No.21163, 113 pp.

5. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

6. Krzyzanowska, T.; Szeliga, J. *Nafta Katowice* <u>1978</u>, *34*, 413-7.

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

ACKNOWLEDGEMENTS

The Evaluator thanks Dr Brian Clare for regression analyses and graphics and Dr Marie-Claire Haulait-Pirson for comments.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1964</u>, *19*, 77-8.

VARIABLES:	PREPARED BY:
Temperature: 53-198.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclopentane in water

$t/°C$	g(1)/100 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
53	0.0427	0.0427	1.10
117	0.151	0.151	3.87
166	0.436	0.434	11.12
198.5	1.288	1.271	32.57

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (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: 0-40°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in cyclopentane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0046	1.79
10	0.0086	3.35
20	0.0142	5.53
30	0.0249	9.69
40	0.0398	15.48

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclopentane in water at 25°C was reported to be 156 mg(1)/kg sln, (0.0156 g/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 4.0×10^{-5}.

The same value is also reported in refs·1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity, used as received. (2) distilled.

	SOURCE AND PURITY cont.

ESTIMATED ERROR:

temp. ± 1.5K
soly. 9 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092.

2. McAuliffe, C. *Amer. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions" U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 pp.

VARIABLES:	PREPARED BY:
Temperature: 278.26-318.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclopentane in water

$T/$ K	g(1)/100 g sln	$10^3 x_1$	$10^4 x_1$ (corrected by compiler)
278.26	0.03386 ± 0.00087	0.8697	0.8697
288.36	0.03417 ± 0.00102	0.8777	0.8777
298.26	0.03419 ± 0.00067	0.8782	0.8782
308.36	0.03685 ± 0.00110	0.9465	0.9465
318.36	0.03415 ± 0.00100	0.8772	0.8772

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Matheson, Coleman & Bell, 90.8%; used as received. (2) laboratory distilled water.
	ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
Temperature: 25-153.1°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of cyclopentane in water at system pressure

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^5 x_1$ (compiler)
25.0	160 ± 2.0	0.0160	4.11
40.1	163 ± 3.0	0.0163	4.19
55.7	180 ± 7.0	0.0180	4.62
99.1	296 ± 16.0	0.0296	7.61
118.0	372 ± 15.0	0.0372	9.56
137.3	611 ± 9.0	0.0611	15.70
153.1	792 ± 74.0	0.0792	20.36

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured 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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

ESTIMATED ERROR:
temp. ± 1K   soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclopentane; C_5H_{10}; [287-92-3] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta Katowice* <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclopentane in water at 25°C was reported
to be 160.0 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 0.0160 g (1)/100 g sln and 4.11×10^{-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).

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

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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. 4.0 mg(1)/kg(2) (standard deviation from 7-9 determinations) **REFERENCES:**

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-2-butene; C_5H_{10}; [513-35-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia. November 1984.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	293	(2) in (1)	analytical
Pavlova *et al.* (ref 2)	293-333	mutual	GLC, Karl Fischer

As only one study of the solubility of (1) in (2) has been reported (ref 2), no Critical Evaluation of those data can be made. The interested user is referred to the relevant data sheet for the experimental values. Solubilities of 2-methyl-2-butene in various aqueous salt solutions have also been reported (ref 3) but will not be considered in this Evaluation.

The reported values for the solubility of (2) in (1) are listed in Table 2 and plotted in Figure 1. The agreement between the values at 293 K of Englin *et al.* (ref 1) and Pavlova *et al.* (ref 2) is reasonable and so the values in Table 2 may be considered "Tentative", subject to further studies.

TABLE 2: Tentative Values of the Solubility of
Water (2) in 2-Methyl-2-butene (1)

T/K	Solubility values		
	Reported values g(2)/100g sln	"Best" values ($\pm \sigma_n$) g(2)/100g sln	$10^3 x_2$
293	0.0435 (ref 1), 0.0388 (ref 2)	0.041 ± 0.02^a	1.6
313	0.0589 (ref 2)	0.059	2.3
333	0.0906 (ref 2)	0.091	3.5

a This "Best" value obtained by averaging; σ_n has no statistical significance.

COMPONENTS:	EVALUATOR:
(1) 2-Methyl-2-butene; C_5H_{10}; [513-35-9] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Australia. November 1984.

CRITICAL EVALUATION: (continued)

FIGURE 1.   Solubility of water (2) in 2-methyl-2-butene: ref 1 (o); ref 2 (x).

REFERENCES

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

2.   Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. *Promyshlennost. Sinteticheskogo Kauchuka* 1966, *3*, 18-20.

3.   Natarajan, G.S.; Venkatachalam, K.A.   *J. Chem. Eng. Data* 1972, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-butene; C_5H_{10}; [513-35-9] (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: One temperature: 20°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in 2-methyl-2-butene at 20°C was reported
to be 0.0435 g(2)/100 g sln.

The corresponding mole fraction, x_2, calculated by the compilers
is 1.69×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-butene; C_5H_{10}; [513-35-9] (2) Water; H_2O; [7732-18-5]	Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. *Promyshlennost. Sinteticheskogo Kauchuka* <u>1966</u>, *3*, 18-20.

VARIABLES:	PREPARED BY:
Temperature: 20-60°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 2-methyl-2-butene in water

$t/°C$	$10^5 x_1$	g(1)/100 g sln (compiler)
20	5.63	0.0215
40	6.06	0.0236
50	6.42	0.0250
60	6.87	0.0267

Solubility of water in 2-methyl-2-butene

$t/°C$	$10^3 x_2$	g(2)/100 g sln (compiler)
20	1.51	0.0388
40	2.29	0.0589
60	3.52	0.0906

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) source not specified; better than 99.7 wt%. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-2-butene; C_5H_{10}; [513-35-9] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9

VARIABLES:	PREPARED BY:
Temperature: 15-25°C	M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of 2-methyl-2-butene in 0.001 mol/L HNO_3 solution.

$t/°C$	10^3 mol/L sln[a]	g(1)/100 g sln[b] (compiler)	$10^5 \, x_1$ (compiler)
15	5.15 ± 0.21	0.037	9.3
20	4.88 ± 0.16	0.035	8.8
25	4.61 ± 0.20	0.033	8.3

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 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^{-1} HCl.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Prepared by dehydration of *t*-amyl alcohol 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:	ORIGINAL MEASUREMENTS:
(1) 3-Methyl-1-butene; C_5H_{10}; [563-45-1] (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 3-methyl-1-butene in water at 25°C was reported
to be 130 g(1)/10^6 g(2).
The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0130 g(1)/100 g sln and 3.34 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 14 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Pentene; C_5H_{10}; [109-67-1] (2) Water; H_2O; [7732-18-5]	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-pentene in water at 25°C was reported
to be 148 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0148 g(1)/100 g sln and 3.80×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 7 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Pentene; C_5H_{10}; [109-68-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 2-pentene in water at 25°C was reported to be 203 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0203 g(1)/100 g sln and 5.21×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 8 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylpropane; C_5H_{12}; [463-82-1] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 2,2-dimethylpropane in water at 25°C was reported to be 33.2 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00332 g(1)/100 g sln and 8.30×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 10 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (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 2-methylbutane (1) and water (2) system have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Black et al. (ref 1)	279-295	(2) in (1)	radiotracer
Englin et al. (ref 2)	273-293	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Pavlova et al. (ref 4)	293-333	mutual	GLC, Karl Fischer
Polak and Lu (ref 5)	273,298	mutual	GLC, Karl Fischer
Price (ref 6)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 7)	298	(1) in (2)	GLC

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation.

In the Tables which follow, solubilities obtained by the Evaluator by graphical interpolation of original measurements in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained, where appropriate, by simple averaging. Uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than error limits.

For convenience, further discussion of this system will be divided into two parts.

1.   THE SOLUBILITY OF 2-METHYLBUTANE (1) IN WATER (2)

The solubility data for 2-methylbutane in water are listed in Table 2 and are also plotted in Figure 1. The data of Krzyzanowska and Szeliga (ref 7) have been excluded from this Evaluation as they do not appear to be independent of those reported by Price (ref 6).

At 298K, where comparison amongst independent values is possible, agreement is excellent. This gives added confidence to the values at other temperatures. A possible exception may be the value of Polak and Lu (ref 5) at 273K which appears a little high (even though some increase in solubility of hydrocarbons in water is usually observed as the temperature approaches 273K, e.g. the benzene-water system).   (continued next page)

COMPONENTS:	EVALUATOR:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (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: Recommended (R) and Tentative Values of the Solubility of 2-Methylbutane (1) in Water (2)

T/K	Solubility values		
	Reported values $10^3 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$)	
		$10^3 g(1)/100g$ sln	$10^5 x_1$
273	7.24 (ref 5)	7.2^a	1.8^a
293	4.69 (ref 4)	4.7	1.2
298	4.78 (ref 3), 4.86* (ref 4), 4.96 (ref 5), 4.8 (ref 6)	4.85 ± 0.07 (R)	1.21 (R)
303	5.06* (ref 4)	5.1	
313	5.77 (ref 4)	5.8	1.4
323	7.01 (ref 4)	7.0	1.8
333	7.93 (ref 4)	7.9	2.0

^{a}Value may be doubtful, see text.
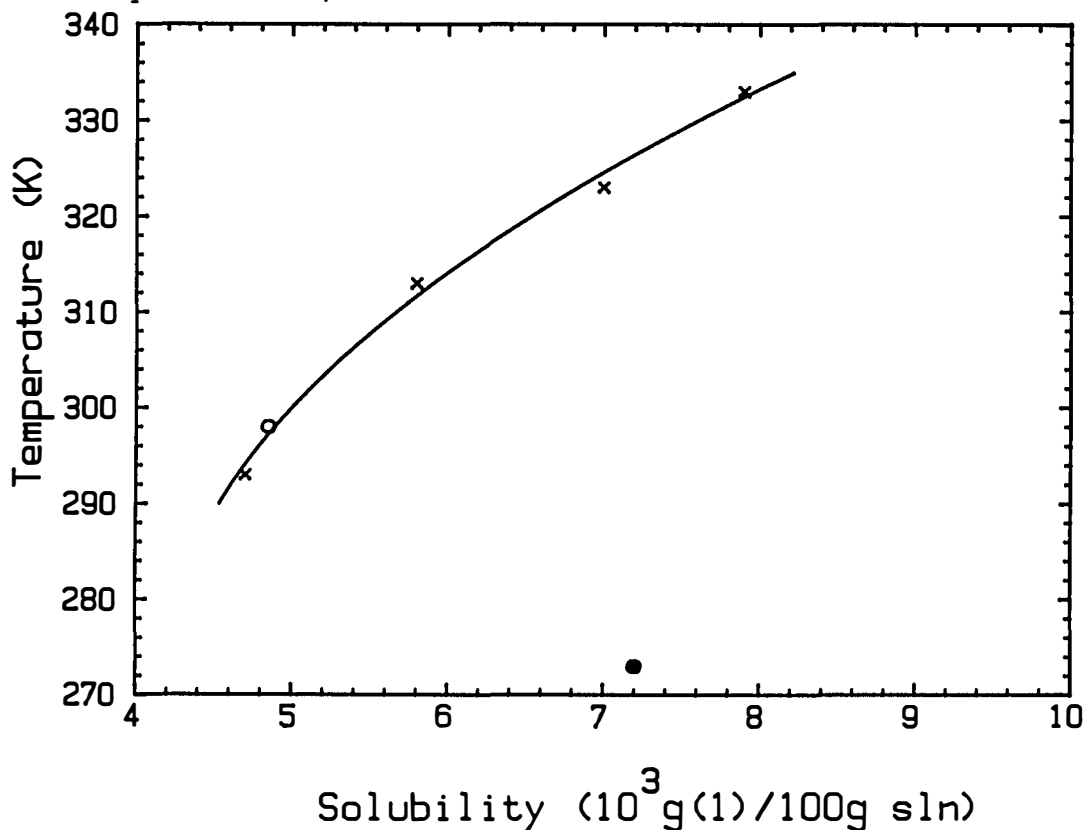
FIGURE 1.   Solubility of 2-methylbutane in water: ref 4 (x); average of ref 3-6 (o); ref 5 (●), but see text.

COMPONENTS:	EVALUATOR:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (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)

2.   THE SOLUBILITY OF WATER (2) IN 2-METHYLBUTANE (1)

The solubility data for water in 2-methylbutane are listed in Table 3 and plotted in Figure 2. In general the reported values are in reasonable agreement. The only exception appears to be the data of Pavlova et al. (ref 4) which are higher than other values. Although there are insufficient independent data to justify outright rejection of the values of Pavlova et al. at this stage, nevertheless, their data have not been used in determining "best" values (Table 3) and should be regarded with caution.

TABLE 3:   Tentative Values of the Solubility of
Water (2) in 2-Methylbutane (1)

T/K	Solubility values		
	Reported values $10^3 g(2)/100g$ sln	"Best" values ($\pm \sigma_n$)[a] $10^3 g(2)/100g$ sln	$10^4 x_2$
273	3.2 (ref 2), 2.8 (ref 5)	3.0 ± 0.2	1.2
278	4.3* (ref 1)	4.3	1.7
283	5.2* (ref 1), 5.9 (ref 2)	5.5 ± 0.4	2.2
288	6.5* (ref 1)	6.5	2.6
293	9.2* (ref 1), 11.2 (ref 2), 16.0 (ref 4)	10 ± 1	4
298	18* (ref 4), 9.6 (ref 5)	10	4
303	20* (ref 4)		
313	25.7 (ref 4)		
323	40* (ref 4)		
333	58.5 (ref 4)		

[a]Data from ref 4 not included in calculation of "best" values, see text.

COMPONENTS:	EVALUATOR:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (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 2. Solubility of water in 2-methylbutane: ref 1 (x); ref 2 (Δ); ref 4 (o), ref 5(●).

REFERENCES

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

3. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

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5. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

6. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

7. Kryzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *34*, 413-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.
VARIABLES:	PREPARED BY:
Temperature: 6-21.8°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2-methylbutane
at a total saturation pressure of 1 atm

$t/°C$	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^4 x_2$ (compiler)
15.3	0.0066*	0.0066	2.6
21.3	0.0096*	0.0096	3.8
21.8	0.0097*	0.0097	3.9
6.0	0.00443	0.00443	1.78
	0.00433	0.00433	1.74
	0.00440	0.00440	1.76
20.0	0.00940	0.00940	3.76
	0.00902	0.00902	3.61
	0.00942	0.00942	7.77
20.5	0.01001	0.01001	4.02

*Determinations made in glass apparatus

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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.* <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A.
(2) Water; H_2O; [7732-18-5]	*Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 42-6.

VARIABLES:	PREPARED BY:
Temperature: 0-20°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2-methylbutane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0032	1.28
10	0.0059	2.37
20	0.0112	4.49

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylbutane in water at 25°C was reported to be 47.8 mg (1)/kg sln, (0.0478 g(1)/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 1.19×10^{-5}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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) drop-lets. 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 frac-tionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.6 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (2) Water; H_2O; [7732-18-5]	Pavlova, S.P.; Pavlov, S.Yu.; Serafimov, L.A.; Kofman, L.S. *Promyshlennost. Sinteticheskogo Kauchuka* 1966, *3*, 18-20.

VARIABLES:	PREPARED BY:
Temperature: 20-60°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of 2-methylbutane in water

$t/°C$	$10^5 x_1$	g(1)/100 g sln (compiler)
20	1.17	0.00469
40	1.44	0.00577
50	1.75	0.00701
60	1.98	0.00793

Solubility of water in 2-methylbutane

$t/°C$	$10^3 x_2$	g(2)/100 g sln (compiler)
20	0.64	0.0160
40	1.03	0.0257
60	2.34	0.0585

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) source not specified; better than 99.7 wt%. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2-methylbutane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	72.4^c	1.81×10^{-5}
25^b	49.6^c	1.24×10^{-5}

Solubility of water in 2-methylbutane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	28^d	1.12×10^{-4}
25^b	96^e	3.85×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
          e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylbutane in water at 25°C and at system pressure was reported to be 48 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.0048 g(1)/100 g sln and 1.20×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 1 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylbutane; C_5H_{12}; [78-78-4] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta Katowice* <u>1978</u>, *12*, 413-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylbutane in water at 25°C was reported
to be 48 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 0.0048 g(1)/100 g sln and 1.2×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 1.44 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Fühner (ref 1)	289	(1) in (2)	titration
Black *et al*. (ref 3)	279-298	(2) in (1)	radiotracer
Namiot and Beider (ref 4)	293-345[a]	(1) in (2)	gas-liq. equilibrium
Wishnia (ref 5)	263-308	(1) in (2)	radiotracer
Barone *et al*. (ref 6)	298	(1) in (2)	GLC
Connolly (ref 7)	573-625[a]	(1) in (2)	cloud point
McAuliffe (ref 8)	298	(1) in (2)	GLC
Nelson and DeLigny (ref 9)	277-303	(1) in (2)	GLC
Pierotti and Liabastre (ref 10)	278-308	(1) in (2)	GLC
Polak and Lu (ref 11)	273,298	mutual	GLC, Karl Fischer
Price (ref 13)	298-423	(1) in (2)	GLC
Korenman and Aref'eva (ref 14)	293	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 15)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 16)	298	(1) in (2)	partition coefficient
Jonsson *et al*. (ref 17)	288-308	(1) in (2)	partition coefficient

[a]Pressure also varied.

Solubility data for pentane in water may also be calculated from the calorimetric data of Gill *et al*. (ref 12). Apart from the work of Scheffer (ref 2) and Roof (ref 18) which did not contain sufficient information to justify inclusion, and Wishnia (ref 5) who reported only graphical information, all the original measurements in the references listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation.

As indicated in the footnote to Table 1, quantitative solubility data for pentane in water at elevated pressures have been reported in the papers by Namiot and Beider (ref 4) and Connolly (ref 7). Since these studies were not carried out under comparable conditions no critical evaluation of their reliability can be made and the interested user is referred to the original measurements in the relevant Data Sheets. Connolly (ref 7) reports an upper critical solution temperature of 624K at 34 MPa whilst Roof (ref 18) reports a three phase critical equilibrium point at 464K and 658 psia (4.5 MPa).

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION: (continued)

In the Tables which follow, solubilities obtained by the Evaluator by graphical interpolation of the original measurements in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits.

For convenience, further discussion of the solubility data for this system will be divided into two parts.

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

Only five studies (ref 9, 10, 11, 13, 17) report the solubility of pentane in water as a function of temperature. The data of Nelson and DeLigny (ref 9), Polak and Lu (ref 11), Price (ref 12) and Jonsson *et al.* (ref 17) are in good agreement with each other given the analytical difficulties at the low concentrations involved. However, the solubilities of Pierotti and Liabastre (ref 10) are approximately twice as high as the other studies (ref 9, 11, 13, 17). Since Pierotti and Liabastre's data are also markedly higher than all other values at 298K (ref 6, 8, 9, 11, 13, 16, 17) and are generally higher than "Recommended" values for well-characterized systems (e.g. benzene in water), their results are rejected.

The data of Fühner (ref 1) at 298K and Korenman and Aref'eva (ref 14) at 293K are also markedly higher than all other values and are therefore rejected. The data of Krzyzanowska and Szeliga (ref 15) do not appear to be independent of those of Price (ref 13) and have therefore been excluded from this Critical Evaluation. All other data are included in Table 2.

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

T/K	Solubility values		
	Reported values 10^3 g(1)/100g sln	"Best" values ($\pm \sigma_n$) 10^3 g(1)/100g sln	$10^5 x_1$
273	6.57 (ref 11)	6.6	1.7
283	4.29 (ref 9)	4.3	1.1
293	3.93 (ref 9), 4.14 (ref 17)	4.0 ± 0.1 (*R*)	1.0 (*R*)
298	4.97 (ref 6), 3.85 (ref 8), 4.05 (ref 9), 4.76 (ref 11), 3.95 (ref 13), 4.06 (ref 16), 4.06 (ref 17)	4.2 ± 0.4	1.1

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION: (continued)

TABLE 2 (continued)

T/K	Solubility values		
	Reported values 10^3g(1)/100g sln	"Best" values ($\pm \sigma_n$) 10^3g(1)/100g sln	$10^5 x_1$
303	4.05 (ref 9), 4.1 (ref 13), 4.03 (ref 17)	4.1 $\pm$ 0.1 (R)	1.0 (R)
313	3.98* (ref 13)	4.0	1.0
323	4.1* (ref 13)	4.1	1.0
333	4.3* (ref 13)	4.3	1.1
343	4.6* (ref 13)	4.6	1.2
353	5.0* (ref 13)	5.0	1.3
363	5.8* (ref 13)	5.8	1.5
383	8.6* (ref 13)	8.6	2.2
403	15.0* (ref 13)	15	3.8
423	30.3* (ref 13)	30	7.5

As is obvious from Table 2, the solubilities at temperatures other than 298K are mainly those of Price (ref 13) and in the absence of confirmatory studies can only be regarded as tentative. However, the agreement with other studies at 298K, as noted above, is quite good and, furthermore, application of the van't Hoff equation to the data listed in Table 2 gives ΔH^∞_{sln} = -4.72 kJ mol^{-1} and $\Delta C^\infty_{p,sln}$ = 379 JK^{-1} mol^{-1} which agree well with the calorimetrically determined values (ref 12) of -2.0 $\pm$ 0.2 kJ mol^{-1} and 400 $\pm$ 70 JK^{-1} mol^{-1}. Thus some confidence can be placed in the "best" values. Selected data are plotted in Figure 1.
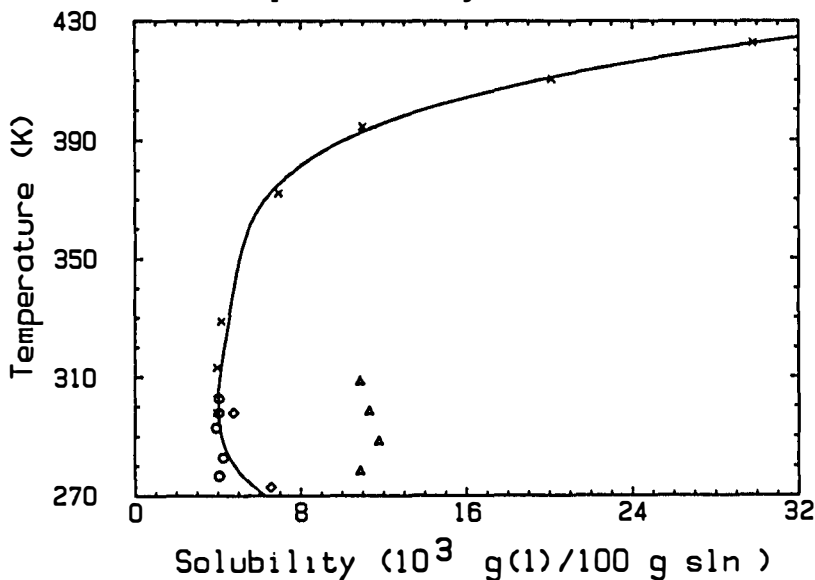
FIGURE 1. Solubility of pentane in water: ref 13 (x); ref 9 (o); ref 11 (◇); ref 10 (△, rejected data, see text). (cont'nued)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION: (continued)

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

The solubility of water in pentane has been reported only by Black *et al.* (ref 3) and Polak and Lu (ref 11). Their results are mutually consistent but in the absence of confirmatory data they must be considered as "Tentative" only. The data are listed in Table 3 and plotted in Figure 2.

TABLE 3:   Tentative Values of the Solubility of
Water (2) in Pentane (1)

T/K	Solubility values		
	Reported values $10^3 g(2)/100g$ sln	"Best" values ($\pm \sigma_n$) $10^3 g(2)/100g$ sln	$10^5 x_2$
273	2.6 (ref 11)		
283	4.2* (ref 3)		
293	8.5* (ref 3		
298	12.2* (ref 3), 10.1 (ref 11)	11 ± 1	4.4
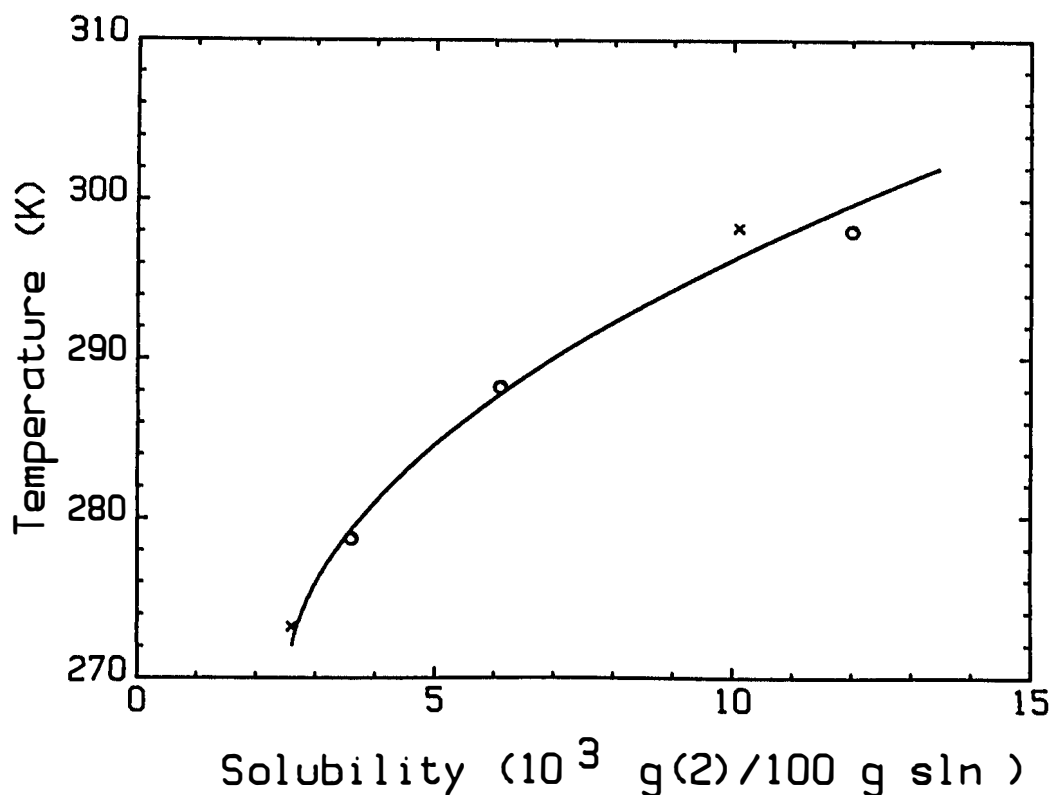
FIGURE 2.   Solubility of water in pentane: ref 3 (o); ref 11 (x). (continued)

COMPONENTS:	EVALUATOR:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. October 1984.

CRITICAL EVALUATION: (continued)

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Fühner, H. *Ber. Dtsch. Chem. Ges.* <u>1924,</u> *57*, 510-15.

VARIABLES:	PREPARED BY:
One temperature: 16°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentane in water at 16°C was reported to be 0.060 mL (1)/100 mL sln or 0.036 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler is 9.0×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; commercial grade; used as received. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.

VARIABLES:	PREPARED BY:
Temperature: 5.5-24.8°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in pentane
at a total saturation pressure of 1 atm

$t/°C$	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^4 x_2$ (compiler)
5.5	0.0036	0.0036	1.44
15.0	0.0061	0.0061	2.45
24.8	0.0119	0.0119	4.77
24.8	0.0120	0.0120	4.81

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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.* <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Namiot, A. Yu; Bender, S. Ya. *Khim. Tekhnol. Topl. Masel* <u>1960</u>, 7, 52-5.
VARIABLES:	PREPARED BY:
Temperature: 20-71.4°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of pentane in water at 32 atm.

$t/°C$	$g(1)/100 \ g \ sln$	$10^5 x_1$
20	0.011	2.7
37.8	0.015	3.9
71.4	0.026	6.4

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

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined from gas-liquid equilibrium measurements in the ternary system pentane-water-methane at 32 atm. in an apparatus described in ref 1. No more details were reported in the paper.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES: 1. Rogov, B.A.; Namiot, A. Yu.; Bondareva, M.M. *Tr. Vses. Neftegazov. Nauch. Issled. Inst.* <u>1958</u>, *15*, 196.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Barone, G.; Crescenzi, V.; Pispisa, B.; Quadrifoglio, F. *J. Macromol. Chem.* 1966, *1*, 761-71.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors report a value of 0.00103 mol(1)/dm³(2) for the solubility of pentane in water at 25°C. This value is the experimental one multiplied by 760/p where p is the partial pressure of (1) over (2). p = 508 mm Hg. The solubility at system pressure calculated by the compiler is 6.88×10^{-4} mol(1)/dm³(2) and the corresponding mass percent and mole fraction, x_1, are 0.00497 g(1)/100 g sln and 1.24×10^{-5} (with the assumption of a solution density of 1 g cm⁻³).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation was carried out by bubbling the vaporized (1) into the solution and letting an excess of the condensed (1) stand in contact with the aqueous phase for more than 12 hr at 25°C under gentle shaking. 0.20 mL samples of (2) saturated with (1) were taken with a calibrated syringe and injected into the chromatographic column packed with 15% of poly(propylene glycol) on chromosorb. A gas chromatography unit having a tungsten-wire katharometer as detector was employed. More details are given in the paper.	(1) RP product, C. Erba, Milan; chromatographically pure. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.02 K soly. ± 4% (type of error not specified).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Connolly, J.F. *J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

VARIABLES:	PREPARED BY:
Temperature: 300-325°C Pressure: 150-700 atm	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

$t/°C$	p/atm	p/MPa (compiler)	g(1)100 g sln	x_1 (compiler)
300	150	15.2	1.3	0.0033
	185	18.7	1.7	0.0043
	350	35.4	1.7	0.0043
	600	60.7	1.6	0.0040
	700	70.9	1.5	0.0038
330	170	17.2	2.1	0.0053
	195	19.7	3.3	0.0084
	220	22.2	4.0	0.0103
	260	26.3	4.6	0.0119
	350	35.4	4.9	0.0127
	485	49.1	4.7	0.0122
	670	67.8	4.0	0.0103
340	230	23.3	5.2	0.0135
	250	25.3	6.1	0.0160
	275	27.8	6.9	0.0182
	330	33.4	7.6	0.0201
	350	35.4	7.6	0.0201
	470	47.6	6.9	0.0182
	620	62.8	5.7	0.0149

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.	(1) Phillips reagent grade; better than 99.8%; used as received. (2) distilled and deaerated.
	ESTIMATED ERROR: temp. ± 0.02 K press. ± 2 atm (accuracy)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0]	Connolly, J.F.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

$t/°C$	p/atm	p/MPa (compiler)	g(1)100 g sln	$x1$ (compiler)
350	240	24.31	7.8	0.0207
	225	25.83	9.0	0.0241
	265	26.84	10.3	0.0279
	280	28.36	12.1	0.0332
	300	30.39	13.9	0.0387
	325	32.92	15.5	0.0438
	350	35.46	15.5	0.0438
	395	40.01	13.9	0.0387
	445	45.08	12.0	0.0329
	510	51.66	10.3	0.0279
	590	59.77	9.0	0.0241
352	280	28.36	15.8	0.0442
	280	28.36	18.4	0.0533
	280	28.36	21.0	0.0622
	280	28.36	23.3	0.0705
	400	40.52	40.7	0.1463
	390	39.51	38.7	0.1362
	385	39.00	36.5	0.1255
	380	38.49	34.0	0.1140
	375	37.99	31.4	0.1026
	375	37.99	28.5	0.0905
	375	37.99	25.4	0.0784
	375	37.99	23.3	0.0705
	380	38.49	21.0	0.0622
	390	39.51	18.4	0.0533
	420	42.55	15.7	0.0444

COMMENTS AND ADDITIONAL DATA:

Upper critical solution temperature: 351°C at p = 340 atm.

The uncertainty in the CST is about 2°C and that of the corresponding pressure about 10 atm.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentane in water at 25°C was reported to
be 38.5 mg (1)/kg sln, (0.0385 g/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler,
is 9.6×10^{-6}.
The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 2 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Nelson, H.D.; De Ligny, C.L. *Rec. Trav. Chim. Pays-Bas* <u>1968</u>, *87*, 528-44.
VARIABLES: Temperature: 4-30°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

$t/°C$	$10^5 x_1$	mg(1)/kg sln (compiler)
4.0	1.02 ± 0.20	40.9
10.0	1.07 ± 0.15	42.9
20.0	0.98 ± 0.19	39.3
25.0	1.01 ± 0.12	40.5
30.0	1.01 ± 0.17	40.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips pure grade. (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 (90% probability interval)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions" U.S. Nat. Tech. Inform. Serv., PB Rep., <u>1972</u>, No. 21163, 113 pp.
VARIABLES: Temperature: 278.26-308.36 K	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

T/ K	g(1)/100 g sln	$10^3 x_1$	g(1)/100 g sln (corrected by compiler)
278.26	0.001094 ± 0.000037	0.02732	0.01094
288.36	0.001180 ± 0.000034	0.02946	0.01180
298.26	0.001128 ± 0.000045	0.02816	0.01128
308.36	0.001089 ± 0.000051	0.02719	0.01089

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Fisher Scientific Co.; certified grade; used as received. (2) laboratory distilled water.
	ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of pentane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	65.7^c	1.64×10^{-5}
25^b	47.6^c	1.19×10^{-5}

Solubility of water in pentane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	26^d	1.04×10^{-4}
25^b	101^e	4.04×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

	ESTIMATED ERROR:
	temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%; e) ± 3.1% (mean)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of pentane in water at system pressure

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^5 x_1$ (compiler)
25.0	39.5 ± 0.6	0.00395	0.99
40.1	39.8 ± 0.9	0.00398	0.99
55.7	41.8 ± 1.3	0.00418	1.04
99.1	69.4 ± 1.1	0.00694	1.73
121.3	110.0 ± 10.0	0.0110	2.74
137.3	201.0 ± 5.0	0.0201	5.01
149.5	298.0 ± 14.0	0.0298	7.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Room-temperature solubilities were determined by use of screw-cap test tubes. The (1) phase floated on top of (2) and ensured 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 al-lowed 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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

ESTIMATED ERROR:
temp. ± 1 K soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	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 pentane in water at 20°C was reported to be
0.7 g(1)dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.07 g(1)/100 g sln and 1.7×10^{-4}. The
assumption that 1 dm^3 sln = 1 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta Katowice* <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of pentane in water at 25°C was reported to be 39 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0039 g(1)/100 g sln and 9.7×10^{-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.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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. 0.8 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of pentane between the gas and aqueous phase. $\alpha = 49 \pm 1$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 512.5$ mm of Hg and $\log C_g = \log p - 4.269$ = -1.56 expressed in moles per liter. Therefore $C_s = 5.63 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0040 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.0×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 10% (estimated by the compiler)
	REFERENCES: 1. Hine, J.; Mooker, P.K. *J. Org. Chem.* <u>1975</u>, *4*, 292.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (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 pentane in water

t/°C	mg(1)/kg sln	10^3g(1)/100g sln (compiler)	$10^5 x_1$ (compiler)
15	42.9	4.29	1.07
20	41.4	4.14	1.03
25	40.6	4.06	1.01
30	40.3	4.03	1.01
35	40.6	4.06	1.01

[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:	SOURCE AND PURITY OF MATERIALS:
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.	(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:	ORIGINAL MEASUREMENTS:
(1) Pentane; C_5H_{12}; [109-66-0] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 1-360 g(2)/kg sln	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Pentane in Aqueous NaCl

Salinity g(2)/kg sln	10^3 g(1)/100 g sln	$10^6 x_1$ (compilers)
1.002	3.68	9.19
10.000	3.45	8.67
34.472[a]	2.76	7.05
50.030	2.26	5.84
125.100	1.09	2.95
199.900	0.591	1.67
279.800	0.264	0.777
358.700	0.201	0.614

[a]Artificial seawater, composition not specified but probably
  similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	(1) commercial, 99 + % pure
	ESTIMATED ERROR: Temperature ± 1 K Solubility ± 10 relative %
	REFERENCES: 1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* <u>1940</u>, *3*, 135.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 the system benzene (1) and water (2) have been reported in the references listed in Table 1.

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

Reference	T/K	Solubility	Method
Herz (ref 1)	295	(1) in (2)	densimetric
Groschuff (ref 2)	278-350	(2) in (1)	titration
Clifford (ref 4)	284-328	(2) in (1)	analytical
Hill (ref 5)	273	(2) in (1)	cryoscopic
Hill (ref 6)	278-343	(1) in (2)	analytical
Jaeger (ref 7)	373-573	(1) in (2)	cloud-point
Milligan (ref 8)	298	(1) in (2)	analytical
Barbaudy (ref 9)	342	mutual	cloud-point
Uspenskii (ref 10)	283,295	mutual	titration, analytical
Rosenbaum and Walton (ref 11)	283-333	(2) in (1)	gasometric
Gross and Saylor (ref 12)	303	(1) in (2)	interferometric
Tarassenkow and Poloshinzewa (ref 13)	278-346	(2) in (1)	synthetic
Robertson (ref 14)	279	(2) in (1)	cryoscopic
Niini (ref 15)	293	mutual	refractometric, pycnometric
Saylor *et al.* (ref 16)	303-308	(1) in (2)	interferometric
Berkengeim (ref 18)	283-323	(2) in (1)	Karl Fischer
Staveley *et al.* (ref 19)	297-344	(2) in (1)	synthetic
Durand (ref 20,25)	289	(1) in (2)	synthetic
Stearns *et al.* (ref 21)	298	(1) in (2)	turbidimetric
Booth and Everson (ref 22,27)	298,333	(1) in (2)	residue volume
Joris *et al.* (ref 23,24)	283-299	(2) in (1)	radiotracer
Andrews and Keefer (ref 26)	298	(1) in (2)	spectrophotometric
Griswold *et al.* (ref 28)	298,323	mutual	cloud-point
Klevens (ref 29)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 30)	273-316	(1) in (2)	spectrophotometric
McBain and Lissant (ref 31)	298	(1) in (2)	synthetic
Staveley *et al.* (ref 32)	295-346	(2) in (1)	synthetic
Donahue and Bartell (ref 33)	298	mutual	interferometric
McDevit and Long (ref 34)	298	(1) in (2)	volumetric
Morrison and Billett (ref 35)	298	(1) in (2)	analytical
McCants *et al.* (ref 36)	311	mutual	titration
Hayashi and Sasaki (ref 37)	293,298	(1) in (2)	titration

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 1 (continued)

Reference	T/K	Solubility	Method
Umano and Hayano (ref 38)	459-554	(2) in (1)	volumetric
Wing and Johnston (ref 39)	298	(2) in (1)	radiotracer
Arnold *et al.* (ref 40)	273-342	(1) in (2)	spectrophotometric
Brady and Huff (ref 41)	298	(1) in (2)	vapor pressure
Pavia (ref 42)	282-388	(2) in (1)	Karl Fischer
Alexander (ref 43)	273-338	(1) in (2)	spectrophotometric
Rebert and Kay (ref 44)	556-580[a]	mutual	synthetic
Caddock and Davies (ref 45)	293	(2) in (1)	radiotracer
Kudchadker and McKetta (ref 46)	311-411[a]	(1) in (2)	not specified
Franks *et al.* (ref 48)	290-336	(1) in (2)	spectrophotometric
Guseva and Parnov (ref 49)	426-537[a]	(1) in (2)	cloud-point
Jones and Monk (ref 50)	298-308	(2) in (1)	radiotracer
McAuliffe (ref 51,60)	298	(1) in (2)	GLC
Schatzberg (ref 52)	293	(2) in (1)	Karl Fischer
Udovenko and Aleksandrova (ref 53)	293-353	(1) in (2).	not specified
Hoegfeldt and Bolander (ref 54)	298	(2) in (1)	Karl Fischer
Thompson and Snyder (ref 55)	311-477[a]	mutual	analytical
Englin *et al.* (ref 56)	273-323	(2) in (1)	analytical
Connolly (ref 57)	533-573[a]	(1) in (2)	cloud-point
Johnson *et al.* (ref 58)	298	(2) in (1)	Karl Fischer
Masterton and Gendrano (ref 59)	298	(2) in (1)	Karl Fischer
Moule and Thurston (ref 61)	282-323	(2) in (1)	radiotracer
Taha *et al.* (ref 62)	298	(1) in (2)	vapor pressure
Alwani and Schneider (ref 63)	523-636[a]	mutual	synthetic
Gregory *et al.* (ref 64)	308	(2) in (1)	Karl Fischer
O'Grady (ref 65)	561-566[a]	mutual	volumetric
Worley (ref 66)	298	(1) in (2)	spectrophotometric
Burd and Braun (ref 67)	359-473[a]	(2) in (1)	GLC
Roddy and Coleman (ref 68)	298	(2) in (1)	gravimetric
Corby and Elworthy (ref 71)	293	(1) in (2)	spectrophotometric
Pierotti and Liabastre (ref 72)	278-319	(1) in (2)	GLC
Ben-Naim *et al.* (ref 73)	283-323	(1) in (2)	spectrophotometric
Bradley *et al.* (ref 74)	298-328[a]	(1) in (2)	spectrophotometric
Filyas (ref 75)	568	(2) in (1)	not specified
Karlsson (ref 76)	287-308	(2) in (1)	Karl Fischer
Leinonen and Mackay (ref 77)	298	(1) in (2)	GLC

(Table 1 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 1 (continued)

Reference	T/K	Solubility	Method
Polak and Lu (ref 78)	273,298	mutual	GLC
Sultanov and Skripka (ref 79,89)	498-533[a]	(2) in (1)	not specified
Brown and Wasik (ref 80)	278-293	(2) in (1)	GLC
Goldman (ref 81)	283-313	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 82)	298	(1) in (2)	GLC
Mackay and Shiu (ref 83)	298	(1) in (2)	GLC
Sada et al. (ref 84)	298	(1) in (2)	titration
Budantseva et al. (ref 85)	293	mutual	GLC
Kirchnerova and Cave (ref 87)	298	(2) in (1)	Karl Fischer
Price (ref 88)	298	(1) in (2)	GLC
Korenman and Aref'eva (ref 90,91)	293,298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 92)	298	(1) in (2)	GLC
May et al. (ref 93)	298	(1) in (2)	GLC
Singh and Sah (ref 94)	303	(2) in (1)	titration
Bittrich et al. (ref 95)	293-333	mutual	GLC
Banerjee et al. (ref 97)	298	(1) in (2)	radiotracer
Schwarz (ref 98)	297	(1) in (2)	chromatographic
Sanemasa et al. (ref 100)	288-318	(1) in (2)	spectrophotometric
Sanemasa et al. (ref 101)	278-318	(1) in (2)	spectrophotometric
Tsonopoulos and Wilson (ref 102)	313-473[a]	mutual	GLC, Karl Fischer
Sanemasa et al. (ref 103)	298	(1) in (2)	spectrophotometric

a. Pressure also varied, see Table 4

Quantitative solubility data for the benzene-heavy water (D_2O) system are given in the papers by Ben-Naim et al. (ref 73), in terms of the Ostwald absorption coefficient, and Backx and Goldman (ref 99). However, these data have not been determined under comparable conditions and thus no Critical Evaluation is possible. The interested user is referred to the relevant Data Sheets for experimental values. Solubility data may also be calculated from the calorimetric data of Gill et al. (ref 86). Bröllos et al. (ref 69) have also reported data on a critical locus in the D_2O-benzene system (cf. Section 3 below).

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

Critical phenomena in the benzene-water system have been reported by Alwani and Schneider (ref 63), Roof (ref 70) and Scheffer (ref 108). These data are discussed along with the solubility data at elevated pressures in Section 3 below.

The extensive information available for the solubility of benzene in brine solutions is considered in a separate Critical Evaluation immediately following the benzene-water Data Sheets.

Apart from the papers by Roof (ref 70) and Scheffer (ref 108) which did not contain sufficient information to justify their inclusion; and the work of Horiba (ref 3), Vermillion (ref 17), Thompson (ref 47) and Herz (ref 107) which were not available for inspection, the original data in all of the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation. The data of Gorbachev *et al.* (ref 109, 110) are noted but arrived too late to be included in this Evaluation.

In the benzene-water system the mutual solubilities are sufficiently low at atmospheric pressures to enable data reported on w/v fractions (or equivalent) to be converted to mass percent solubilities with reasonable precision by assuming solution densities to be the same as the pure solvents. These conversions are given on the Data Sheets and data are included in this Evaluation. The data of Herz (ref 1), Jaeger (ref 7), Milligan (ref 8), Durand (ref 20,25), Booth and Everson (ref 22,27), Jones and Monk (ref 50) and Sada *et al.* (ref 84) given in v/v fractions have not been converted and so have been excluded.

For convenience, further discussion of this system will be divided into three parts: the solubility of benzene in water and of water in benzene at atmospheric pressure, and their mutual solubilities at higher temperatures and pressures.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation of the original measurements compiled in the data sheets are indicated by an asterisk (*). The uncertainty limits (given as standard deviations, σ_n) attached to the mean "Best" values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits. Where relevant, 95% confidence intervals have been calculated for the mass percentage solubilities, as error estimates using the *t*-distribution and are given along with the mean values. Error estimates have not been included for mole fraction

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

solubilities because of space limitations but may be assumed to be the same (proportionately) as those given for the mass percentage solubilities. The letter (R) indicates "Recommended" data. Data are "Recommended" if σ_n is less than 5% (relative) of the average solubility. All other data are regarded as Tentative.

1.   THE SOLUBILITY OF BENZENE (1) IN WATER (2) AT ATMOSPHERIC PRESSURE

Table 1 shows a plethora of studies of the solubility of benzene in water: 29 independent values have been reported at 298K! Most of the data are in good agreement enabling solubilities to be "Recommended" over almost the entire liquid range at atmospheric pressure.

The data of Niini (ref 15), Stearns *et al.* (ref 21), McBain and Lissant (ref 31), Hayashi and Sasaki (ref 37), Kudchadker and McKetta (ref 46, atmospheric pressure data only), Udovenko and Aleksandrova (ref 53), Worley (ref 68), Pierotti and Liabastre (ref 72), Krasnoshchekova and Gubergrits (ref 82), Korenman and Aref'eva (ref 90,91), Schwarz (ref 98) and Sanemasa *et al.* (ref 100,101,103), reported mainly at 293 or 298K, disagree markedly with other studies and have therefore been rejected.

The approximate solubilities of Griswold *et al.* (ref 28), Taha *et al.* (ref 62) and Budantseva *et al.* (ref 85) have been excluded from consideration because of the abundance of more precise values.

All other data on the solubility of benzene in water are included in Table 2. Also included in Table 2 are the mean "Best" values and the 95% confidence intervals.

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

	Solubility values		
T/K	Reported values[a] g(1)/100g sln	"Best" values ± σ_n (C.I.)[b] g(1)/100g sln	$10^4 x_1$
273[c]	0.153 (ref 5), 0.185 (ref 43), 0.168 (ref 78)	0.169 ± 0.013(0.032)[c]	3.90
278	0.181* (ref 30), 0.172 (ref 40), 0.182* (ref 43), 0.185 (ref 80)	0.180 ± 0.005(0.005)(R)	4.15(R)
283	0.175 (ref 10), 0.180 (ref 30), 0.173* (ref 40), 0.179* (ref 43), 0.181* (ref 80)	0.178 ± 0.003(0.004)(R)	4.11(R)

(Table 2 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 (continued)

T/K	Reported values[a] g(1)/100g sln	"Best" values $\pm \sigma_n$(C.I.)[b] g(1)/100g sln	$10^4 x_1$
288	0.178* (ref 30), 0.173 (ref 40), 0.178* (ref 43), 0.170* (ref 48), 0.179* (ref 80)	0.176 ± 0.003(0.004)(R)	4.06(R)
293	0.178* (ref 30), 0.171 (ref 40), 0.178* (ref 43), 0.172* (ref 48), 0.177* (ref 80), 0.179 (ref 95).	0.176 ± 0.003(0.003)(R)	4.06(R)
298	0.174 (ref 26), 0.186 (ref 29), 0.179 (ref 30), 0.182 (ref 33), 0.172 (ref 35), 0.180 (ref 37), 0.175* (ref 40), 0.176 (ref 41), 0.180* (ref 43), 0.173* (ref 48), 0.178 (ref 51,60), 0.170 (ref 71), 0.177 (ref 77), 0.176 (ref 78), 0.178 (ref 83), 0.174 (ref 88), 0.174 (ref 92), 0.179 (ref 93), 0.175 (ref 97)	0.177 ± 0.004(0.002)(R)	4.09(R)
303	0.185 (ref 12), 0.184 (ref 16), 0.184* (ref 30), 0.177 (ref 40), 0.182* (ref 43), 0.176* (ref 48)	0.181 ± 0.004(0.005)(R)	4.18(R)
308	0.190 (ref 16), 0.189* (ref 30), 0.182 (ref 40), 0.187* (ref 43), 0.181* (ref 48)	0.186 ± 0.004(0.006)(R)	4.30(R)
313	0.195* (ref 30), 0.188 (ref 40), 0.194* (ref 43), 0.188* (ref 48), 0.203 (ref 95), 0.192[d] (ref 102)	0.193 ± 0.005(0.006)(R)	4.46(R)
318	0.197 (ref 40), 0.203* (ref 43), 0.196* (ref 48), 0.201[d] (ref 102)	0.199 ± 0.003(0.006)(R)	4.60(R)
323	0.205* (ref 40), 0.212* (ref 43), 0.205* (ref 48), 0.209[d] (ref 102)	0.208 ± 0.003(0.006)(R)	4.81(R)
328	0.216* (ref 40), 0.223* (ref 43), 0.216* (ref 48), 0.220[d] (ref 102)	0.219 ± 0.003(0.006)(R)	5.06(R)
333	0.227* (ref 40), 0.238* (ref 43), 0.228* (ref 48), 0.231[d] (ref 102)	0.231 ± 0.004(0.007)(R)	5.34(R)
338	0.242* (ref 40), 0.236* (ref 43), 0.241* (ref 48), 0.245[d] (ref 102)	0.241 ± 0.003(0.006)(R)	5.57(R)
343	0.281 (ref 9), 0.261* (ref 40), 0.259[d] (ref 102)	0.267 ± 0.010(0.03) (R)	6.17

a Values marked with an asterisk (*) have been graphically interpolated by the Evaluator from the authors' original data.
b Obtained by averaging; figures in parentheses are the 95% confidence intervals (t - test).   c Refers to supercooled liquid (1).
d Calculated from original authors' fitting equation over the range of their experimental investigation.   (continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 plots the mean solubility values as a function of temperature. Using non-linear regression, these values can be fitted to an equation of the form:

$$s\,(g(1)/100g\ sln) = 5.5773 - 4.6067 \times 10^{-2}T + 1.2504 \times 10^{-4}T^2 - 1.0489 \times 10^{-7}T^3 \quad [1]$$

(Range T: 273-343K, std. error of estimate = 0.0008 g(1)/100g sln., correlation coefficient = 0.9995).

A similar equation was obtained by Arnold et al. (ref 40) from a least squares treatment of their own data:

$$s\,(g(1)/100g\ sln) = 0.1784 - 7.436 \times 10^{-4}t + 1.906 \times 10^{-5}t^2 + 1.217 \times 10^{-7}t^3 \quad [2]$$

(Range t: 5-70°C, std. dev. 0.0028 g(1)/100g sln).
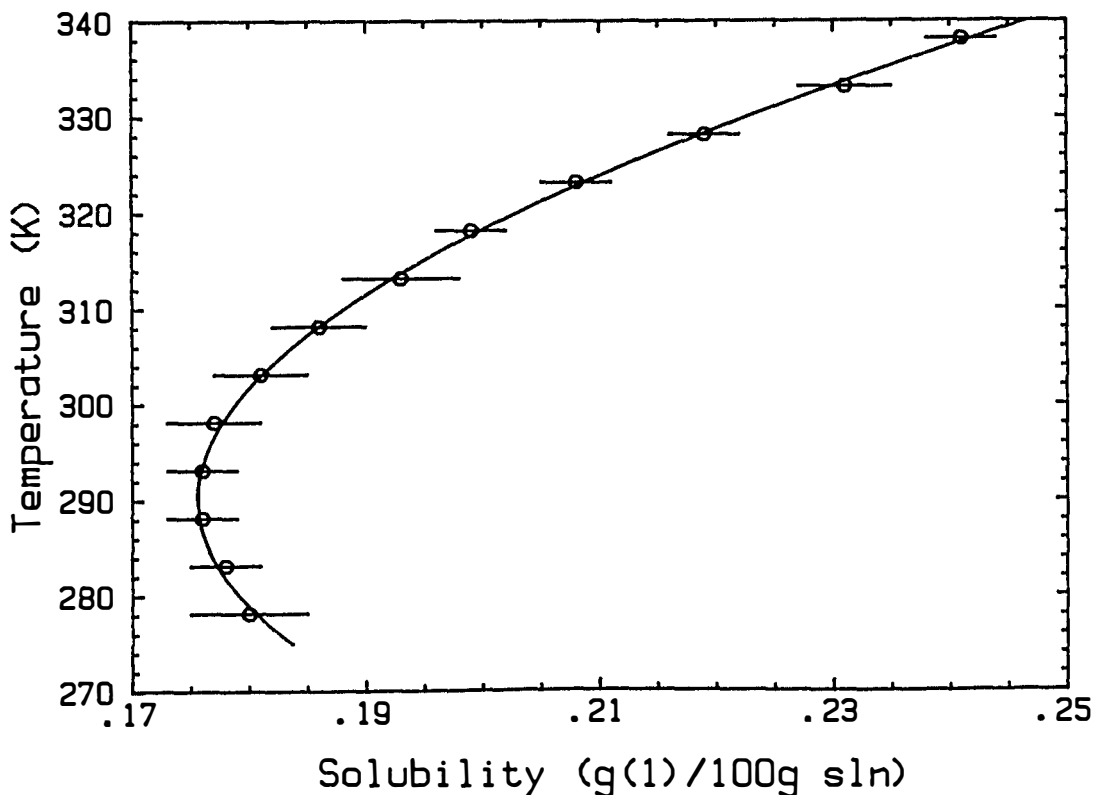
FIGURE 1. Solubility of benzene in water: "Best" values. Error bars represent $\pm\sigma_n$.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

Solubilities calculated from equation [2] are generally 2% (relative) lower than those obtained from equation [1], *i.e.* within the limits of precision of the Recommended values in Table 2.

Gill *et al.* (ref 86) present an alternative equation derived from calorimetric studies of the enthalpy and heat capacity of solution of benzene in water between 288 and 303 K.

$$\ln\{x_1(T)/x_1(T^\dagger)\} = (\Delta C^\infty_{p,\text{sln}}/R)\{\ln(T/T^\dagger) + (T^\dagger/T) - 1\} \qquad [3]$$
$$(\Delta C^\infty_{p,\text{sln}} = 225 \text{ J K}^{-1} \text{ mol}^{-1}, \; T^\dagger = 289.0 \text{ K}, \; \ln x_1(T^\dagger) = -7.843)$$

where $\Delta C^\infty_{p,\text{sln}}$ is the infinite dilution heat capacity for benzene in water and $T^\dagger$ the temperature of the solubility minimum. Solubilities calculated from this equation are in good agreement (typically lower by 2% relative) with equation [1] over the range 288-303 K. However, they show a systematically increasing deviation at higher temperatures rising to -5.3% at 333 K, *i.e.* slightly outside the precision limits of the recommended values although well within the 95% confidence interval.

Consistent with these findings, application of the van't Hoff equation to the recommended solubilities (Table 2) gives $\Delta H^\infty_{\text{sln}} = 2.07$ kJ mol^{-1} and $\Delta C^\infty_{p,\text{sln}} = 232$ J K^{-1} mol^{-1} for the dissolution of benzene in water in good agreement with the experimental values of Gill *et al.* No evidence was found for any dependence of $\Delta C^\infty_{p,\text{sln}}$ on temperature.

Finally, it is worthwhile noting that Green and Frank (ref 96) have concluded from Henry's law measurements and other thermodynamic data that benzene dissolves in water in monomeric form. These authors also show that solubility determinations based on the measurement of benzene in the vapor-phase by UV spectrophotometry (*e.g.* ref 73) may be seriously in error.

2. THE SOLUBILITY OF WATER (2) IN BENZENE (1) AT ATMOSPHERIC PRESSURE

Despite the many studies of the solubility of water in benzene the reported values are in only fair agreement. This is probably a reflection of the difficulties of quantitating the relatively low water solubility. Thus, the *absolute* uncertainty in the averaged solubility of (2) in (1) is virtually independent of the magnitude of the solubility thereby increasing the *relative* uncertainty at lower solubilities.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

The wealth of publications reporting solubility as a function of temperature (ref 2, 5, 6, 13, 19, 32, 56, 61, 81) enables a particularly critical appraisal of all reported solubilities. Hence data which might be acceptable in less well investigated systems have been rejected if they deviate significantly from averaged values. This procedure has a small effect on the mean value but often results in a substantial decrease in the uncertainty (σ_n).

On this basis the data of Clifford (ref 4), Rosenbaum and Walton (ref 11; data below 303 K retained), Tarassenkow and Poloshinzewa (ref 13; data above 283 K retained), Berkengeim (ref 18), Joris *et al.* (ref 23, 24), Wing and Johnston (ref 39), Englin *et al.* (ref 56; data below 303 K retained), Budantseva *et al.* (ref 85) and Bittrich (ref 95) have been rejected. Most of these data are lower than the mean values. The approximate values of Griswold *et al.* (ref 28) and McCants *et al.* (ref 36) have also been excluded as more precise data are available. All other data are included in Table 3.

It is interesting to note that the average solubilities reported in the more recent studies (ref 58, 59, 61, 64, 68, 76, 78, 81, 87, 94, 102) tend to be somewhat higher than the overall average and with considerably smaller σ_n (see Table 3). The reasons for these differences are unclear but could be due to improved analytical or purification techniques. If only the more recent data are considered then the averaged values could be "Recommended" between 283 and 298 K. However, comparison of the earlier data (with ref 58 arbitrarily chosen as the cut off) with the more recent values by standard statistical procedures (*t*-test or *F*-test) indicates that these two data sets differ significantly $(P < 0.05)$ only at 298 K and possibly 288 K. Further careful measurements are required to resolve this situation.

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

T/K	Reported values[a] g(2)/100g sln	"Best" values $\pm \sigma_n$ (C.I.)[b] g(2)/100g sln	$10^3 x_2$
273	0.029* (ref 2), 0.0400 (ref 56), 0.0302 (ref 78)	$0.033 \pm 0.005(0.012)$	1.4
278	0.032* (ref 2), 0.034* (ref 6), 0.035 (ref 14), 0.042* (ref 56)	$0.036 \pm 0.004(0.006)$	1.6

(Table 3 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 3 (continued)

T/K	Reported values[a] g(2)/100g sln	"Best" values $\pm \sigma_n$ (C.I.)[b] g(2)/100g sln	$10^3 x_2$
	Solubility values		
283	0.038* (ref 2), 0.042* (ref 6), 0.051 (ref 10), 0.0451 (ref 11), 0.040 (ref 18), 0.0425* (ref 42), 0.0446 (ref 56), 0.045 (ref 61), 0.0440 (ref 81)	0.044 ± 0.003(0.002) [0.0445 ± 0.0005][b]	1.9 [1.93]
288	0.045* (ref 2), 0.052* (ref 6), 0.057* (ref 10), 0.050* (ref 11), 0.043* (ref 13), 0.046* (ref 18), 0.0510* (ref 42), 0.051* (ref 56), 0.0530 (ref 61), 0.0533 (ref 76), 0.0522 (ref 81)	0.050 ± 0.004(0.003) [0.0528 ± 0.0005][b]	2.2 [2.29]
293	0.055* (ref 2), 0.064* (ref 6), 0.064* (ref 10), 0.0573 (ref 11), 0.054* (ref 13), 0.059 (ref 15), 0.053 (ref 18), 0.053* (ref 32), 0.0603* (ref 42), 0.052 (ref 45), 0.0532 (ref 52), 0.0582 (ref 56), 0.0635* (ref 61), 0.0631 (ref 76), 0.0618 (ref 81), 0.0586 (ref 95)	0.058 ± 0.006(0.003) [0.062 ± 0.002][b]	2.5 [2.69]
298	0.066* (ref 2), 0.077* (ref 6), 0.065* (ref 11), 0.065* (ref 13), 0.069* (ref 19), 0.067* (ref 32), 0.072 (ref 33), 0.0710* (ref 42), 0.066* (ref 54), 0.065 (ref 56), 0.0719 (ref 58), 0.0715 (ref 59), 0.0740* (ref 61), 0.0747 (ref 68), 0.0725* (ref 76), 0.0691 (ref 78), 0.0725 (ref 81), 0.0719 (ref 87)	0.070 ± 0.004(0.002) [0.0722 ± 0.0016][b]	3.0 [3.13]
303	0.080* (ref 2), 0.090* (ref 6), 0.077* (ref 13), 0.082* (ref 19), 0.083* (ref 32), 0.0828* (ref 42), 0.0860* (ref 61), 0.0854 (ref 76), 0.082 (ref 81), 0.082 (ref 94)	0.083 ± 0.003(0.002)(R) [0.084 ± 0.002][b]	3.60(R) [3.64]
308	0.095* (ref 2), 0.105* (ref 6), 0.089* (ref 13), 0.097* (ref 19), 0.097* (ref 32), 0.0970* (ref 42), 0.102 (ref 61), 0.097 (ref 64), 0.102 (ref 76), 0.0979 (ref 81)	0.098 ± 0.004(0.003)(R) [0.099 ±0.002][b]	4.23(R) [4.30]
313	0.114 (ref 2), 0.122* (ref 6), 0.102 (ref 13), 0.114* (ref 19), 0.114* (ref 32), 0.112* (ref 42), 0.118* (ref 61), 0.110 (ref 81), 0.112 (ref 102)	0.113 ± 0.005(0.004)(R)	4.87(R)
318	0.134* (ref 2), 0.140* (ref 6), 0.126 (ref 13), 0.135* (ref 19), 0.135* (ref 32), 0.131* (ref 42), 0.138 (ref 61), 0.133[c] (ref 102)	0.134 ± 0.004(0.004)(R)	5.78(R)

(Table 3 continued next page)

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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 3 (continued)

/K	Solubility values		
	Reported values[a] g(2)/100g sln	"Best" values $\pm \sigma_n$(C.I.)[b] g(2)/100g sln	$10^3 x_2$
323	0.158* (ref 2), 0.156* (ref 6), 0.150* (ref 13), 0.160* (ref 19), 0.156* (ref 32), 0.152* (ref 42), 0.160* (ref 61), 0.152[c] (ref 102)	0.156 ± 0.003(0.003)(R)	6.74(R)
328	0.184 (ref 2), 0.173* (ref 6), 0.175 (ref 13), 0.223 (ref 19), 0.210* (ref 32), 0.201* (ref 42), 0.203[c] (ref 102)	0.179 ± 0.006(0.006)(R)	7.76(R)
333	0.213* (ref 2), 0.198* (ref 6), 0.203* (ref 13), 0.223 (ref 19), 0.210* (ref 32), 0.201* (ref 42), 0.203[c] (ref 102)	0.207 ± 0.008(0.008)(R)	8.96(R)
338	0.246* (ref 2), 0.230* (ref 6), 0.234* (ref 13), 0.256* (ref 19), 0.242* (ref 32), 0.226* (ref 42), 0.233[c] (ref 102)	0.238 ± 0.010(0.010)(R)	10.0(R)
343	0.283* (ref 2), 0.270* (ref 6), 0.279* (ref 9), 0.272* (ref 13), 0.290* (ref 19), 0.280* (ref 32) 0.266[c] (ref 102)	0.277 ± 0.008(0.008)(R)	11.9(R)

a Values marked with an asterisk (*) have been graphically interpolated by the Evaluator from the authors' original data.
b Figures in round parentheses () are 95% confidence intervals (t-test). Values in square parentheses [] are averages $\pm \sigma_n$ of the most recent determinations (ref 58, 59, 61, 64, 68, 76, 78, 81, 87, 94, 102).
c Calculated from the original authors' fitting equation over the range of their experimental data.

Figure 2 plots the mean solubility values as a function of temperature. These values can be fitted to an equation of the form:

$$s \text{ (g(2)/100g sln)} = -5.6667 + 6.3536 \times 10^{-2}\, T - 2.4024 \times 10^{-4}\, T^2 + 3.0752 \times 10^{-7}\, T^3$$

(Range: T = 273 - 343 K, std. error of estimate = 0.001 g(2)/100g sln, correlation coefficient = 0.9998).

A similar expression was obtained by Hill (ref 6) by fitting his own data:

$$s \text{ (g(2)/100g sln)} = 0.03294 + 6.449 \times 10^{-4}\, t + 3.728 \times 10^{-5}\, t^2$$

(Range: t = 5 - 70°C).

Staveley et al. (ref 32) present an alternative equation, in terms of mole fraction, based on their data:

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2); [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.
	June 1986.

CRITICAL EVALUATION: (continued)

$$\log x_2 = 2.237 - (1427/T)$$
over the range $T = 295 - 346$ K.

Application of the van't Hoff equation to the mean values in Table 3 gives $\Delta H^\infty_{sln} = 24.0$ kJ mol^{-1} and $\Delta C^\infty_{p,sln} = 89$ J K^{-1} mol^{-1} for the dissolution of water in benzene ($R^2 = 0.9995$).
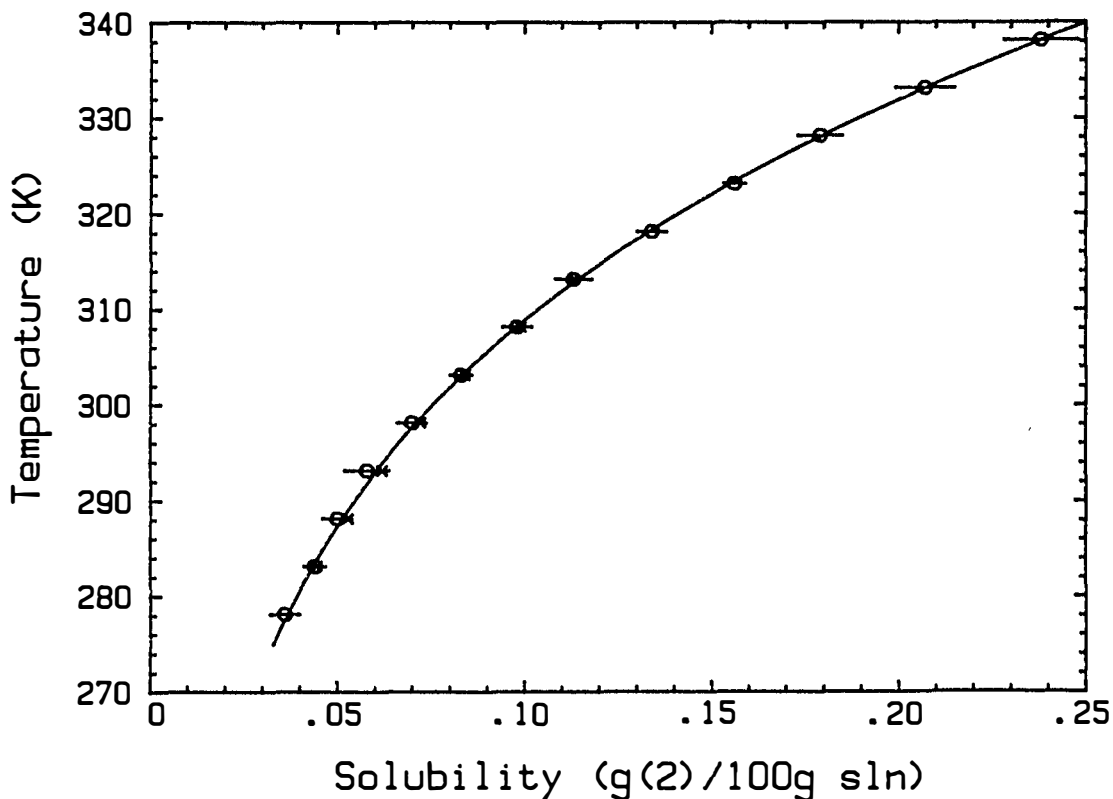
FIGURE 2. Solubility of water in benzene: average of all determinations (o); average of more recent determinations (x). Error bars represent $\pm\sigma_n$.

3. THE MUTUAL SOLUBILITIES OF BENZENE (1) AND WATER (2) AT ELEVATED PRESSURES

To clarify the relationship between the phases in equilibrium in this system it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram. On such a projection, phases with the same values of pressure and temperature but different composition will be located at the same point. Benzene + water has type III phase behaviour, using Scott and von Konynenburg's classification (ref 105 106). This type of phase behaviour is characterised by two critical loci, one starting at the critical point of the least volatile component, water in the present

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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.
	June 1986.

CRITICAL EVALUATION: (continued)

case, and eventually approaching high pressures. The other critical locus starts at the critical point of the other component and ends on a three phase (liquid-liquid-vapor) line at a critical end point. Type III phase behaviour is illustrated in Figure 3. It is important to note that the three phase line on a pressure-temperature projection corresponds to three lines on the pressure-temperature-composition diagram. In the region above the three phase line on the pressure-temperature projection, the pressure is greater than the vapor phase and 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 also possible to have one or two phases present depending on the over-all composition.
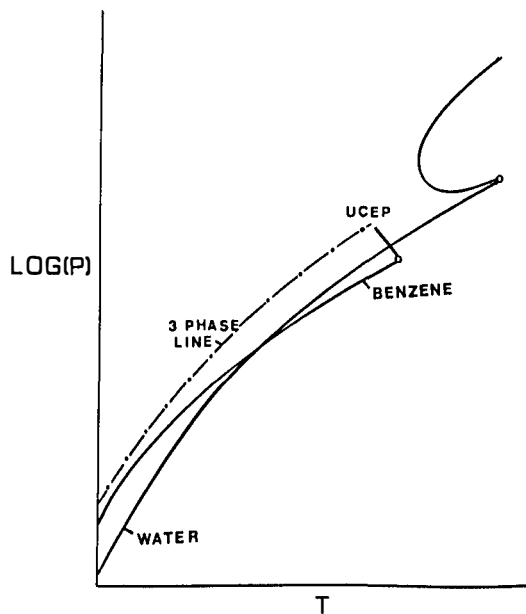
FIGURE 3. Pressure-temperature projection of the equilibrium pressure-temperature-composition surface for the benzene-water system.

Solubility data for the benzene-water system at elevated pressures have been reported in the publications listed in Table 4.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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.
	June 1986.

CRITICAL EVALUATION: (continued)

TABLE 4: Solubility Studies of the Benzene-Water System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Umano and Hayano (ref 38)	-[a]	459-554	(2) in (1)
Rebert and Kay (ref 44)	12-16	560-579	mutual
Kudchadker and McKetta (ref 46)	0.1-6	311-411	(1) in (2)
Guseva and Parnov (ref 49)	-[b]	426-527	(1) in (2)
Thompson and Snyder (ref 55)	7,36	311-477	mutual
Connolly (ref 57)	10-80	533-573	(1) in (2)
Alwani and Schneider (ref 63)	15-302	523-636	mutual
O'Grady (ref 65)	25	561,566	mutual
Burd and Braun (ref 67)	0.2-3	359-473	(2) in (1)
Bradley et al. (ref 74)	6	298-328	(1) in (2)
Filyas (ref 75)	1	568	(2) in (1)
Sultanov and Skripka (ref 79,89)	5-79	498-533	(2) in (1)
Tsonopoulos and Wilson (ref 102)	0-3[a]	377-485	mutual

a Along three phase line.
b Unspecified but presumably at pressures along the three phase line.

As Table 4 shows, almost none of the solubility data collected at elevated pressures have been obtained under comparable conditions thus making evaluation of their reliability difficult. Although some of the data are in reasonable agreement (e.g. the value of 22 g(1)/100g sln at 574.85 K and 14.6 MPa (ref 44) and 22.8 g(1)/100g sln at 573.15 K and 14.7 MPa (ref 57), most are not. Thus the interpolated solubilities of ref 46 and ref 55 at 311K and 5 MPa are 0.336 and 0.187 g(1)/100g sln respectively and other broadly comparable data (e.g. ref 55 and ref 57) are only in fair agreement. It should also be noted that the atmospheric pressure data of Kudchadker and McKetta (ref 46) are in poor agreement with the "Recommended" values in Tables 2 and 3.

Table 5 summarizes solubilities of benzene and water as a function of temperature and pressure. All values were obtained by double graphical interpolation (temperature and pressure) to produce data at convenient intervals. The interested user is referred to the original measurements in the Data Sheets for more comprehensive values. For the reasons given above all the values in Table 3 should be regarded as very tentative, subject to further investigations.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_8; [71-43-2] (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. June 1986.

CRITICAL EVALUATION: (continued)

TABLE 5: Tentative Values of the Mutual Solubilities of Benzene and Water at High Pressures[a]

T/K	p/MPa			
	1	10	20	30

(a) Benzene (1) in water (2), g(1)/100g sln

T/K	1	10	20	30
313	0.26[b]	0.20	0.22	0.23
373	0.40	0.41	0.50	0.56
423	1.0	1.1	1.1	1.3
473	3.0	3.3	3.5	3.2
523	6.5[c]	6.6[c]	6.9[c]	6.5[c]

(b) Water (2) in benzene (1), g(2)/100g sln

T/K	1	10	20	30
313	0.10	0.10	0.09	0.09
373	0.60	0.60	0.55	0.55
423	1.7	1.7	1.6	1.6
473	4.5	4.4	4.4	4.2
523	-	13.2[d]	11.5[d]	10.2[d]

[a] Data from ref 55 unless otherwise indicated.
[b] Averaged value of ref 46, 55.
[c] Data from ref 57.
[d] Data from ref 79, 89.

Figure 4 plots the mutual solubilities of benzene and water at elevated temperatures and pressures. The chief effect is to make the solution composition at the (projected) upper critical solution temperature more benzene-rich. This is because the solubility of benzene in water shows a smaller dependence on pressure than the solubility of water in benzene at temperatures near the UCST.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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.
	June 1986.

CRITICAL EVALUATION: (continued)
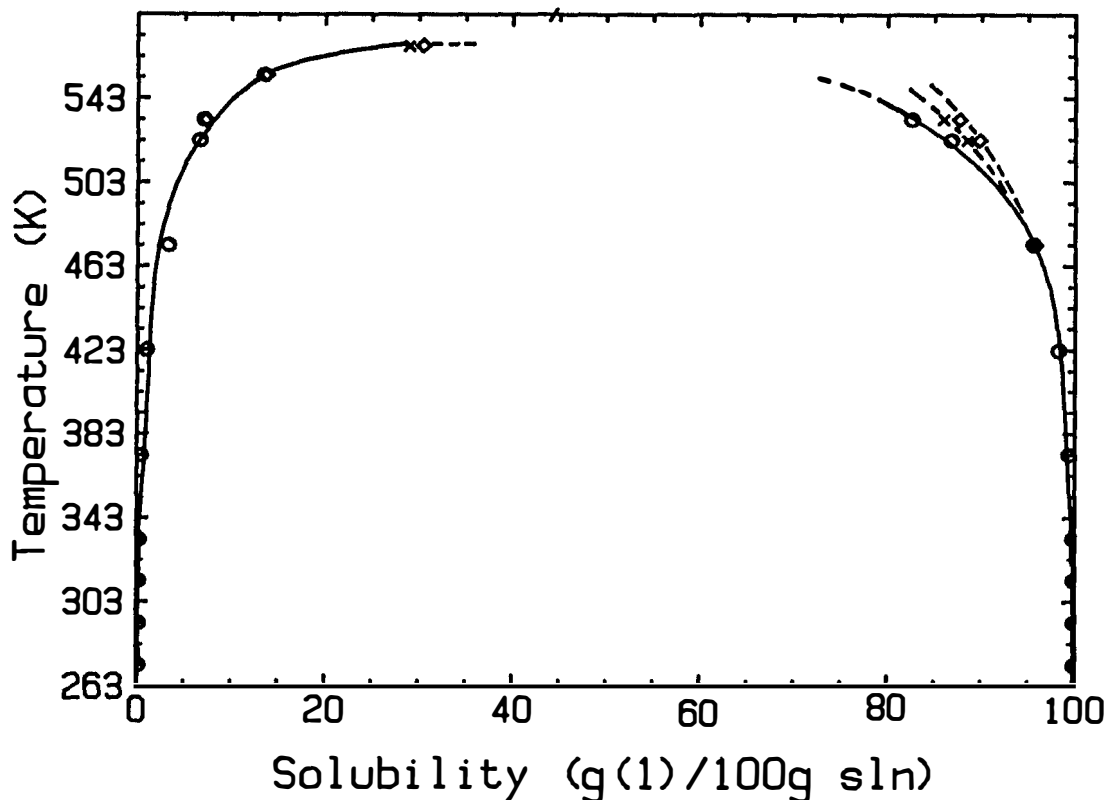
FIGURE 4. Mutual solubility of benzene (1) and water (2) at elevated temperatures and pressures: 0.1 or 10 MPa (o); 20 MPa (x); 30 MPa (◊).

A number of workers (ref 47, 49, 102) have studied the solubility of benzene in water along the three phase equilibrium locus (Figure 3). The data are summarized graphically in Figure 5 and are seen to be in only fair agreement (note that the solubility is represented logarithmically and that the data from ref 47 is only approximate, see Figure 5 caption). The interested user is referred to the relevant Data Sheets (ref 49, 102) for experimental values.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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. June 1986.

CRITICAL EVALUATION: (continued)
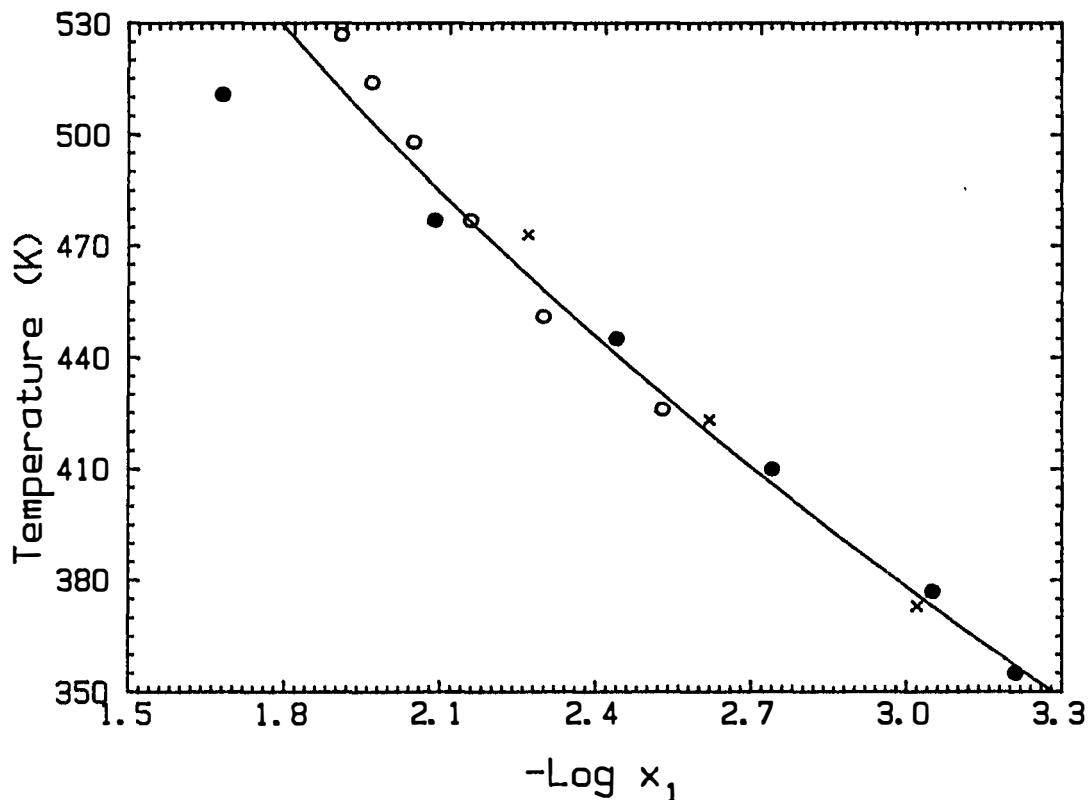
FIGURE 5.   Solubility of benzene in water at three phase equilibrium pressures: ref 47 (o, data obtained graphically from ref 102);   ref 49 (●); ref 102 (x).

The solubility of water in benzene along the three phase equilibrium locus has also been reported by three groups (ref 38, 47, 102). The data are summarized graphically in Figure 6 and are seen to be in reasonable agreement. Again it should be noted that the data from ref 47 are approximate only, having been obtained graphically from ref 102. The interested user is referred to the relevant Data Sheets (ref 38, 102) for experimental values.

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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.
	June 1986.

CRITICAL EVALUATION: (continued)
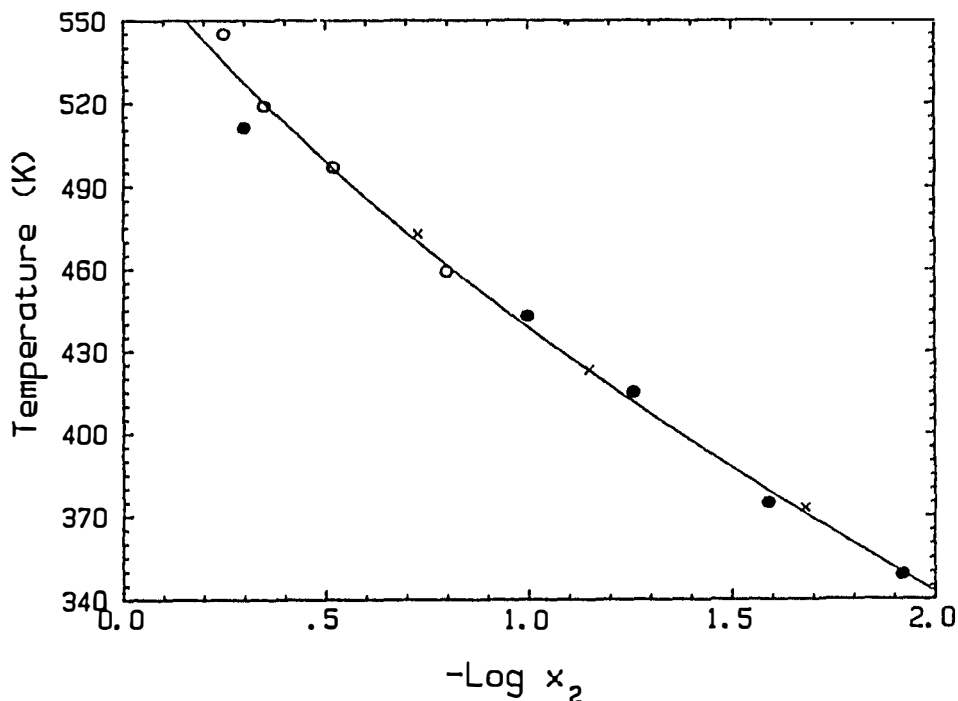
FIGURE 6. Solubility of water in benzene at three phase equilibrium pressures: ref 38 (o); ref 55 (●); ref 102 (x).

For the benzene + water system three workers have determined the temperature and pressure of the critical end point and these are given in Table 6. The values are in surprisingly good agreement.

Alwani and Schneider (ref 63) have reported detailed measurements in the high pressure region to the left of the critical line starting at the critical point of benzene (Figure 3). These data are for the one phase-two phase boundary and at the pressures and temperatures studied (Table 4), the phases are at liquid-like densities. These data are classified as Tentative as they were determined using a well-tested experimental method.

TABLE 6: Critical End Point Properties of the Benzene-Water System

Reference	T/K	p/MPa
Rebert and Kay (ref 44)	541.5	9.404
Roof (ref 70)	542.6	9.460
Scheffer (ref 108)	541.0	9.39

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. June 1986.

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

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COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (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)

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Herz, W. *Ber. Dtsch. Chem. Ges.* <u>1898</u>, *31*, 2669-72.

VARIABLES:	PREPARED BY:
One temperature: 22°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 22°C was reported to be 0.082 mL(1)/100 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The composition of the saturated solution was evaluated by extrapolation of calibration density measurements (carried out on a series of synthetic solutions) to the measured density of the saturated solution. The maximum difference between the actual and the synthetic densities was a few units in the third decimal place.	(1) not specified. (2) d^{22} 0.9980 g/cm^3.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Groschuff, E. von *Z. Elektrochem.* <u>1911</u>, *17*, 348-54.

VARIABLES:	PREPARED BY:
Temperature: 3-77°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene

$t/$°C	g(2)/100 g sln	x_2 (compiler)
3	0.030	0.0013
23	0.061	0.0026
40	0.114	0.0049
55	0.184	0.0079
66	0.255	0.0110
77	0.337	0.0145

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In 1 dm^3 long-necked flask (1) was placed and (2) was added dropwise.	(1) Kahlbaum; stored over Na; distilled twice from K-Na alloy; m.p. 5.4°C, (2) not specified.

ESTIMATED ERROR:

temp. ± 1-2 K

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Clifford, C.W. *Ind. Eng. Chem.* <u>1921</u>, *13*, 631-2.

VARIABLES:	PREPARED BY:
Temperature: 21-55°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	x_2 (compiler)
21.0	0.046	0.0020
26.6	0.055	0.0024
42.0	0.088	0.0038
55.0	0.113	0.0049

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A current of air predried by cal-cium chloride was passed through a sample. The moisture abstracted from the sample by this air was ab-sorbed in calcium chloride tubes. The amount of water was calculated from the weights of these tubes. This method is described in ref 1.	(1) source not specified; 100 percent benzene; dehy-drated with metallic sodium; purity not specified. (2) not specified.

ESTIMATED ERROR:
Not specified.

REFERENCES:
1. Clifford, C.W.; *Ind. Eng. Chem.* <u>1921</u>, *13*, 628.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Hill, A.E. *J. Am. Chem. Soc.* <u>1922</u>, *44*, 1163-93.

VARIABLES:	PREPARED BY:
One temperature: 0°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 0°C was reported to be
0.153 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by compiler is
3.53×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Three determinations of freezing point of (2) saturated with (1) gave 0.037°C as the average depression.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Hill, A.E. *J. Am. Chem. Soc.* <u>1923</u>, *45*, 1143-55.

VARIABLES:	PREPARED BY:
Temperature: 5.4-69.5°C	A. Maczynski and A. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	g(2)/100 g sln	$10^3 x_2$ (compiler)
5.4 a)	0.034	1.5
15.0	0.054	2.3
25.0	0.073	3.2
37.5	0.115	5.0
50.0	0.156	6.7
57.5	0.185	8.0
65.0	0.230	9.9
69.5 b)	0.265	11.4

$$S = 0.03294 + 0.0006449t + 0.00003728t^2$$
$$(S = g(2)/100 \text{ g sln})$$

a) quadruple point
b) boiling point of 2-liquid system

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was mechanically stirred at various temperatures and, after saturation was obtained, was transferred to small cylinders, treated with weighed amounts of silver perchlorate and the solubility of the salt in the mixed solvent determined at 25°C. After a correction for the amount of (1) present in the solid phase, the original (2) content of the saturated solution could be determined from the reference curve.	(1) source not specified; purified by recrystallization; dried over calcium chloride and finally over bright sodium wire; m.p. 54°C or higher. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Jaeger, A. *Brennst. Chem.* <u>1923</u>, *4*, 259.
VARIABLES: Temperature: 100-300°C	**PREPARED BY:** A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	mL(1)/100 mL(2)
100	0.2
150	0.6
200	2.1
250	7.3
285	10.6
300	14.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Milligan, L.H. *J. Phys. Chem.* <u>1924</u>, *28*, 494-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.07 mL (1)/100 mL (2).

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

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
20 cm^3 of benzene/air vapor were introduced into a glass cell, containing 120 cm^3 of air-saturated distilled water in a thermostatted water bath. The apparatus was removed from the bath and shaken for two minutes to bring about equilibrium. Benzene solubility in water was determined by analysis of the vapor by combustion in a Haldane apparatus before and after equilibration.	(1) Not specified. (2) Distilled.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Barbaudy, J. *J. Chim. Phys.* 1926, *23*, 289-91.
VARIABLES: One temperature: 69.25°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 69.25°C was reported to be
0.281 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by compiler
is 6.49×10^{-4}.

The solubility of water in benzene at 69.25°C was reported to be
0.279 g(2)/100 g sln.
The corresponding mole fraction, x_2, calculated by compiler
is 0.0120.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Sealed glass tubes were heated in a paraffinic oil bath for a long time above the cloud point and then cooled to turbidity.	(1) Poulenc, cryoscopic grade; thiophene free; dried over $CaCl_2$ and distilled; purity not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Uspenskii, S.P. *Neft. Khoz.* <u>1929</u>, *11-12*, 713-7.

VARIABLES:	PREPARED BY:
Temperature: 10 and 22°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
10	0.175 ± 0.001	4.04
22	0.1865 ± 0.0015	4.306

Solubility of water in benzene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
10	0.051 ± 0.0011	2.2
22	0.0662 ± 0.0008	2.86

AUXILIARY INFORMATION

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

The solubility of (1) in (2) was determined by titration. The solubility of (2) in (1) was determined by Clifford's (ref 1), method. Dried air was passed through the vessel with a saturated solution of (2) in (1) and U-tubes with $CaCl_2$ and next the adsorbed (2) was weighed.	(1) source not specified;
	    b.p. 79.8°C at 740 mm Hg,
	
	    d_4^{22} 0.8768, d_4^{10} 0.8887.
	
	(2) not specified.

	ESTIMATED ERROR: soly. see experimental values above.
	REFERENCES: 1. Clifford, C.W. *Ind. Eng. Chem.* <u>1921</u>, *13*, 628.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Rosenbaum, C.K.; Walton, J.H. *J. Am. Chem. Soc.* <u>1930</u>, *52*, 3568-73.

VARIABLES:	PREPARED BY:
Temperature: 10-60°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/100 g (1)	$10^3 x_2$ (compiler)
10	0.0451	1.95
20	0.0573	2.48
30	0.0746	3.22
40	0.0953	4.12
50	0.1271	5.48
60	0.1637	7.05

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The organic phase was first saturated by shaking with water in a flask at a high temperature and then allowing the flask to cool in a thermostat to the desired temperature, with the resulting separation of excess water. After one day or more the solution was allowed to react with added calcium hydride in dry solvent. Hydrogen was evolved and the gas volume was read.	(1) source not specified; reagent grade; free from thiophene; b.p.79.6°C m.p. 5.4°C; used as received. (2) not specified.

ESTIMATED ERROR:
not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Gross, P.M.; Saylor, J.H. *J. Am. Chem. Soc.* <u>1931</u>, *53*, 1744-51.
VARIABLES:	PREPARED BY:
One temperature: ´30°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 30°C was reported to be 1.85 g(1)/kg (2) and 0.0237 mol (1)/kg (2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.185 g(1)/100 g solution and 4.27×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions were prepared by shaking in a thermostat and were analyzed by means of an inter-ferometer. The instrument used was a combination liquid and gas interferometer made by Zeiss.	(1) Eastman Kodak Co., best grade; distilled; m.p. 5.40°C, (2) distilled.
	ESTIMATED ERROR: soly. 1.0% (from values of duplicate determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Tarassenkow, D.N.; Poloshinzewa, E.N. *Ber. Dtsch. Chem. Ges.* <u>1932</u>, *65B*, 184-6.
VARIABLES:	PREPARED BY:
Temperature: 5-73°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
5	0.024	1.0
9.5	0.034	1.5
14.5	0.041	1.8
22.5	0.060	2.6
32	0.082	3.5
40	0.102	4.4
56	0.181	7.8
67.5	0.251	10.8
73	0.300	12.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Alexejew's method was used (ref 1). No additional details were reported in the paper.	(1) Kahlbaum, CP; dried over calcium chloride and distilled from sodium; purity not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 0.01% (not specified).
	REFERENCES: 1. Alexejew, W. *Wied. Ann. Physik* <u>1886</u>, *28*, 35.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Robertson, J.B. *Sth. African J. Sci.* <u>1933</u>, *30*, 187-95.

VARIABLES:	PREPARED BY:
One temperature: 5.4°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of water in benzene at 5.4°C was reported to be 0.035 per cent, corresponding to 0.035 g(2)/100 g sln.

The corresponding mole fraction (x_2), calculated by the compiler, is 1.5×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Moist benzene-saturated air was allowed to bubble through moist benzene in a freezing-point tube until a constant freezing point was obtained. A few drops of distilled water were then added and the solution stirred "for some time" and the freezing point re-determined. The water content of the saturated sln was calculated from the freezing point depression (relative to pure benzene) by assuming the water to be monomolecular in solution.	(1) Kahlbaum, "pro-analysi", used without further purification. (2) Distilled, purity not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Niini, A. *Suomen Kemistilehti A* <u>1938</u>, *11*, 19-20.
VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 20°C was reported to be 0.085 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by compiler is 2.0×10^{-4}.

The solubility of water in benzene at 20°C was reported to be 0.059 g(2)/100 g sln.
The corresponding mole fraction, x_2, calculated by compiler is 2.6×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The weight concentration was determined by combined refractometry and pycnometry.	(1) Kahlbaums; analytical grade; dried with P_2O_5 and distilled; purity not specified. (2) not specified.
	ESTIMATED ERROR:
	soly. ± 0.005 g(2)/100 g sln (type of error not specified).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) Benzene; C_6H_6; [71-43-2]
 	
(2) Water; H_2O; [7732-18-5]
	Saylor, J.H.; Stuckey, J.M.;
	  Gross, P.M.
	
	J. Am. Chem. Soc. <u>1938</u>, *60*,
	  373-6.

VARIABLES:	PREPARED BY:
Temperature: 30 and 35°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	mol(1)/1000 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
30	0.0236	0.184	4.25
35	0.0243	0.190	4.38

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A large quantity of (1) was brought to equilibrium with a limited quantity of (2). Analyses were made by comparing the readings of the solutions in a Zeiss combination interferometer with those of known standards made by dissolving weighed quantities of (1) in known weights of (2) as described in ref 1.	(1) source not specified; purified; m.p. 5.48°C (2) distilled.

ESTIMATED ERROR:

Presumably:
   temp. ± 0.01 K
   soly. ± 0.005 g(1)/100 g(2)

REFERENCES:

1. Gross, P.M.; Saylor, J.H.
   J. Am. Chem. Soc. <u>1931</u>, *53*,
   1747.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6 [71-43-2] (2) Water; H_2O; [7732-18-5]	Berkengeim, T.I. *Zavod. Lab.* **1941**, *10*, 592-4.

VARIABLES:	PREPARED BY:
Temperature: 10-50°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
10	0.040	1.7
20	0.053	2.3
30	0.066	2.9
40	0.084	3.6
50	0.114	4.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) source not specified; CP reagent; b.p. 80.4°C; used as received. (2) not specified

	ESTIMATED ERROR:
	not specified.

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Staveley, L.A.K.; Jeffes, J.H.E.; Moy, J.A.E. *Trans. Faraday Soc.* <u>1943</u>, *39*, 5-13.
VARIABLES:	PREPARED BY:
Temperature: 24-71°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/kg(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
24.7	0.685	0.0685	2.96
41.4	1.213	0.1212	5.23
44.0	1.296	0.1294	5.88
50.4	1.619	0.1616	6.97
58.2	2.073	0.2069	8.91
58.5	2.190	0.2185	9.41
71.0	2.976	0.2967	12.74

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 50 cm^3 of (1) was introduced into a clean dry glass tube about 3.5 cm in diameter with a narrow inlet, a small amount of (2) was added from a weighted pipette, and the tube at once sealed off. It was then agitated at a sufficiently high temperature until all (2) had gone into solution, placed in a bath of water, and allowed to cool slowly. The temperature at which (1) was saturated with respect to (2) was taken to be that at which opalescence appeared.	(1) source not specified; dried over sodium wire; distilled from sodium powder. (2) not specified.
	ESTIMATED ERROR: temp. ± 1.5 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Stearns, R.S.; Oppenheimer, H.; Simon, E.; Harkins, W.D. *J. Chem. Phys.* <u>1947</u>, *15*, 496-507.
VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and D. Shaw

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
0.086 and 0.085 g(1)/100 g sln.
The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.085 g(1)/100 g sln and 2.0×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Mixtures of (1) in (2) of known composition were shaken for at least 48 hours. The turbidity was then measured with a photo-meter. Turbidities of several mixture compositions were plotted and the sharp break point taken as the solubility.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: temp. ± 3 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.
VARIABLES: Temperature: 10-26°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
10	0.030	0.030	1.30
20	0.0425	0.0425	1.84
20	0.0445	0.0445	1.93
26	0.054	0.054	2.34

(at total saturation pressure of 1 atm)

The same data are reported in ref (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Air saturated with radioactive water vapor was bubbled through (1) until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred into the counter by equilibration with ethanol vapor. The method is described in ref (1).	(1) Ohio State University under an American Petroleum Institute project, purity not specified; used as received. (2) not specified.

	ESTIMATED ERROR:
	soly. ± 1% (type of error not specified)

	REFERENCES:
	1. Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.
VARIABLES: One temperature: 25.0°C (298.2K)	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25.0°C was reported to be 0.16 mg (1)/100 mL (2). The solubility of (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate was also reported to be 0.37 mL (1)/100 mL sulfonate sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 0.02 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 neck of the tube from the total added.	(1) "Highest grade commercial sample available"; no other details given. (2) Distilled.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Durand, R. *C.R. Hebd. Seances Acad. Sci.* <u>1948</u>, *226*, 409-10.
VARIABLES: One temperature: 16°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 16°C was reported to be
1.65 cm^3(1)/dm^3(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titration method described in ref 1 was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.	(1) not specified. (2) distilled.
	ESTIMATED ERROR: soly. ± 0.05 cm^3(1)/dm^3(2)
	REFERENCES: 1. Durand, R. *C.R. Hebd. Seances Acad. Sci.* <u>1946</u>, *223*, 898-900.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* <u>1949</u>, *71*, 3644-77.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 0.174 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 4.02×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Eastman Kodak Co. best grade; washed successively with concentrated sulfuric acid, water, and dilute sodium hydroxide; dried, and distilled b.p. 80°C. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Booth, H.S.; Everson, H.E.
(2) Water; H_2O; [7732-18-5]	*Ind. Eng. Chem.* <u>1949</u>, *41*, 2627-8.

VARIABLES:	PREPARED BY:
Temperature: 25 and 60°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	mL(1)/100 mL(2)
25	0.11
60	0.19

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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. Then the mixture was separated by gentle rotation. After this treatment, the volume was determined directly.	(1) Source not specified; CP or highest commercial grade; used as received. (2) Distilled.

ESTIMATED ERROR:
temp. ± 0.1 K at 25°C
soly. ± 0.1 mL(1)/100 mL(2).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Griswold, J.; Chew, J.-N.; Klecka, M.E. *Ind. Eng. Chem.* <u>1950</u>, *42*, 1246-51.

VARIABLES:	PREPARED BY:
Temperature: 25 and 50°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100 g sln	$10^4 x_1$ (compiler)
25	0.18	4.2
50	0.22	5.5

Solubility of water in benzene

t/°C	g(2)/100 g sln	$10^3 x_2$ (compiler)
25	0.06	2.6
50	0.15	6.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Samples of (1) or (2) were placed in glass-stoppered flasks mounted on a rotating shaft and immersed in a water bath. Compositions were obtained by titrating a known sample, alternately adding the major and minor components from microburets until the two-phase point was found accurately. The flask was reimmersed in the bath after each titration to maintain thermal equilibrium. Finally, one drop of reagent would cause the second phase to appear or to disappear.	(1) Koppers Co., industrial pure grade; purified by azeotropic distillation with acetone and refractionated; purity 99.7%, (2) not specified.

	ESTIMATED ERROR:
	temp. ± 0.05 K soly. ± 0.1% (not specified)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* <u>1950</u>, *54*, 283-98.
VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
1.86 g(1) dm^{-3} sln and 0.0239 mol(1) dm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.186 g(1)/100 g sln and 4.31 x 10^{-4}.
The assumption that 1.00 dm^3 sln = 1.00 kg sln was used in this
calculation.

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 spectrophotometry.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* <u>1951</u>, *73*, 1571-8.

VARIABLES:	PREPARED BY:
Temperature: 0.4-42.8°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	g(1)/100g sln^a (compiler)	$10^4 x_1$ (compiler)
0.4	0.174^b	4.01
5.2	0.181	4.17
10.0	0.180	4.15
14.9	0.178	4.10
21.0	0.179	4.13
25.0	0.179^c	4.13^c
25.6	0.179	4.13
30.2	0.184	4.24
34.9	0.189	4.36
42.8	0.200	4.61

^{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 the solubility of solid (1) in (2).

^{c}Given in the original paper as 1.79g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Baker and Adamson, purified by recrystallization from ethanol, washing, filtering through silica gel then distilling. 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:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	McBain, J.W.; Lissant, K.J. *J. Phys. Colloid. Chem.* <u>1951</u>, *55*, 665-62.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to
be 0.151 g(1)/100 mL sln.

The corresponding mass percent and mole fraction solubilities, calculated
by the compilers assuming a solution density of 1.00 kg dm^{-3}, are
0.151 g(1)/100 g sln and $x_1 = 3.48 \times 10^{-4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL portions of (2) are pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.	(1) C.P. grade. (2) distilled and boiled to remove CO_2.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Staveley, L.A.K; Johns, R.G.S.; Moore, B.C. *J. Chem. Soc.* <u>1951</u>, 2516-23.

VARIABLES:	PREPARED BY:
Temperature: 22.7-73.2°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	$10^3 x_2$	g(2)/100 g sln (compiler)
22.7	2.606	0.0602
30.5	3.674	0.0849
33.0	3.784	0.0875
40.6	5.041	0.1167
41.9	5.153	0.1193
45.9	6.064	0.1405
51.9	6.902	0.1600
52.2	7.078	0.1641
53.2	7.211	0.1672
54.7	7.521	0.1744
60.9	9.294	0.2158
65.3	10.50	0.2441
67.2	11.21	0.2607
73.2	13.02	0.3032

$$\log x_2 = 2.237 - 1427/(t/°C + 273.1)$$

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A synthetic mixture of known amounts of (2) and (1) was heated in a sealed tube until homogeneous and then the temperature of phase splitting on cooling was determined. The apparatus and procedure are described in ref 1.	(1) source not specified; stored over phosphoric oxide. (2) not specified.

ESTIMATED ERROR:
temp. ± 0.1 K   soly. ± 0.2% (type of error not   specified)

REFERENCES:

1. Staveley, Jeffes, and Moy
    Trans. Faraday Soc. <u>1943</u>, *39*,
    5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Donahue, D.J.; Bartell, F.E. *J. Phys. Chem.* <u>1952</u>, *56*, 480-4.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
$x_1 = 4.2 \times 10^{-4}$.

The corresponding mass percent calculated by compiler is
0.182 g(1)/100 g sln.

The solubility of water in benzene at 25°C was reported to be
$x_2 = 0.0031$.

The corresponding mass percent calculated by compiler is
0.072 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Samples of (1) with (2) were placed in glass stoppered flasks and were shaken intermittently for at least three days in a water-bath held at 25°C. The (1)-rich phases were analyzed for (2) content by the Karl Fischer method and the (2)-rich phases were analyzed interferometrically.	(1) source not specified; best reagent grade; purified by fractional distillation and treatment with silica gel; purity not specified. (2) purified.
	ESTIMATED ERROR: temp. ± 0.1 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	McDevit, W.F.; Long, F.A. *J. Am. Chem. Soc.* <u>1952</u>, *74*, 1773-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
1.775 mol(1) dm^{-3} sln.

Presumably this should be 1.775 g(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler assuming a solution density of 1.000 g mL^{-1} are
0.1775 g(1)/100 g sln and 4.091 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by a variation of the Euler method in which a measured excess volume of (1) is added to (2), and after equilibration, the volume of undissolved (1) is determined by measuring its length in a precision bore tube which leads from the top of the apparatus.	(1) source not specified, reagent grade; thiophene-free; distilled; purity not specified. (2) doubly distilled.

ESTIMATED ERROR:
temp. ± 0.02 K soly. ± 0.5% (from duplicate determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Morrison, T.J.; Billett, F. *J. Chem. Soc.* <u>1952</u>, 3819-22.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
0.0220 mol(1)/1000 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by compilers are 0.172 g(1)/100 g sln and $x_1 = 3.96 \times 10^{-4}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; purest obtainable material; distilled; purity not specified. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.1 K soly. ± 0.5% (mean of large numbers of determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	McCants, J.F.; Jones, J.H.; Hopson, W.H. *Ind. Eng. Chem.* <u>1953</u>, *45*, 454-6.

VARIABLES:	PREPARED BY:
One temperature: 100°F (311 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 100°F (311 K) was reported to be 0.5 g(1)/100 g sln. The corresponding mole fraction, x_1, calculated by the compiler, is 1.2×10^{-3}.

The solubility of water in benzene at 100°F (311 K) was reported to be <0.3 g(2)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is $<1.3 \times 10^{-2}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was essentially that of ref. 1 and involved titration of the second component to the cloud point, in a constant temperature bath.	(1) Baker; thiophene free; used without further purification; n_D^{20} 1.5004. (2) Distilled.
	ESTIMATED ERROR: Not specified.
	REFERENCES: 1. Washburn, E.R.; Hnizda, V.; Vold, R.D. *J. Am. Chem. Soc.* <u>1931</u>, *53*, 3232.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Hayashi, M.; Sasaki, T. *Bull. Chem. Soc. Japan* <u>1956</u>, *29*, 857-9.

VARIABLES:	PREPARED BY:
Temperature: 20 and 25°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
20	0.137	3.16
25	0.180	4.16

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experiment has been described for the determination of the solubility in a ternary system (1)-(2)-Tween 80.	(1) source not specified; shaken repeatedly with concentrated H_2SO_4, boiled with H_2O, re-crystallized several times and distilled over Na metal. (2) not specified.

	ESTIMATED ERROR:
	soly. more than 0.4 g(1)/100 g sln (type of error not specified).

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Sodium chloride; NaCl; [76-14-5] (3) Water; H_2O; [7732-18-5]	Umano, S.; Hayano, I. *Kogyo Kagaku Zasshi* <u>1957</u>, *60*, 1436-7.

VARIABLES:	PREPARED BY:
Temperature: 20-284°C Concentration of NaCl	H. Miyamoto and G.T. Hefter

EXPERIMENTAL VALUES:
Solubility of water in benzene at system pressure

Concn. NaCl[a]	t/°C	g(3)/100 g sln	$10^2 x_3$ (compilers)
0.0	281.0	28.46	63.29
	271.5	25.11	59.24
	250.1	17.22	47.41
	223.0	8.98	29.95
	186.0	4.42	16.7
9.939	78.0	0.240	0.103
	66.0	0.189	0.814
	40.0	0.0762	3.29
	20.2	0.042	1.82
10.0	284.0	27.44	62.11
	265.0	18.91	50.27
	249.0[b]	13.02	39.35
	223.0[c]	7.65	26.4
	183.5	3.70	14.3

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
At higher temperatures: (1) and the aqueous brine were placed in an autoclave, described in detail in the paper, and equilibrated by stirring. After settling, the solubility of (3) in (1) was determined volummetrically by withdrawing layers from the auto-clave into a burette. At lower temperatures: (1) and the aqueous solution were refluxed in a flask at constant temperature. After equilibration, an aliquot of the water rich layer was withdrawn and analysed argentometrically and the solubility of (3) in (1) calculated. The solubility of NaCl in benzene was determined to be negligible in these experiments (8 x 10^{-5} mol dm^{-3} at 223°C and 54.23 atm.).	(1) : c.p. grade, source not specified; purified by single fractional distillation. (2) : not specified. (3) : c.p. grade, source not specified; recrystallized.
	ESTIMATED ERROR: Not specified
	REFERENCES:

(1) Benzene; C_6H_6; [71-43-2]
(2) Sodium chloride; NaCl; [76-14-5]
(3) Water; H_2O; [7732-18-5]

(continued)

Concn. NaCl[a]	t /°C	g(3)/100 g sln	$10^2 x_3$ (compilers)
19.200	81.0	0.155	0.67
	63.0	0.079	0.34
	40.0	0.037	0.16
	21.0	0.024	0.10
20.0	280.0	17.93	48.6
	265.0	13.56	40.5
	245.0	7.96	27.3
	221.0	3.98	15.2
	178.0	1.52	6.3
20.0	277.5	15.17	43.7
	268.5	12.47	38.2
	245.5	6.69	23.7
	219.0	3.85	14.8
	178.0	1.58	6.5

a Stated as % in paper: presumably g(2)/100 g sln (compilers).
b Given as 294.0 in the original (corrected in personal communication by the authors to H. Miyamoto).
c p = 54.23 atm.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Wing, J.; Johnston, W.H. *J. Am. Chem. Soc.* <u>1957</u>, *79*, 864-5.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be
0.0554 mL(2)/100 mL sln and 0.0635 mL(2)/100 g(1).
The corresponding mass percent and mole fraction, x_2, calculated
by the compilers are 0.114 g(2)/100 g sln and 4.9×10^{-3}. The
assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small amount of (2) was equi- librated with 20 mL of (1) using a Teflon stirrer in a 100 mL flask in a Sargent constant temperature bath. At the end of two hours, the mixture was poured into a test tube immersed in the bath and the organic phase separated from water by gra- vitation. The determination of THO in the organic phase was done by isotopic dilution with a large excess of H_2O. The tritium activ- ities in the tritiated water samples were determined by the acetylene method described in ref 1.	(1) source not specified, chemical grade; redistilled in a column of 50 theoretical plates; purity not specified. (2) Tracerlab, Inc., tritiated water with an activity of approximately 1 µCi/mL.
	ESTIMATED ERROR:
	temp. ± 0.02 K soly. 0.9% (st. dev. from 6 deter- minations).
	REFERENCES:
	1. Wing, J; Johnson, W.H. *Science* <u>1955</u>, *121*, 674.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Arnold, D.S.; Plank, C.A.; Erickson, E.E.; Pike, F.P. *Chem. Eng. Data Ser.* <u>1958</u>, *3*, 253-6.

VARIABLES:	PREPARED BY:
Temperature: 0.4-69°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of benzene in water

Solid, gaseous benzene plus water and air

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
0.4	0.168	3.88
3.0	0.170	3.92
3.9	0.176	4.06
4.5	0.172	3.97

Solid, liquid, gaseous benzene plus water and air

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
4.9	0.172	3.97

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a thermostatted 3 L borosilicate glass flask (2) was saturated with (1), the water phase stirred very slowly, then the flask left quiescent, and the saturated solution sampled repeatedly and analyzed on a Beckman model DU unit until a constant benzene concentration response was achieved on successive days. Many details are given in the paper.	(1) the Barrett Division of Allied Chemical and Dye Corp., thiophene-free, 1°; water washed and distilled; for two determinations (a) thrice crystallized. (2) distilled; electrical conductivity confirmed its high quality.

ESTIMATED ERROR:
temp. ± 0.05 K   soly. 0.0028 g(1)/100 g sln (standard deviation).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) Benzene; C_6H_6; [71-43-2]
 	
(2) Water; H_2O; [7732-18-5]
	Arnold, D.S.; Plank, C.A.;
	   Erickson, E.E.; Pike, F.P.
	Chem. Eng. Data Ser. <u>1958</u>, *3*,
	   253-6.

Solubility of benzene in water

Liquid, gaseous benzene plus water and air

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
5.6	0.174	4.02
6.7	0.174	4.02
9.0	0.173	3.99
12.5	0.172	3.97
15.0	0.173	3.99
20.0	0.171	3.95
20.6	0.172	3.97
24.8	0.171	3.95
24.9	0.174	4.02
27.3	0.174	4.02
30.0	0.177	4.09
30.0	0.176	4.06
35.0	0.182	4.20
39.9	0.188	4.34
45.0	0.197	4.55
45.0	0.196	4.53
49.8	0.204	4.71
54.5	0.215	4.97
59.8	0.226	5.22
64.8	0.241	5.57
69.0	0.260	5.67

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Brady, A.P.; Huff, H. *J. Phys. Chem.* <u>1958</u>, *62*, 644-9.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.76 g(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.176 g(1)/100 g sln and 4.06×10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) has been extrapolated from vapor-pressure measurements. The vapor pressure apparatus used the same principle as that of ref 1.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly: 0.03 (standard deviation)

	REFERENCES:
	 1. McBain, J.W.; O'Connor, J.J.
	   J. Am. Chem. Soc. <u>1936</u>, *58*,
	   2610.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Pavia, R.A. *"The Solubility of Water in Benzene"*, M.S. Thesis, 1958, North Carolina State College, Raleigh, N.C., U.S.A.
VARIABLES: Temperature: 9.3-65°C	PREPARED BY: C. Tsonopoulos and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	p_1^S/mm Hg	g(2)/100 g sln[a]	$10^3 \, x_2$ (compilers)
9.28	8.774	0.04117	1.783
20.00	17.535	0.05989	2.592
20.00	17.535	0.06076	2.629
30.17	32.136	0.08318	3.597
40.15	55.764	0.11216	4.845
49.97	92.37	0.15222	6.567
59.90	148.70	0.2010	8.657
65.00	187.54	0.2261	9.730

a Average of three separate analyses.

Results were represented with a "probable deviation of 0.8%" by the equation

$$\log_{10} (100 \, s) = 0.117135 + 0.5162095 \log_{10} p_1^S + 0.0127866 (\log_{10} p_1^S)^2$$

where s is the solubility of water in benzene in g(2)/100 g sln and p_1^S is the equilibrium vapour pressure of the solution.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Water and benzene were equilibrated in a 4-L pyrex vessel fitted with a stirrer. Equilibration typically required about 100 h of stirring. Care was taken to avoid condensation of water on the vessel lid and selective adsorption of water on the glass walls. Samples for analysis were withdrawn by air pressure. Water was determined by Karl Fischer titration.

SOURCE AND PURITY OF MATERIALS:

(1) Distilled in a tinned Barnstead still (specific conductivity 5-20 x 10^{-7} Ω^{-1}).

(2) Allied Chemical: purified by triple fractional crystallization; purity 99.99 mol %; n_0^{25} = 1.49806.

ESTIMATED ERROR:
temp. ± 0.01°C
soly. ± 1% relative; type of error not stated

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Alexander, D.W. *J. Phys. Chem* <u>1959</u>, *63*, 1021-2.

VARIABLES:	PREPARED BY:
Temperature: 0.8 - 65.4°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	g(1)/100g sln	$10^4 x_1$ (compiler)
0.8	0.184*	4.25
9.4	0.179	4.13
16.8	0.177	4.09
24.0	0.180	4.16
31.0	0.183	4.23
38.0	0.192	4.50
44.7	0.203	4.69
51.5	0.214	4.94
58.8	0.234	5.40
65.4	0.257	5.94

*supercooled liquid

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was based on that of Bohon and Claussen (1). Absorbance was determined with a Beckman model D.U. ultraviolet spectrophotometer.	(1) Analar benzene; shaken with mercury and purified according to the method of Mair *et al.* (2); purity not specified. (2) not specified.

ESTIMATED ERROR:

soly. ±0.5% (type of error not specified).

REFERENCES:

1. Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* <u>1951</u>, *73*, 1517.

2. Mair, B.J.; Termini, D.J.; Willingham, C.B.; Rossini, F.D. *J. Research Natl. Bur. Standard* <u>1946</u>, *37*, 229.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Rebert, C.J.; Kay, W.B. *A. I. Ch. E. J.* 1959, *5*, 285-9.

VARIABLES:	PREPARED BY:
Temperature: 282.8-306.4°C Pressure: 11.51-15.87 MPa	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	p/psia	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
287.5	1763	12.16	11.7	0.030
301.7	2118	14.60	22	0.061
306.4	2301	15.86	35.1	0.111
306.4*	2302	15.87	41	0.138

Solubility of water in benzene

$t/°C$	p/psia	p/MPa (compiler)	g(2)/100 g sln	x_2 (compiler)
282.8	1670	11.51	29.9	0.649
297.5	1992	13.73	31.6	0.667
306	2302	15.87	50.9	0.818
306.4*	2302	15.87	59	0.862

*upper critical solution temperature

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus employed was a modification of that described in refs 1 and 2 for P-T-x studies. A schematic diagram and construction details amply reported.	(1) source not specified, reagent grade; dried over P_2O_5 and distilled; purity not specified. (2) freshly prepared, conductivity grade.

ESTIMATED ERROR:
soly. ± 0.022 wt. fraction
temp. ± 0.05 K
pressure ± 1 lb/sq.in.

REFERENCES:
1. Young, S. *Stoichiometry* Longmans, Green, New York, 1918, p. 122.
2. Kay, W.B. *Ind. Eng. Chem.* 1938, *30*, 450.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Caddock, B.D.; Davies, P.L. *J. Inst. Petrol.* <u>1960</u>, *46*, 391-6.

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 20°C was reported to be
52 mg(2)/100 g(1).

The corresponding mass percent and mole fraction, x_2, calculated
by the compiler are 0.052 g(2)/100 g sln and 0.0022.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A sample of (1) was equilibrated at 20°C with an air stream containing a known amount of water vapor tagged with HTO. At equilibrium a sample of (1) was taken and its (2) content determined by liquid scintillation counting.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

temp. ± 0.01 K

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Kudchadker, A.P.; McKetta, J.J. *Petrol Refiner* <u>1962</u>, *41*, 191-2.

VARIABLES:	PREPARED BY:
Temperature: 37.8 - 137.8°C Pressure: 0.1 - 5.7 MPa	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°F$	$t/°C$ (compiler)	p/psia	p/MPa (compiler)	$10^4 x_1$	g(1)/100 g sln (compiler)
100	37.8				
		15.8	0.109	1.24	0.0538
		20.2	0.139	1.32	0.0572
		37.9	0.261	1.57	0.0681
		49.2	0.339	1.66	0.0720
		97.1	0.669	2.06	0.0893
		161.35	1.112	2.61	0.113
		225.7	1.556	3.28	0.142
		244.2	1.684	3.43	0.149
		308.2	2.125	4.01	0.174
		373.7	2.577	4.84	0.201
		406.3	2.801	4.98	0.216
		486.4	3.354	5.78	0.250
		554.8	3.825	6.41	0.277
		635.2	4.380	6.84	0.296
		743.23	5.124	7.87	0.340
		822.7	5.672	8.5	0.38

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experimental apparatus and analytical technique are described in ref 1. The equilibrium apparatus consisted of a jacketed cell with an internal heating coil. The mixing of the contents of the cell was achieved by a rocking mechanism.	(1) Phillips Petroleum Co., purity 99.0 mole percent; used as received. (2) distilled and boiled to remove any dissolved gases.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Davis, J.E., The Solubility of Methane and Ethylene in Water, M.S. Thesis, the University of Texas, Austin, Tex., 1959.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Kudchadker, A.P.; McKetta, J.J.
(2) Water; H_2O; [7732-18-5]	*Petrol Refiner* <u>1962</u>, *41*, 191-2.

Solubility of benzene in water

$t/°F$	$t/°C$ (compiler)	p/psia	p/MPa (compiler)	$10^4 x_1$	g(1)/100 g sln (compiler)
160	71.1	19.8	0.137	1.75	0.0758
		17.7	0.122	1.91	0.0828
		23.8	0.164	1.88	0.0815
		27.5	0.190	2.01	0.0871
		37.6	0.259	2.24	0.0971
		74.0	0.510	2.81	0.1218
		209.8	1.447	4.80	0.2078
		260.2	1.794	5.71	0.2471
		314.3	2.167	6.39	0.2765
		390.6	2.693	7.69	0.3327
		449.1	3.096	8.58	0.3710
		509.8	3.536	10.00	0.4326
		607.2	4.186	12.23	0.5283
220	104.4	29.4	0.203	2.35	0.1018
		36.25	0.250	2.93	0.1270
		46.2	0.319	3.50	0.1516
		49.9	0.344	3.80	0.1646
		84.8	0.585	4.89	0.2127
		165.2	1.139	7.68	0.332
		195.0	1.344	8.49	0.367
		204.6	1.411	9.39	0.406
		218.2	1.504	9.40	0.406
		259.3	1.788	10.75	0.465
		283.1	1.952	11.62	0.502
		327.8	2.260	13.28	0.573
		372.6	2.569	14.68	0.633
		447.5	3.085	16.85	0.727
		548.2	3.780	21.49	0.925
280	137.8	61.3	0.423	3.92	0.170
		76.2	0.525	5.84	0.253
		78.5	0.541	6.10	0.264
		103.7	0.715	7.78	0.337
		112.0	0.772	8.11	0.351
		114.9	0.792	8.28	0.358
		137.5	0.948	9.0	0.389
		170.0	1.172	10.55	0.456
		195.2	1.346	11.59	0.501
		265.1	1.766	14.28	0.616
		316.2	2.180	16.22	0.700
		325.1	2.241	16.98	0.732
		356.2	2.456	18.39	0.793
		402.6	2.776	20.20	0.870
		462.5	3.189	23.0	0.990

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Kudchadker, A.P.; McKetta, J.J.
(2) Water; H_2O; [7732-18-5]	*Petrol. Refiner* 1962, *4l*, 191-2

Author's smoothed values

$p/psia$	$10^4 x_1$
	100°F	160°F	220°F	280°F
14.7	1.18	1.56		
20.0	1.33	1.80	1.01	
40.0	1.58	2.22	3.16	
60.0	1.75	2.58	4.16	3.52
80.0	1.92	2.89	4.88	6.20
100.0	2.10	3.17	5.61	7.53
150.0	2.58	3.89	7.18	9.71
200.0	3.03	4.60	8.61	11.82
250.0	3.50	5.52	10.61	13.74
300.0	3.98	6.24	12.32	15.80
350.0	4.41	7.20	14.03	17.84
400.0	4.85	8.15	15.80	20.00
450.0	5.30	9.05	17.61	22.38
500.0	5.77	10.00	19.56	
550.0	6.21	11.06	21.54	
600.0	6.68	12.01		
650.0	7.13			
700.0	7.54			
750.0	7.94			
800.0	8.35			

Author's smoothed values calculated by compiler

p/MPa	g(1)/100 g sln
	37.8°C	71.1°C	104.4°C	137.8°C
0.101	0.0512	0.0676	-	-
0.138	0.0577	0.0780	0.0438	-
0.276	0.0685	0.0962	0.1369	-
0.414	0.0758	0.1109	0.1802	0.1525
0.552	0.0832	0.1252	0.2113	0.2683
0.689	0.0910	0.1373	0.2428	0.3258
1.034	0.1118	0.1685	0.3107	0.4198
1.379	0.1313	0.1992	0.3723	0.5106
1.724	0.1516	0.2390	0.4585	0.5975
2.068	0.1724	0.2701	0.5321	0.6817
2.413	0.1910	0.3115	0.6057	0.7691
2.758	0.210	0.3525	0.6817	0.8615
3.103	0.229	0.3913	0.7593	0.9634
3.447	0.250	0.4323	0.8428	-
3.792	0.269	0.4779	0.9275	-
4.137	0.289	0.5188	-	-
4.482	0.308	-	-	-
4.826	0.326	-	-	-
5.171	0.343	-	-	-
5.551	0.361	-	-	-

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Franks, F.; Gent, M.; Johnson, H.H. *J. Chem. Soc.* <u>1963</u>, 2716-23.

VARIABLES:	PREPARED BY:
Temperature: 17-63°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

T/K	$10^4 x_1$	g(1)/100 g sln (compiler)
290.2	3.95	0.171
295.2	3.97	0.172
299.2	3.99	0.173
302.2	4.02	0.174
305.2	4.12	0.178
308.2	4.20	0.182
313.7	4.39	0.190
315.2	4.40	0.191
317.2	4.45	0.193
319.2	4.57	0.198
324.2	4.78	0.207
329.2	5.03	0.218
334.2	5.31	0.230
336.2	5.42	0.235

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The absorbance of saturated solutions of (2) in (1) were measured directly at 254 nm on a Unicam S.P. 500 spectrophotometer.	(1) source not specified; thiophene-free; recrystallized twice from ethanol, washed, filtered through silica gel and distilled. (2) deionized and doubly distilled from alkaline potassium permanganate and aqueous phosphoric acid.
	ESTIMATED ERROR: temp. ± 0.05 K absorbance ± 0.5%
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1963</u>, *18*, 76-9.

VARIABLES:	PREPARED BY:
Temperature: 153-254°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	g(1)/100 g sln	$10^3 x_1$ (compiler)
153	1.283	2.978
178	1.913	5.044
204	2.902	6.844
225	3.790	9.000
241	4.471	10.67
254	5.073	12.17

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in sealed glass tubes. No more details were reported in the paper.	(1) source not specified; n_D^{20} 1.5011, (2) doubly distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Jones, J.R.; Monk, C.B. *J. Chem. Soc.* <u>1963</u>, 2633-5.
VARIABLES: Temperature: 25-35°C	PREPARED BY: A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	10^4 mL (2)/mL (1)
25	5.7
30	6.5
35	7.5

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 quenching effects (due to solvent) on the scintillator.	(1) 'AnalaR' grade repurified by conventional methods ref 1. (2) not specified.

ESTIMATED ERROR:
soly. 5% ± 1% (average deviation)

REFERENCES:
1. Vogel 'Practical Organic Chemistry', Longmans, Green and Co., London, 1956.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092-3. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported
to be 0.1780 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compilers
is 4.11 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+%; used as received. (2) distilled.
	ESTIMATED ERROR:
	temp. ± 1.5 K soly. 0.0045 (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Schatzberg, P.J. *J. Phys. Chem.* <u>1963</u>, *67*, 776-9.

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 20°C was reported to be
532 mg(2)/kg(1).
The corresponding mass percent and mole fraction calculated
by the compilers are 0.0532 g(2)/100 g sln and 2.30 x 10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a serum cap-sealed 4-oz. brown glass bottle immersed in a water bath, (1) was saturated with (2) at 20 ± 0.02°C for 7 days. A 20-mL sample was withdrawn with a silicone-hydrophobized hypodermic syringe pushed about 2/3 of the way into the hydrocarbon liquid. 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 with a 5-mL micro-buret.	(1) Matheson, Coleman and Bell Chromatoquality reagent, 99+ mole%; used as received. (2) distilled and deionized.

ESTIMATED ERROR:
temp. ± 0.02 K   soly. ± 3 mg(2)/kg(1) (type of error not specified).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Udovenko, V.V.; Aleksandrova, L.P. *Zh. Fiz. Khim.* 1963, 37, 52-6.

VARIABLES:	PREPARED BY:
Temperature: 20-79.5°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	g(1)/100 g sln	$10^4 x_1$ (compiler)
20.0	0.210	4.85
30.0	0.227	5.24
40.5	0.248	5.73
44.5	0.259	5.98
56.5	0.288	6.65
60.0	0.300	6.93
65.0	0.319	7.37
79.5	0.373	8.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The polythermic method of Alekseev was used. No details were reported in the paper.	(1) source not specified; dried over metallic sodium, and distilled; n_D^{20} 1.5013; d_4^{30} 0.8661. (2) not specified.

	ESTIMATED ERROR:
	not specified.

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Hoegfeldt, E.; Bolander, B. *Ark. Kemi* <u>1964</u>, *21*, 161-86.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene was reported to be

0.032 mol(2) dm^{-3} sln at 25°C.

The corresponding mass percent and mol fraction, x_2, calculated

by the compilers are 0.066 g(2)/100 g sln and 2.9×10^{-3}.

The assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The water determination was carried out according to Johansson's modification of the Karl Fischer titration in ref 1, 2.	(1) source not specified, 0.04% of toluene; purity 99.6%; used as received. (2) not specified.

	ESTIMATED ERROR:
	temp. ± 0.3 K soly. ± 0.001 mol(2) dm^{-3} sln (type of error not specified)

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Thompson, W.H.; Snyder, J.R. *J. Chem. Eng. Data* <u>1964</u>, *9*, 516-20.
VARIABLES: Temperature: 37.9-204.3°C Pressure: 7 and 34.6 MPa	PREPARED BY: A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:
  Mutual solubility of benzene and water at 1000 psig (7 MPa compiler)

$t/°F$	$t/°C$ (compiler)	$10^4 x_2$ (1)-rich phase	$10^4 x_1$ (2)-rich phase	g(2)/100 g sln (compiler) (1)-rich phase	g(1)/100 g sln (compiler) (2)-rich phase
99.9	37.7	41.6	4.33	0.0962	0.187
99.9	37.7	41.8	4.61	0.0967	0.200
100.1	37.8	46.6	4.54	0.1078	0.197
100.3	37.9	48.7	4.34	0.1127	0.188
101.0	38.3	42.1	4.60	0.0974	0.199
101.5	38.6	43.3	-	0.1002	-
160.3	71.2	124	6.63	0.289	0.287
218.0	103.3	-	9.84	-	0.425
219.0	103.8	274	8.56	0.645	0.370
280.0	137.8	558	-	1.344	-
280.3	137.9	-	14.3	-	0.617
281.0	138.3	-	18.6	-	0.802
339.3	170.7	-	41.6(a)	-	1.780
339.3	170.7	-	42.7(a)	-	1.826
340.0	171.1	1000	44.2(a)	2.498	1.889
340.3	171.3	-	46.5(a)	-	1.986
341.0	171.7	-	36.0(a)	-	1.543
396.3	202.4	-	85.3	-	3.60
397.3	202.9	1770	-	4.724	-
398.0	203.3	-	94.2(a)	-	3.96
399.0	203.9	-	72.6	-	3.07
399.7	204.3	-	81.0	-	3.42

  (a) results known to be high due to a high analytical blank   (continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
About 70 mL each of (1) and (2) were placed in a high-pressure equilibrium cell. The cell was installed in the phase-contacting equipment, pressurized with nitrogen, heated and kept horizontal with no agitation for min. 24 hr, then rotated and kept vertical for 3 hr to ensure complete phase separation. Each phase was sampled (20 mL) and the sample volume measured under the experimental conditions. The (1)-rich phase was analyzed for (2) by the Karl Fischer method and the (2)-rich phase for (1) via combustion at 1450-1500°F over CuO, absorption of CO_2 and back-titration of NaOH.	(1) Phillips Petroleum Co.; pure grade, 99+ mole%; used as received. (2) distilled and redistilled in the absence of carbon dioxide. ESTIMATED ERROR: not specified. REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Thompson, W.H.; Snyder, J.R.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* <u>1964</u>, *9*, 516-20.

Mutual solubility of benzene and water at 500 psig (34.6 MPa compiler)

$t/°F$	$t/°C$ (compiler)	$10^4 x_2$ (1)-rich phase	$10^4 x_1$ (2)-rich phase	g(2)/100 g sln (compiler) (1)-rich phase	g(1)/100 g sln (compiler) (2)-rich phase
100.3	37.9	38.1	5.61	0.0881	0.243
159.7	70.9	-	8.95	-	0.387
160.3	71.3	110	-	0.256	-
161.0	71.7	105	-	0.244	-
219.7	104.3	-	14.1	-	0.609
220.7	104.8	263	-	0.619	-
279.3	137.4	505	22.8	1.211	0.981
339.3	170.7	959	43.1	2.387	1.843
400.7	204.8	1530	98.3	3.998	4.13
459.7	237.6	4320	248	14.92	9.93
460.7	238.1	4600	265	16.42	10.56

Author's smoothed values of the mutual solubility of benzene and water at 1000 psig (7 MPa)

$t/°F$	$t/°C$	$10^4 x_2$ (1)-rich phase	$10^4 x_1$ (2)-rich phase	g(2)/100 g sln (1)-rich phase	g(1)/100 g sln (2)-rich phase
100	38	42.3	4.46	0.0978	0.193
160	71	121	6.65	0.282	0.288
220	104	274	10.1	0.645	0.436
280	138	558	18.6	1.34	0.801
340	171	1000	36.0	2.50	1.54
400	204	1780	82.0	4.75	3.46

Author's smoothed values of the mutual solubility of benzene and water at 5000 psig (34.6 MPa)

$t/°F$	$t/°C$	$10^4 x_2$ (1)-rich phase	$10^4 x_1$ (2)-rich phase	g(2)/100 g sln (1)-rich phase	g(1)/100 g sln (2)-rich phase
100	38	38.1	5.61	0.0880	0.243
160	71	106	9.05	0.246	0.392
220	104	245	14.1	0.575	0.608
280	138	500	22.8	1.20	0.980
340	171	905	43.0	2.24	1.84
400	204	1620	98.0	4.45	4.11
460	238	4500	255	15.90	10.20

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (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: 0-50°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
0	0.03996	1.730
10	0.0446	1.93
20	0.0582	2.52
30	0.0749	3.24
40	0.0948	4.10
50	0.1177	5.09

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Connolly, J.F. *J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

VARIABLES:	PREPARED BY:
Temperature: 260-300°C Pressure: 100-800 atm	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
260	100	10.1	7.1	0.0173
	250	25.3	7.3	0.0178
	500	50.7	7.2	0.0176
	800	81.1	6.6	0.0160
281	150	15.2	13.7	0.0353
	250	25.3	13.8	0.0356
	500	50.7	13.3	0.0342
	600	60.8	12.7	0.0325
287.5	165	16.7	17.2	0.0457
	195	19.8	18.1	0.0485
	320	32.4	18.1	0.0485
	380	38.5	17.3	0.0460
	735	74.5	13.9	0.0359
295	135	13.7	18.2	0.0488
	160	16.2	22.8	0.0638
	185	18.7	27.0	0.0786
	210	21.3	31.3	0.0951
	225	22.8	34.0	0.1062
	230	23.3	35.3	0.1117
	240	24.3	35.5	0.1126
	250	25.3	35.3	0.1117
	265	26.8	34.0	0.1062

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected until either a cloud or a small droplet of a second phase appeared at the top of the cell. Then mercury was injected to change pressure, more (1) was injected and the measurement was repeated.	(1) Phillips reagent grade; better than 99.8%; used as received. (2) distilled and deaerated.
	ESTIMATED ERROR: temp. ± 0.02 K pressure ± 2 atm.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Connolly, J.F.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

Solubility of benzene in water

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
295	290	29.4	31.3	0.0951
	350	35.5	27.0	0.0786
	450	45.6	22.9	0.0641
	690	69.9	18.2	0.0488
300	145	14.7	22.8	0.0638
	155	15.7	27.3	0.0797
	160	16.2	30.9	0.0935
	160	16.2	34.3	0.1074
	165	16.7	37.5	0.1216
	165	16.7	40.0	0.1332
	160	16.2	43.0	0.1482
	160	16.2	46.1	0.1647
	490	49.6	56.0	0.2269
	480	48.6	52.5	0.2031
	470	47.6	49.5	0.1843
	470	47.6	46.1	0.1647
	470	47.6	43.0	0.1482
	470	47.6	40.0	0.1332
	480	48.6	37.5	0.1216
	490	49.6	34.3	0.1074
	505	51.2	31.0	0.0939
	555	56.2	27.3	0.0797
	665	67.4	22.9	0.0641

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Johnson, J.R.; Christian, S.D.; Affsprung, H.E. *J. Chem. Soc. A.* <u>1966</u>, 77-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be 0.0349 mol(2)/dm^3 sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0719 g(2)/100 g sln and 3.11×10^{-3}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus described in ref 1 was used without modification. Samples were equilibrated in a constant-temperature water-bath maintained at 25 ± 0.1°C. Water solubilities were determined by using a Beckman Model KF-3 Aquameter.	(1) source not specified; certified or reagent grade; distilled through a 30-plate Oldershaw column. (2) not specified.
	ESTIMATED ERROR:
	temp. ± 0.1 K soly. ± 0.0005 mol(2)dm^3 sln (type of error not specified)
	REFERENCES:
	1. Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Worley, J.D. *J. Chem. Educ.* <u>1963</u>, *40*, 419.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Masterton, W.L.; Gendrano, M.C. *J. Phys. Chem.* <u>1966</u>, *70*, 2895-8.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be
0.0347 mol(2) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_2, calculated
by the compilers are 0.0715 g(2)/100 g sln and 3.09 x 10^{-3}. The
assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Equilibration of (1) and (2) was allowed to take place for at least 2 days. The organic phase was analyzed for water by the Karl Fischer method.	(1) source not specified; free from thiophene; used as received. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.05 K soly. 0.0002 mol(2) dm^{-3} (mean deviation from duplicate determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Moule, D.C.; Thurston, W.M. *Can. J. Chem.* <u>1966</u>, *44*, 1361-7.
VARIABLES: Temperature: 9.44-49.45°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in benzene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
9.44	442.5	0.0443	1.92
14.98	530.2	0.0530	2.30
20.10	639.2	0.0639	2.77
24.54	726.0	0.0726	3.14
29.52	848.0	0.0848	3.67
34.88	1017.1	0.102	4.40
40.06	1177.8	0.117	5.09
43.78	1333.7	0.133	5.76
49.45	1570.6	0.157	6.78

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A method based on an isotope dilution procedure was used. This method involves the exchange of the water present in the sample with D_2O determined by infrared difference spectroscopy.	(1) Fischer Certified reagent grade; distilled twice and dried over molecular sieve (Linde No. 4A). (2) from Ottawa River (0.0146 mole % D_2O; distilled from alkaline permanganate).

ESTIMATED ERROR:
temp. ± 0.05 K
soly. ± 0.8% (mean of three
      determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Taha, A.A.; Grigsby, R.D.; Johnson, J.R.; Christian, S.D.; Affsprung, H.E. *J. Chem. Educ.* <u>1966</u>, *43*, 432-5.
VARIABLES: One temperature: 25°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported as 0.022 mol/L sln. The corresponding mass per cent and mole fraction solubility, x_1, calculated by the compiler are, assuming a solution density of 1.00 kg L^{-1}, 0.16 g(1)/100 g sln and 4.0 x 10^{-4} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubility of (1) in (2) was determined from vapor pressure measurements. 190 mL of pure water were placed in a glass manometric apparatus of known vapor volume. The apparatus is described in detail in the paper. The apparatus was evacuated, benzene added (probably as a liquid), and the pressure measured.	(1) Source and purity not specified. (2) Pure; purity not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Alwani, Z.; Schneider, G.M. *Ber. Bunsenges. Phys. Chem.* <u>1969</u>, *73*, 294-301.
VARIABLES: Critical temperature and pressure	PREPARED BY: C.L. Young

EXPERIMENTAL VALUES:

Values of Critical Temperatures and Pressures

T/°C	T/K	P/bar
339,5	612.7	2000
329,7	602.9	1600
320,2	593.4	1200
309,5	582.7	800
297,1	570.3	400
294,2	567.4	200
297,4	570.6	170
304,9	578.1	154
325,4	598.6	171
363,0	636.2	210

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Steel optical cell in large aluminum block furnace. Cell contents stirred by magnetically operated stirrer. Pressure measured using a movable piston and Boardon gauge. Temperature measured using a steel-sheathed thermocouple. Components charged into cell and one phase-two phase boundaries observed visually. Critical properties determined from boundary envelopes.	(1) Analytical grade product fractionally distilled, purity 99.9 mole per cent. (2) Distilled and degassed.
	ESTIMATED ERROR: $\delta T/K = 0.4$ $\delta P/P = \pm 0.02$ (estimated by compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Gregory, M.D.; Christian, S.D.; Affsprung, H.E. *J. Phys. Chem.* <u>1967</u>, *71*, 2283-9.
VARIABLES: One temperature: 35°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 35°C was reported to be 0.0465 mol(2) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0970 g(2)/100 g sln and 4.19 x 10^{-3}.

The assumption that 1 dm^3 sln = 863 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A solution of (2) in (1) was obtained using solute isopiestic equilibrator described in ref 1. Water concentration was determined with a Beckman KF-3 aquameter by the Karl Fischer analysis.	(1) source not specified, reagent grade; fractionally distilled using a 30-plate Oldershaw, (2) not specified.
	ESTIMATED ERROR: temp. ± 0.05 K
	REFERENCES: 1. Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Warley, J.D. *J. Chem. Educ.* <u>1963</u>, *40*, 419.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	O'Grady, T.M. *J. Chem. Eng. Data* <u>1967</u>, *12*, 9-12.

VARIABLES:	PREPARED BY:
Temperature: 288 and 293°C Pressure: 3600 psig (24.9 MPa)	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°F$	$t/°C$	p/psig	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
550	288	3600	24.9	19.0	0.0513
560	293	3600	24.9	26.3	0.0751

Solubility of water in benzene

$t/°F$	$t/°C$	p/psig	p/MPa (compiler)	g(1)/100 g sln	x_2 (compiler)
550	288	3600	24.9	32.6	0.677
560	293	3600	24.9	41.0	0.751

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measured amounts of (1) and (2) of known composition were pumped into the extractor and mixed for 1 or 2 hours. The phases were allowed to settle for about 2 hours; then the contents were slowly (1.5 mL per minute) displaced at constant pressure with mercury. The product was collected in 2-5 mL cuts in burets with 0.1 mL subdivisions. The (1) - (2) composition could be read directly.	(1) Phillips research grade; less than 0.2% impurities; used as received. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 0.1°F pressure ± 10 psi soly. ± 0.02 mL(2)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Worley, J.D. *Can. J. Chem.* <u>1967</u>, *45*, 2465-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 2.17 g(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, values calculated by the compiler are 0.217 g(1)/100 g sln and 5.01 x 10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The isotopic solute transfer technique of Christian *et al.* (refs 1, 2), was used. This method consists of vapor phase equilibrations of water with solutions of benzene-dinonylphthalate in closed containers. The benzene absorbance was measured at 254 nm with a Cary 14 spectrophotometer.	(1) source not specified; reagent grade; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 0.2 K
	REFERENCES: 1. Christian, S.D. *et al.* *J. Chem. Educ.* <u>1963</u>, *40*, 419. 2. Christian, S.D.; Affsprung, H.E.; Johnson, J.R. *J. Chem. Soc.* <u>1963</u>, 1896.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Burd, S.D.Jr.; Braun, W.G. *Proc. Div. Refining.*, *Am. Petrol.* *Inst.* <u>1968</u>, *48*, 464-76.

VARIABLES:	PREPARED BY:
Temperature: 359 - 473 K Pressure: 0.17 - 2.76 MPa	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in benzene

p/psia	p/MPa (compiler)	t/°F	T/K (compiler)	g(2)/100 g sln	x_2 (compiler)
25	0.17	187	359	0.33	0.014
50	0.34	233	385	0.63	0.027
100	0.69	283	413	1.08	0.045
150	1.03	321	434	1.54	0.064
200	1.38	337	443	1.75	0.072
250	1.72	356	453	2.08	0.084
300	2.07	371	461	2.25	0.091
350	2.41	385	469	2.60	0.104
400	2.76	392	473	2.80	0.111

AUXILIARY INFORMATION

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

The measurements were carried out in the autoclave for vapor-liquid equilibrium determination. The solubility points were obtained by incremental addition of (2) followed by stirring, settling, sampling and analysis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. The samples were analyzed by glc.	(1) Phillips Petroleum Co.;
	    99.0% by glc; used as
	    received.
	
	(2) distilled

ESTIMATED ERROR:
temp. ± 0.5°F. soly. ± 0.004 g(2)/100 g sln.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Roddy, J.W.; Coleman, C.F. *Talanta* <u>1968</u>, *15*,1281-6.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be
x_2 = 3.23 x 10^{-3} and 0.0363 mol(2) dm^{-3} sln.
The corresponding mass percent value calculated by the compilers
is 0.0747 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A method for measuring the solubility of (2) in (1) was based on the use of tritium tracer to monitor the recovery of (2) in a conventional gravimetric method and to measure tritium distribution between the aqueous and the organic phases.	(1) source not specified; thiophene free reagent; recrystallized three times. (2) HTO at 5 Ci/mL, New England Corp.; diluted to about 1 mCi/mL.

	ESTIMATED ERROR:
	soly. better than 1% (type of error not specified).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Corby, T.C.; Elworthy, P.H. *J. Pharm. Pharmacol.* <u>1971</u>, *23 suppl.* 39 S-48 S.

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 20°C was reported to be 0.0218 mol dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.170 g(1)/100 g sln and 3.9×10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small excess of (1) was equili-brated with (2) by shaking at 20°C until saturation was attained. The saturated aqueous phase was analysed by ultraviolet spectrophotometry.	(1) W. Jarvie Ltd., cyrstalizable; distilled before use; n_D^{18} 1.5028. (2) distilled once from glass.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., <u>1972</u>, No. 21163, 113 p.
VARIABLES:	PREPARED BY:
Temperature: 278.26-318.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of benzene in water

T/K	g(1)/100 g sln	$10^3 x_1$
278.26	0.2071 ± 0.0052	0.4776
288.06	0.2078 ± 0.0055	0.4792
293.06	0.2085 ± 0.0040	0.4809
298.16	0.2088 ± 0.0038	0.4815
308.26	0.2102 ± 0.0046	0.4848
318.86	0.2300 ± 0.0054	0.5304

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 ml serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Matheson, Coleman & Bell; Chromatoquality; 99+mole%; used as received. (2) laboratory distilled water.
	ESTIMATED ERROR:
	soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Ben-Naim, A.; Wilf, J.; Yaacobi, M. *J. Phys. Chem.* <u>1973</u>, *77*, 95-102.

VARIABLES:	PREPARED BY:
Temperature: 10-50°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water is expressed in terms of the standard free energy of solution; $\Delta\mu_s^o$, determined as:

$$\Delta\mu_s^o = \lim_{\rho_s \to 0} [-RT \ln(\rho_s^\ell/\rho_s^g)_{eq}]$$

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:

$$\Delta\mu_s^o = -9536.2 + 37.122\, t - 0.02666\, t^2$$

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:	SOURCE AND PURITY OF MATERIALS:
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.	(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 x 10^{-6} S cm^{-1}.
	ESTIMATED ERROR: Temperature: ±0.05 K Solubility: std. dev. in $\Delta\mu_s^o$, 8.788 cal/mol
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Bradley, R.S.; Dew, M.J.; Munro, D.C. *High Temp. High Press.* 1973, 5 169-76.

VARIABLES:	PREPARED BY:
Temperature: 25-55°C Pressure: 1-1200 bar	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	p/bar[b]	mol/L sln	g(1)/100g sln[a] (compiler)	$10^4 x_1$[a] (compiler)
25	1	0.0234	0.183	4.21
45	1	0.0277	0.216	4.99
55	1	0.0305	0.238	5.49
45	625	0.0268	0.209	4.82
55	625	0.0326	0.254	5.87

[a] Assuming a solution density of 1.00kg/L at all temperatures and pressures.

[b] 1 bar = 0.1 MPa exactly.

Data at other pressures are presented in graphical form. Data are also presented for the solubility of (1) in aqueous solutions of $AgNO_3$ and KNO_3 at various temperatures and pressures.

AUXILIARY INFORMATION	

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) at room temperature and pressure was determined in a stoppered 1mm silica cuvette placed in a Unicam SP500 spectrophotometer and stirred magnetically. Measurements were made until a constant concentration was reached. The value was cross-checked against a 2-L sample of saturated solution which had been equilibrated for some months. Solubilities at higher temperatures and pressures were similarly determined in a special cell fitted into the spectrophotometer. Many details of the apparatus are given in the paper.	(1) A.R. grade, thiophene-free, no further details given. (2) Distilled, air-free

	ESTIMATED ERROR: Not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Filyas, Yu.I. *Sb. Nauch. Tr. Vses. Neftegazov. Nauch.-Issled. Inst.* <u>1973</u>, *45*, 68-70.
VARIABLES: One temperature: 295°C One pressure: 10 atm	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 295°C and 10 atm was reported to be 0.318 g(2)/g(1).

The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 24.1 g(2)/100 g sln and 0.580 at 1.01 MPa.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing is specified in the paper	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Karisson, R. *J. Chem. Eng. Data* <u>1973</u>, *18*, 290-2.

VARIABLES:	PREPARED BY:
Temperature: 14-35°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	mg(2)/kg(1)	10^2 g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
14.97	533.0	5.33	2.31
17.94	591.3	5.91	2.56
20.05	631.4	6.31	3.74
22.95	686.7	6.87	2.98
24.90	724.8	7.24	3.14
27.97	803.2	8.03	3.14
29.95	853.5	8.53	3.70
31.96	915.8	9.16	3.97
35.06	1021.1	10.21	4.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The determination of the solubility of (2) in (1) was based on an accurate method for determining small amounts of water via coulometrically generated iodine at a controlled potential in a Karl Fischer reagent as described in ref(1,2). Two 100-mL Erlenmeyer flasks, each containing 10 mL of (2) and 40 mL of (1), were placed in a water bath. The temperatures were measured with a platinum resistance thermometer. When equilibrium was reached, samples were withdrawn from the benzene phase with a dried Agla microsyringe and immediately added through a membrane to the electrolysis cell.	(1) Fisher Scientific Co., thiophene-free; twice recrystallized. (2) twice distilled.

ESTIMATED ERROR:
temp. ± 0.3 K   soly. ± 0.3% (type of error not specified).

REFERENCES:
1. Karisson, R. *Talanta* <u>1972</u>, *19*, 1639.   2. Karisson, R.; Karrman, K.J. *Talanta* <u>1951</u>, *18*, 459.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* <u>1973</u>, *51*, 230-3.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
1765 mg(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.1765 g(1)/100 g sln and 4.07 x 10^{-4}.

The compiler's calculation assumes a solution density of 1.000 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was equilibrated at 25 ± 0.1°C for a minimum of 12 hrs in a 200-mL Teflon-stoppered vessel (25 cm long and 3.5 cm across) with gentle shaking, allowed to settle for 6 hrs and tested for the absence of emulsion (Tyndall effect). The aqueous and organic phases were analyzed by glc (with internal standardization) on a Hewlett-Packard Model 700 instrument equipped with a 15% SE-30 on 60/80 mesh acid-washed $(CH3)_2Cl_2Si$-treated Chromosorb P column (steel capillary 10 ft x 0.125 inch). The (1) in the aqueous phase was extracted into 5 ml of heptane and the extract analyzed by glc.	(1) Phillips Petroleum Co. research grade, 99+ mole%; used as received. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1 K soly. 30 mg(1) dm^{-3} (two standard deviations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C.-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.
VARIABLES: Temperature: 0-25°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of benzene in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
0† (a)	1678 (c)	0.167	3.87
25 (b)	1755 (c)	0.175	4.05

Solubility of water in benzene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
0‡ (a)	302 (d)	0.030	1.31
25 (b)	692 (e)	0.069	2.99

†Benzene was at supercooled liquid state.
‡Solubility in supercooled liquid.
a-e see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99+%); shaken three times with distilled water. (2) distilled.

ESTIMATED ERROR:
temp. (a) ± 0.02 K, (b) ± 0.01 K
soly. (c) ± 1.7%, (d) ± 4.7%,
(e) ± 3.1% (from two or three determinations)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Brown, R.L.; Wasik, S.P. *J. Res. Natl. Bur. Stds. A.* <u>1974</u>, *78*, 453-60.

VARIABLES:	PREPARED BY:
Temperature: 4.5-20.1°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of Benzene in Water

t/°C	g(1)/100 g sln		$10^4 x_1$ (compiler)
4.5	0.184	0.0033	4.25
6.3	0.185	0.0033	4.27
7.1	0.181	0.0055	4.18
9.0	0.181	0.0034	4.18
11.8	0.177	0.0041	4.09
12.1	0.177	0.0035	4.09
15.1	0.179	0.0038	4.14
17.9	0.179	0.0038	4.14
20.1	0.176	0.0032	4.07

a Errors given as standard deviations.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 cm³ 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.	(1) 99.99 mole per cent purity; source and methods of purification not specified. (2) Distilled.

ESTIMATED ERROR:
Temperature: ±0.01 K   Solubility: see Table above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Goldman, S. *Can. J. Chem.* <u>1974</u>, *52*, 1668-80.

VARIABLES:	PREPARED BY:
Temperature: 10-40°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	mol(2) dm^{-3} sln	g(2)/100 g sln (compiler)	$10^3 \, x_2$ (compiler)
10	0.02171	0.0440	1.91
15	0.02561	0.0522	2.26
20	0.03017	0.0618	2.67
25	0.03518	0.0725	3.14
30	0.03950	0.0820	3.55
35	0.04690	0.0979	4.23
40	0.05243	0.1101	4.76

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 175-mL milk-dilution bottle fitted with a bakelite screw cap and a Teflon insert and rotated end-over-end at 20 min^{-1}, (1) was equilibrated with an excess of (2) at 25 ± 0.02°C, sampled (5 mL ± 0.2%) with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.	(1) certified grade; washed successively with conc. H_2SO_4, H_2O, 1N NaOH, H_2O, dried with silica gel, and distilled; d_4^{25} 0.87365, (2) distilled.

ESTIMATED ERROR:
temp. ± 0.02 K   soly. 0.00039 (st. dev.)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Vodnye. Resursy.* <u>1975</u>, *2*, 170-3.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to
be 1.000 mg(1) cm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.1000 g (1)/100 g sln and 2.305×10^{-4}.
The compiler's calculation assumes a solution density of 1.000 g mL^{-1}.

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

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) described in ref 1. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1 K
	REFERENCES:
	1. Kresnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* <u>1973</u>, *13*, 885.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* <u>1975</u>, *53*, 239-41.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1.7795 g(1) dm^{-3}.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.178 g(1)/100 g sln and 4.11 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubility of (1) in (2) was determined by gas chromatography. The gas chromatograph was Hewlett-Packard Model 5750 equipped with a hydrogen flame ionization detector. Many details were given in the paper.	(1) Phillips Petroleum Co., research grade; 99.9+%; used as received. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.1 K soly. ± 0.0164 g(1) dm^3
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Sada, E.; Kito, S.; Ito, Y. *J. Chem. Eng. Data* <u>1975</u>, *20*, 373-5.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 2.0403 mL(1)/1000 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Sudan IV was used to dye (1). The experimental apparatus and procedure used in this work were similar to those of Sobotka and Khan (ref 1). To make the measurements more accurate, the apparatus used consisted of a 1-liter dissolution flask and a 2-mL microburet. The scale was calibrated in advance by use of mercury. The dissolution flask was immersed in a water bath controlled thermostatically at 25°C. To avoid condensation of (1) from the gas phase, the temperature of gas phase in the dissolution flask was kept 1°C higher than that of the liquid phase. The dissolution flask and the microburet were connected tightly.	(1) source not specified; reagent grade; used as received; purity not specified. (2) pure.

	ESTIMATED ERROR:
	temp. ± 0.01 K soly. less than 0.008 mL(1)/1000 mL sln (type of error not specified)

REFERENCES:
1. Sobotka, H.; Kahn, J. *J. Am. Chem. Soc.* <u>1948</u>, *53*, 2935.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [77-43-2] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* __1976__, *50*, 1344. *Deposited doc.* __1976__, VINITI 438-76
VARIABLES: One temperature: 20°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 20°C was reported to be $x_1 = 4 \times 10^{-4}$.

The corresponding mass percent calculated by the compiler is 0.17 g(1)/100 g sln.

The solubility of water in benzene at 20°C was reported to be $x_2 = 0.0026$.

The corresponding mass percent calculated by the compiler is 0.060 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.	(1) source not specified; pure or analytical reagent grade; purity <99.9%. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* <u>1976</u>, *54*, 3909-16.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in benzene at 25°C was reported to be 0.0349 mol(2) dm^{-3} sln. The corresponding mass percent and mole fraction, x_2, calculated by the compilers are 0.0719 g(2)/100 g sln and 3.11 x 10^{-3}.

The assumption that 1 dm^3 sln = 874 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 submerged 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.	(1) Fisher B-245; purified by double crystallization; d_4^{25} 0.87378. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.1 K soly. 0.0002 mol(2) dm^{-3} sln (standard deviation from 5 determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C and at system pressure was reported to be 1740 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.174 g(1)/100 g sln and 4.01×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.

ESTIMATED ERROR:
temp. ± 1 K soly. ± 17 mg(1)/kg(2)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water, H_2O; [7732-18-5]	Skripka, V.G. *Tr. Vses. Neftegazov. Nauch. Issled.* *Inst.* <u>1976</u>, *61*, 139-51. Sultanov, R.G.; Skripka, V.G. *Zh. Fiz. Khim.* <u>1973</u>, *47*, 1035.
VARIABLES: Temperature: 225-260°C Pressure: 4.7-78.5 MPa	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in benzene

$t/°C$	$p/kg\ cm^{-2}$	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
225	48	4.7	0.256	7.35
	100	9.8	0.250	7.14
	150	14.7	0.242	6.86
	200	19.6	0.228	6.37
	300	29.4	0.227	6.34
	400	39.2	0.217	6.01
	500	49.0	0.209	5.74
	600	58.8	0.200	5.45
	700	68.6	0.191	5.16
	800	78.5	0.183	4.91
250	75	7.4	0.410	13.81
	100	9.8	0.399	13.27
	150	14.7	0.378	12.29
	200	19.6	0.361	11.52
	300	29.4	0.332	10.28
	400	39.2	0.314	9.55
	500	49.0	0.312	9.47
	600	58.8	0.291	8.64
	700	68.6	0.280	8.23
	800	78.5	0.270	7.86

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experimental technique was described in ref 1. No details reported in the paper.	(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.* <u>1971</u>, *4*, 6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Skripka, V.G. *Tr. Vses. Neftegazov. Nauch. Issled. Inst.* <u>1976</u>, *61*, 139-51.
(2) Water; H_2O; [7732-18-5]	Sultanov, R.G.; Skripka, V.G. *Zh. Fiz. Khim.* <u>1973</u>, *47*, 1035.

$t/°C$	$p/\text{kg cm}^{-2}$	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
260	84.5	8.3	0.491	18.19
	100	9.8	0.479	17.49
	150	14.7	0.442	15.44
	200	19.6	0.416	14.10
	300	29.4	0.381	12.43
	400	39.2	0.363	11.61
	500	49.0	0.352	11.13
	600	58.8	0.342	10.70
	700	68.6	0.332	10.28
	800	78.5	0.321	9.83

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* <u>1978</u>, *51*, 957-8.
VARIABLES: Temperature: 25°C	**PREPARED BY:** A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be
0.82 g(1)dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.084 g(1)/100 g sln and 1.94 x 10^{-4}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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).	(1) not specified. (2) not specified.

	ESTIMATED ERROR: soly. 0.01 g (1)dm^{-3} sln (standard deviation from 6 determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (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 benzene in water at 25°C was reported

to be 1740.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated

by compiler are 0.174 g(1)/100 g sln and 4.02×10^{-4}.

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:	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. 35.0 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* <u>1978</u>, *50*, 997-1000.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 1791 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, values calculated by compiler are 0.1791 g(1)/100 g sln and 4.130×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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 K soly. ± 10 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.* <u>1975</u>, *13*, 535.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Singh, R.P.; Sah, R.
(2) Water; H_2O; [7732-18-5]	*Indian J. Chem.* <u>1978</u>, *16A*, 692-4.

VARIABLES:	PREPARED BY:
One temperature: 303.15 K	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in benzene at 303.15 K was reported to be
0.064 g(2)/mol(1).
The corresponding mass percent and mole fraction, x_2, values
calculated by compiler are 0.082 g(2)/100 g sln and 0.0035.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The titrations were carried out in well stoppered volumetric flasks in order to check for loss due to vaporization. Shaking after each addition of water was done in an ultrasonic shaker for at least 30 min. The contents were equilibrated in a thermostat. The final end point was determined when a second phase appeared and the volume of the water added was noted. Each titration was repeated at least three times to check the reproducibility of the results.	(1) BDH, analar quality; purified; purity not specified. (2) conductivity water.
	ESTIMATED ERROR: temp. ± 0.05 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Bittrich, H.J.; Gedan, H.; Feix, G. Z. Phys. Chem., Leipzig 1979, 260 1009-13.

VARIABLES:	PREPARED BY:
Temperature: 20 - 40°C	A. Maczynski and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln	$10^4 x_1$ (compiler)
20	1790	0.1790	4.133
40	2025	0.2025	4.676
60	2442	0.2442	5.641

Solubility of water in benzene

$t/°C$	mg(2)/kg(2)	g(2)/100 g sln	$10^3 x_2$ (compiler)
20	586	0.0586	2.54
40	712	0.0712	3.08
60	860	0.0860	3.72

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was shaken at a specified temperature and then thermostatted for 48 h. The equilibrated phases were sampled and analyzed by flame-ionization glc using 3-m steel columns of 10% SE 30-on-Chromaton N (90°C) and 1.5 g + 10% SE 30-on-Chromaton N (120°C) for (1) and (2), respectively.	(1) source not specified; distilled and crystallized; glc pure. (2) not specified.

ESTIMATED ERROR:
soly. ± 5% (type of error not specified).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (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 benzene in water was reported to be 2.24×10^{-2} 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 0.175 g(1)/100 g sln and 4.05×10^{-4} respectively.

AUXILIARY INFORMATION

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

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of ^{14}C-labelled benzene 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.	(1) ^{14}C-labelled benzene: New
	     England Nuclear, used without
	     further purification.
	
	(2) Distilled.

ESTIMATED ERROR:
Temperature: ±0.2 K
Solubility: ±0.7% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Schwarz, F. P. *Anal. Chem.* <u>1980</u>, *52*, 10-15.
VARIABLES: One temperature: 23.5°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of benzene in water at 23.5°C

g(1)/100 g sln	$10^4 x_1$ (compiler)
0.188 ± 0.005*a	4.34
0.188 ± 0.009 b	4.34
0.182 ± 0.007 c	4.20
0.193 ± 0.011 d	4.45
0.190 ± 0.007 e	4.38

*values determined for different masses of (1) coated into the inert
 support. a: 0.014; b: 0.0154; c: 0.0124; d:0.0464; e: 0.0526 g/cm

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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.	(1) spectral grade used without further purification (2) distilled
	ESTIMATED ERROR: temp. ± 1.5°C soly. 4% (average std. dev.)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Chem. Lett.* <u>1981</u>, 225-8.

VARIABLES:	PREPARED BY:
Temperature: 15-45°C	M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of benzene in water

$t/°C$	$g(1)/L$	$g(1)/100\ g\ sln^a$	$10^4 x_1{}^a$
15	1.54 ± 0.04	0.154	3.56
25	1.61 ± 0.09	0.161	3.72
35	1.76 ± 0.06	0.177	4.09
45	1.85 ± 0.11	0.187	4.32

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Bull. Chem. Soc. Jpn.* <u>1982</u>, *55*, 1054-62.

VARIABLES:	PREPARED BY:
Temperature: 5-45°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)[a]	10^4 x_1 (compiler)[a]
5	20.7	0.162	3.73
15	20.2 ± 0.3	0.158	3.65
25	20.7[b] ± 0.1	0.162	3.74
35	21.8 ± 0.6	0.171	3.94
45	22.8 ± 0.5	0.180	4.15

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

[b] No error estimate given.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 99.5%, used without further purification. (2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified.
<u>temp. ± 0.01°C.</u>

REFERENCES:

1. Kell, G.S.
   J. Chem. Eng. Data <u>1975</u>, *20*, 97.

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* <u>1983</u>, *29*, 990-9.

VARIABLES:	PREPARED BY:
Temperature: 313-473 K Pressure: 0.03-3.0 MPa	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water

T/K	p^a/MPa	$10^3\ x_1$	g(1)/100 g sln (compiler)
313.15	0.03054	0.4435	0.192
373.15	0.2758	0.949	0.412
423.15	1.0549	2.42	1.05
473.15	3.020	5.40	2.34

The solubility of water in benzene

T/K	p^a/MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
313.15	0.03054	0.471,0.501	0.112^b
373.15	0.2758	1.81,2.08	0.448^b
423.15	1.0549	7.13	1.64
473.15	3.020	18.5	4.26

a Absolute pressure

b Average value

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
All experimental details are given in an Appendix deposited in a Documentation Centre rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, whilst that of (2) in (1) was measured by Karl Fischer titration.	(1) No details given (2) No details given

ESTIMATED ERROR:
soly. ± 5% relative; repeatability of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

(1) Benzene; C_6H_6; [71-43-2]
(2) Water; H_2O; [7732-18-5]

(continued)

The three phase critical point was reported to be 541.7K, 9.42 MPa and $x_1 = 2.528 \times 10^{-2}$ (10.1 g(1)/100 g sln, compiler).

The authors also report equations fitted to their own and literature data over the range 273-542K, *viz*.

$$\ln x_1 = -170.04018 + 6922.912/T + 24.398795 \ln T$$

$$\ln x_2 = -1.64055 - 2029.41/T + 0.00900544 \ T$$

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* <u>1984</u>, *57*, 1539-44.
VARIABLES: One Temperature: 25°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of benzene in water at 25°C was reported to be 2.07×10^{-2} mol(1)/dm^3 sln. Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 0.162 g(1)/100 g sln, $x_1 = 3.73 \times 10^{-4}$, calculated by the compiler.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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.* <u>1982</u>, *55*, 1054-62.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Water-d_2; D_2O; [7789-20-0]	Brollos, K.; Peter, K.; Schneider, G. M. *Ber. Bunsenges. Phys. Chem.* <u>1970</u>, *74*, 682-6.
VARIABLES: Pressure and temperature on one phase-two phase boundary.	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
339.1	2445	0.25	56.5
337.5	2300		
333.4	2000		
328.0	1750		
323.9	1530		
314.9	1100		
308.4	840		
303.8	655		
300.1	490		
295.6	220		
326.1	170		
315.9	158		
355.2	2855	0.546	82.4
351.0	2600		
348.2	2450		
342.4	2095		
337.9	1850		
332.4	1585		
330.4	1480		
324.9	1300		
319.6	1100		
311.8	790		

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measurements were made in a steel optical cell within an aluminum block furnace. The cell contents were stirred magnetically. Pressure was measured using a movable piston and Bourdon gauge. Temperature was measured with a steel-sheathed thermocouple. Components were charged into the cell and the transition from one phase to two phases was observed visually.	1. Merck sample, purity 99.9 mole per cent. 2. Isotopic purity 99.7 mole per cent.
	ESTIMATED ERROR: δT/K = ±0.1 $\delta P/P$ = ±0.01 (estimated by compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2]	Brollos, K.; Peter, K.; Schneider, G. M.
(2) Water-d_2; D_2O; [7789-20-0]	*Ber. Bunsenges. Phys. Chem.* 1970, 74, 682-6.

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
303.4	521	0.546	82.4
297.0	300		
296.2	250		
300.2	181		
312.2	166		
325.2	182		
330.3	2750	0.755	92.3
327.4	2600		
322.9	2300		
318.9	2000		
310.0	1500		
313.1	1700		
304.4	1200		
298.9	990		
296.4	840		
288.1	540		
281.0	290		
275.4	168		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Deuterium oxide (heavy water); D_2O; [7789-20-0]	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 benzene in heavy water is reported in terms of the standard free energy of solution, $_s$, determined as:

$$\Delta\mu_s = \lim_{\rho_s \to o} [-RT \ln(\rho_s^\ell/\rho_s^g)_{eq}]$$

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:

$$\Delta\mu_s^o = -10657.5 + 44.618\ t - 0.03864\ t^2$$

where t is in °C (10 < t < 50°C) and $\Delta\mu_s^o$ is in cal/mol (1 cal = 4.187 J).

Values of the Ostwald absorption coefficient are also reported.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubilities were determined spectro-scopically. 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 spectro-photometer with a thermostatted cell holder. Establishment of equili-brium was checked by use of a special three compartment cell, details of which are given in the paper.	(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 $\Delta\mu_s^o$, 15.103 cal/mol.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Deuterium oxide (heavy water); D_2O; [7789-20-0]	Backx, P.; Goldman, S. *J. Phys. Chem.* <u>1981</u>, *85*, 2975-9.

VARIABLES:	PREPARED BY:
Temperature: 283-313 K	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of deuterium oxide in benzene

T/K	$10^3 x_2$	std. dev.	10^3 g(2)/100 g sln (compiler)
283	1.70	0.03	0.436
288	1.91	0.03	0.490
293	2.17	0.04	0.557
298	2.68	0.06	0.689
303	3.02	0.04	0.776
308	3.56	0.04	0.915
313	4.12	0.08	1.057

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 175-ml milk-dilution bottle fitted with a Bakelite screw cap and a Teflon insert and rotated end-over-end, (1) was equilibrated with an excess of (2), sampled with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.	(1) certified grade; washed successfully with conc. H_2SO_4, H_2O, 1 N NaOH, again H_2O, dried with silica gel, and distilled; d^{25} 0.87365. (2) obtained from the manufacturer; minimum isotopic purity of 99.7 atom % D.

	ESTIMATED ERROR:
	Temp. ± 0.01 K Std. dev. of soly calcd from 25-36 determinations reported above.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Benzene; C_6H_6; [71-43-2] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of benzene (1) in seawater (2) at 298 K has been reported by the following workers:

Authors	Method	Salinity g salts/kg sln	g(1)/100 g sln
Mackay and Shiu (ref 2)	GLC	35	0.1340
Price (ref 3)	GLC	34.472	0.1391
May *et al.* (ref 4)	HPLC	35	0.1365

These three determinations made by two methods agree within their experimental error of 8 to 10%. Each group of workers has also determined the solubility of benzene in pure water and obtained results within the same error of the value recommended in this volume. Therefore, the mean of the reported values, 0.135 g(1)/100 g sln, is accepted as the recommended value at the indicated temperature and salinity. These studies measured solubility over a range of salinities. Mackay and Shiu and May *et al.* reported their data in terms of the Setschenow equation. Their values of K_s (0.1836 and 0.175 L/mol) indicate the same (within experimental error) dependence of solubility on salinity and may be used to interpolate solubilities at other salinities up to 200 g salts/kg sln.

  Brown *et al.* (ref 1) determined the solubility of benzene in seawater at a salinity of 34.42 g salts/kg sln over the temperature range 273 to 293 K. Linear extrapolation by the evaluator of these results to 298 K gives a value of 0.127 g(1)/100 g sln. This suggests that the results of Brown *et al.* may be slightly low.

SOLUBILITY OF BENZENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	35	0.136

Since the solubility of seawater (1) and benzene (2) has been reported only by Umano and Hayano (ref 5), no critical evaluation is possible. The interested reader is referred to the relevant data sheet which is included with the preceeding benzene-water system.

REFERENCES

1. Brown, R.L.; Wasik, S.P.; *J. Res. Natl. Bur. Stds.* A. <u>1974</u>, *78*, 453-60.
2. Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* <u>1975</u>, *53*, 239-42.
3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.
4. May, W.E.; Wasik, S.P.; Freeman, D.H. *Anal. Chem.* <u>1978</u>, *50*, 997-1000.
5. Umano, S.; Hayano, I.; *Kogyo Kagaku Zasshi* <u>1957</u>, *60*, 1436-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-42-2] (2) Artificial seawater	Brown, R.L.; Wasik, S.P. *J. Res. Natl. Bur. Stds. A.* <u>1974</u>, *78*, 453-60.

VARIABLES:	PREPARED BY:
Temperature: 0-20°C Salinity: 34.42 g salts/kg sln	G.T. Hefter and D.G. Shaw

EXPERIMENTAL VALUES:

Solubility of benzene in artificial seawater

t/°C	g(1)/100 g sln[a]	$10^4 x_1$ (compiler)
0.19	0.1323 (0.0017)	3.129
5.32	0.1376 (0.0022)	3.255
10.05	0.1347 (0.0023)	3.186
14.96	0.1318 (0.0025)	3.117
20.04	0.1296 (0.0022)	3.065

[a] numbers in parentheses are standard deviations from 4 observations

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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 cm³ 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.	(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 <u>1942</u>, Prentice-Hall, Englewood Cliffs, New Jersey p186.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* 1975, *53*, 239-42.

VARIABLES: One temperature: 25°C Salinity: 0-200 g(2)/kg sln	PREPARED BY: M. Kleinschmidt and W. Shiu

EXPERIMENTAL VALUES:

The solubility of benzene in solutions of 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 benzene in water (mg/L)

S is the solubility of benzene in solution (mg/L)

K_s is the Setschenow constant (L/mol)

C_s is the concentration of sodium chloride (L/mol)

evaluating the equation for S over the range of C_s 0-4 mol/L, K_s = 0.1836 ± 0.0072 (standard error) with S_o = 1779.5 ± 16.4.

The corresponding mass percent and mole fraction, x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 0.1340 g(1)/100 g sln and 3.227 x 10^{-4} assuming a solution density of 1.025 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubility was determined by vapor phase extraction and gas chromatographic analysis. This method does not require the preparation of saturated solutions and thus avoids one of the major sources of error of other methods.	(1) research grade, 99.9+%, from Phillips Petroleum Co. (2) and (3) not specified

	ESTIMATED ERROR: temp. ± 0.1 K soly. 95% confidence limit is about 8%
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 1-360 g(2)/kg sln	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Benzene in Aqueous NaCl

Salinity g(2)/kg sln	Mass Percent g(1)/100 g sln	Mole fraction $10^4 x_1$ (compilers)
1.002	0.1718	3.96
10.000	0.1628	3.78
34.472[a]	0.1391	3.28
50.030	0.1194	2.85
125.100	0.0593	1.48
199.900	0.0388	1.01
279.800	0.0214	0.581
358.700	0.0134	0.378

[a]Artificial seawater, composition not specified but probably
  similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	(1) commercial, 99 + % pure

ESTIMATED ERROR:

Temperature ± 1 K

Solubility ± 10 relative %

REFERENCES:

1. Lyman, J.; Fleming, R.H.; *J. Mar.
    Res.* <u>1940</u>, *3*, 135.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzene; C_6H_6; [71-43-2] (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 benzene 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 = 0.175 with S_o = 1791.

The corresponding mass percent and mole fraction x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 0.1365 g(1)/100 g sln and 3.22 x 10^{-4}.

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 K K_s ± 0.006 S_o ± 10
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1984.

CRITICAL EVALUATION:

Quantitative data for the solubility of 1,4-cyclohexadiene (1) in water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of 1,4-Cyclohexadiene (1) in Water (2)

Reference	T/K	Method
McAuliffe (ref 1)	298	GLC
Pierotti and Liabastre (ref 2)	278–318	GLC

The original data in these publications are compiled in the Data Sheets immediately following this Critical Evaluation. No data appear to have been reported for the solubility of water in 1,4-cyclohexadiene.

The solubility values of (1) in (2) are listed in Table 2. The data are in poor agreement, with those of Pierotti and Liabastre (ref 2) being approximately 20% (relative) higher than those of McAuliffe (ref 1). This situation is typical for a large number of hydrocarbon-water systems investigated by these authors and is discussed in greater detail in the Critical Evaluation of the cyclopentane-water system. In general the values of McAuliffe are much closer to accepted values (in well-characterised systems) than those of Pierotti and Liabastre. However, in the absence of confirmatory studies, the data of Pierotti and Liabastre are not rejected although they should probably be regarded only as order-of-magnitude values. The datum of McAuliffe may be considered as "Tentative".

TABLE 2: Solubility Values of 1,4-Cyclohexadiene (1) in Water (2)

T/K	Solubility values		
	Reported values[a] g(1)/100g sln	"Best" value ($\pm \sigma_n$)[b] g(1)/100g sln	$10^4 x_1$
278	0.085* (ref 2)	0.09	1.9
288	0.094* (ref 2)	0.09	2.1
298	0.070 (ref 1), 0.093*(ref 2)	0.08 ± 0.01	2.1
308	0.09* (ref 2)	0.1	2.2
318	0.101 (ref 2)	0.1	2.3

Note: Footnotes to Table 2 on next page.

COMPONENTS:	EVALUATOR:
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1984.

CRITICAL EVALUATION: (continued)

TABLE 2 (continued)

a   Values marked with asterisk (*) obtained by Evaluator by graphical interpolation of original measurements.

b   See comments in text regarding reliability of "Best" values; σ_n has no statistical significance.

REFERENCES

1.   McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

2.   Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water solutions.* U.S. Nat. Tech. Inform. Serv., PB Rep. 1972, No. 21163, 113 pp.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,4-cyclohexadiene in water at 25°C was reported to be 700 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0700 g(1)/100 g sln and 1.57 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.

ESTIMATED ERROR:
temp. ± 1.5 K   soly. 16 g(1)/10^6 g(2)   (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,4-Cyclohexadiene; C_6H_8; [628-41-1] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., <u>1972</u>, No. 21163, 113 p.
VARIABLES: Temperature: 278.26-318.36 K	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 1,4-cyclohexadiene in water

T/K	g(1)/100 g sln	$10^3 x_1$
278.26	0.08519 ± 0.0019	0.1915
288.36	0.09585 ± 0.0028	0.2155
298.26	0.09362 ± 0.0023	0.2105
308.36	0.09634 ± 0.0023	0.2166
318.36	0.10100 ± 0.0023	0.2271

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Columbia Organic Chemicals Co., Inc.; 99%; used as received. (2) laboratory distilled water.
	ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1984.

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
McBain and Lissant (ref 1)	298	(1) in (2)	synthetic
Duque-Estrada *et al.* (ref 2)	298	(1) in (2)	GLC
Englin *et al.* (ref 3)	283-313	(2) in (1)	analytical
Farkas (ref 4)	298	(1) in (2)	GLC
McAuliffe (ref 5)	298	(1) in (2)	GLC
Pierotti and Liabastre (ref 6)	278-318	(1) in (2)	GLC
Budantseva *et al.* (ref 7)	293	mutual	GLC, Karl Fischer
Schwarz (ref 8)	297	(1) in (2)	chromatographic

The original data in all these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Solubilities of cyclohexene in various aqueous salt solutions have also been reported (ref 9) but will not be considered in this Evaluation. For convenience, further discussion of this system will be divided into two parts.

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

The solubility data for cyclohexene in water are listed in Table 2. There are too few values to justify plotting them in a Figure.

At 298 K, the results of Pierotti and Liabastre (ref 6) appear to be much higher than all other values. This situation is typical of the large number of hydrocarbon-water systems investigated by these authors and is discussed in greater detail in the Critical Evaluation for the cyclopentane-water system. On the other hand, Pierotti and Liabastre's results at other temperatures are in reasonable agreement with the other available data (ref 7,8). This probably means that these data are also higher than "true" values. However, in the absence of confirmatory studies it is not possible to reject these data (ref 6,7,8). They are included in Table 2 but excluded in the determination of "Best" values.

COMPONENTS:	EVALUATOR:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1984.

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Value of the Solubility of Cyclohexene (1) in Water (2)

T/K	Solubility values		
	Reported values g(1)/100g sln	"Best" value g(1)/100g sln	$(\pm \sigma_n)^a$ $10^5 x_1$
278	0.028 (ref 6)		
288	0.029 (ref 6)		
293	0.023 (ref 4)		
298	0.013 (ref 1), 0.014 (ref 2), 0.016 (ref 4), 0.021 (ref 5), 0.030 (ref 6), 0.028^b (ref 8)	0.016 ± 0.003	3.5
308	0.030 (ref 6)		
318	0.031 (ref 6)		

a Obtained by averaging reported values excluding those of ref 6 (see text) and ref 8 (297K datum). σ_n values do not have statistical significance.

b 297 K datum.

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

The solubility data for water in cyclohexene are listed in Table 3. The results of Englin *et al.* (ref 6) and Budantseva *et al.* (ref 7) at 293 K are only in fair agreement.

It should be noted that in a number of well-characterised systems (e.g. benzene-water) the data of Englin *et al.* are usually reliable when $T < 300$ K but are much higher than "Recommended" values when $T > 300$ K. Thus, in the absence of confirmatory studies, all the data in Table 3 should be regarded very cautiously.

COMPONENTS:	EVALUATOR:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, Western Australia. November 1984.

CRITICAL EVALUATION: (continued)

TABLE 3: Tentative Solubility Values of Water (2) in Cyclohexene (1)

		Solubility values		
		Reported values $10^2 g(2)/100g$ sln	"Best" values (± σ_n)^a	
			$10^2 g(2)/100g$ sln	$10^3 x_2$
283		2.52 (ref 3)	2.5	1.2
293		3.17 (ref 3), 4.2 (ref 7)	3.7 ± 0.5	1.7
298		3.70^b (ref 3)	3.7	1.7
303		4.24 (ref 3)	4.2	1.9
313		5.62 (ref 3)	5.6	2.6

a See text, however; σ_n has no statistical significance.
b Interpolated graphically by the Evaluator.

REFERENCES

1. McBain, J.W.; Lissant, K.J. *J. Phys. Chem.* 1951, *55*, 655-62.

2. Duque-Estrada, E.; Bayne, A.H.; Manakan, D.A. Instr. Lab. Rept., Dept. Chem. Eng. MIT, April 22, 1964. (*cf.* ref 4).

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

4. Farkas, E.J. *Anal. Chem.* 1965, *37*, 1173-5.

5. McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

6. Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water solutions.* U.S. Nat. Tech. Inform. Serv., PB Rep. 1972, No. 21163, 113 pp.

7. Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344; Deposited Doc. 1976, VINITI 438-76.

8. Schwarz, F.P. *Anal. Chem.* 1980, *52*, 10-15.

9. Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	McBain, J.W.; Lissant, K.J. *J. Phys. Colloid. Chem.* <u>1951</u>, *55*, 665-62.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water at 25°C was reported to be 0.013 g(1)/100 mL sln.

The corresponding mass percent and mole fraction (x_1), calculated by the compilers assuming solution density to be the same as pure water (1.00 g mL^{-1}), are 0.013 g(1)/100 g sln and 2.9 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL portions of (2) was pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.	(1) Eastman No. 1043. (2) distilled and boiled to remove CO_2.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Duque-Estrada, E.; Bayne, A.H.; Manalan, D.A. Instr. Lab. Rept., Dept. Chem. Eng., MIT, April 22, 1964.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water at 77°F was reported to be 0.000107 lb mol(1) ft^{-3} sln.

The corresponding temperature, mass percent, and mole fraction, x_1, values calculated by compilers are 25°C, 0.014 g(1)/100 g sln, and 3.1×10^{-5}.

The assumption 1 ft^3 sln = 28.32 kg sln was used in the calculation.

The data are taken from ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The analytical (glc) method was used. Nothing more was reported in ref 1.	(1) not specified in ref 1. (2) not specified in ref 1.
	ESTIMATED ERROR:
	not specified in ref 1.
	REFERENCES:
	1. Farkas, E.J. *Anal. Chem.* <u>1965</u>, *37*, 1173.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (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: Temperature: 10-40°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in cyclohexene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
10	0.0252	1.15
20	0.0317	1.44
30	0.0424	1.93
40	0.0562	2.56

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Farkas, E.J. *Anal. Chem.* <u>1965</u>, *37*, 1173-5.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water at 77°F was reported to be 0.000114, 0.000121, and 0.000128 lb mol(1) ft^{-3} sln.

The corresponding temperature, mass percent, and mole fraction, x_1, calculated by compilers at 25°C, 0.016 g(1)/100 g sln, and 3.5×10^{-5}. The assumption that 1 ft^3 sln = 28.32 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) has been evaluated from vapor pressure measurements in a specially constructed reactor described in the paper. Theoretical basis is included.	(1) not specified. (2) not specified.

ESTIMATED ERROR:
soly. ± 6%   (mean from three determinations)   (compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8]	McAuliffe, C.
(2) Water; H_2O; [7732-18-5]	*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 cyclohexene in water at 25°C was reported to be 213 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0213 g(1)/100 g sln and 4.67×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 10 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9
VARIABLES: One temperature 30°C	PREPARED BY: M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water was reported to be 4.950×10^{-3} mol L^{-1} at 30°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, 0.0406 g(1)/100 g sln and 8.91×10^{-5}.

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:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Prepared by dehydration of cyclohexanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography. (2) Not specified.
	ESTIMATED ERROR: Temp. ± 0.05 K Soly. not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 p.
VARIABLES: Temperature: 278.26-318.36 K	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexene in water

T/K	g(1)/100 g sln	$10^3 x_1$
278.26	0.02800 ± 0.00069	0.06141
288.36	0.02985 ± 0.00061	0.06546
298.26	0.02990 ± 0.00082	0.06557
308.36	0.03025 ± 0.00070	0.06634
318.36	0.03105 ± 0.00093	0.06809

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Eastman Organic Chemicals, No. 1043; washed with water to remove stabilizing agent. (2) laboratory distilled water.
	ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344. *Deposited doc.* 1976, VINITI 438-76.

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of cyclohexene in water at 20°C was reported to be
$x_1 = 5 \times 10^{-5}$.

The corresponding mass percent calculated by the compiler is
0.023 g(1)/100 g sln.

The solubility of water in cyclohexene at 20°C was reported to be
$x_2 = 0.0019$.

The corresponding mass percent calculated by the compiler is
0.042 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.	(1) source not specified; pure or analytical reagent grade; purity <99.9%. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexene; C_6H_{10}; [110-83-8] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *Anal. Chem.* <u>1980</u>, *52*, 10-15.

VARIABLES:	PREPARED BY:
One temperature: 23.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexene in water at 23.5°C

g(1)/100 g sln	$10^5 x_1$ (compiler)
0.0281 ± 0.0005	6.16
0.0286 ± 0.0013	6.27

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.	(1) reagent grade used without further purification (2) distilled
	ESTIMATED ERROR: temp. ± 1.5°C soly. 3% (average std. dev.)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,5-Hexadiene; C_6H_{10}; [592-42-7] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.

VARIABLES:	PREPARED BY:
Temperature: 13.5 and 20.2°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in 1,5-hexadiene

$t/°C$	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
13.5	0.0618	0.0618	2.81
20.2	0.0969	0.0962	4.37

(at total saturation pressure of 1 atm)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Air saturated with radioactive water vapor was bubbled through (1) until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred into the counter by equilibration with ethanol vapor. The method is described in ref (1).	(1) Harvard University; purity not specified; used as received. (2) not specified.

ESTIMATED ERROR:
soly. ± 1% (type of error not specified)

REFERENCES:
1. Joris, G.G.; Taylor, H.S.   *J. Chem. Phys.* <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,5-Hexadiene; C_6H_{10}; [592-42-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,5-hexadiene in water at 25°C was reported to be 169 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0169 g(1)/100 g sln and 3.70 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 6 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexyne; C_6H_{10}; [693-02-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-hexyne in water at 25°C was reported to be 360 $g(1)/10^6$ $g(2)$.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0360 g(1)/100 g sln and 7.89×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 17 $g(1)/10^6$ $g(2)$ (standard deviation of mean)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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. November 1984

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	335-487	(1) in (2)	synthetic?
Englin *et al*. (ref 2)	283-303	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Price (ref 4)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 5)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 6)	298	(1) in (2)	partition coefficient

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 METHYLCYCLOPENTANE (1) IN WATER (2)

The solubility data for methylcyclopentane in water at 298K are listed in Table 2. The datum of Krzyzanowska and Szeliga (ref 5) has been excluded from consideration as it does not appear to be independent of that of Price (ref 4). The high temperature data of Guseva and Parnov (ref 1) presumably made in sealed tubes are rejected because of inadequate specification of system conditions (especially pressure). All other data are given in Table 2.

TABLE 2:   Recommended Value of the Solubility
of Methylcyclopentane (1) in Water (2)

T/K	Solubility values		
	Reported values 10^3g(1)/100g sln	"Best" values (± σ_n)[a] 10^3g(1)/100g sln	$10^6 x_1$
298	4.2 (ref 3), 4.18 (ref 4), 4.5 (ref 6)	4.3 ± 0.1	9.2

[a] Obtained by averaging, σ_n has no statistical significance.

COMPONENTS:	EVALUATOR:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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. November 1984

CRITICAL EVALUATION: (continued)

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

The solubility of water in methylcyclopentane has been reported in only one publication: Englin *et al.* (ref 2), and thus no Critical Evaluation can be given. However, it should be noted that in well characterized systems (e.g. benzene-water), the data of Englin *et al.* are generally reliable at lower temperatures but are higher than "Recommended" values when $T > 300K$. The interested user is referred to the appropriate data sheet for the original values.

REFERENCES

1.   Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1964</u>, *19*, 77-8.

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

3.   McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1967-75.

4.   Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

5.   Krzyzanowska, T.; Szeliga, J. *Nafta Katowice* <u>1978</u>, *34*, 413-7.

6.   Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1964</u>, *19*, 77-8.

VARIABLES:	PREPARED BY:
Temperature: 61.5-214°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of methylcyclopentane in water

$t/°C$	g(1)/100 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
61.5	0.0229	0.0229	0.490
146	0.155	0.155	3.31
184	0.457	0.457	9.76
214	1.479	1.457	31.20

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Guseva, A.N.; Parnov, E.I.
    Vestn. Mosk. Univ. Khim. <u>1963</u>,
    18, 76.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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 methylcyclopentane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.073	3.4
20	0.0131	6.12
30	0.0205	9.58

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of methylcyclopentane in water at 25°C was reported to be 42 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 9.0×10^{-6}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.6 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of methylcyclopentane in water at 25°C and at system pressure was reported to be 41.8 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00418 g(1)/100 g sln and 8.95×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1 K soly. ± 1 mg(1)/kg(2)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (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 methylcyclopentane in water at 25°C was reported to be 41.8 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00418 g(1)/100 g sln and 8.95×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 1.05 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of methylcyclopentane between the gas and aqueous phase. $\alpha = 14 \pm 1$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 137.5$ mm of Hg and $\log C_g = \log p - 4.269 = -2.13$ expressed in moles per liter. Therefore $C_s = 5.29 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0045 g(1)/100 g sln and the corresponding mole fraction, x_1, is 9.6×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 10% (estimated by the compiler)
	REFERENCES: 1. Hine, J.; Mooker, P.K. *J. Org. Chem.* <u>1975</u>, *4*, 292.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclopentane; C_6H_{12}; [96-37-7] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 1-360 g(2)/kg sln	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Methylcyclopentane in Aqueous NaCl

Salinity g(2)/kg sln	Mass Percent g(1)/100 g sln	Mole fraction $10^6 x_1$ (compilers)
1.002	0.00380	8.14
10.000	0.00363	7.82
34.472[a]	0.00292	6.40
50.030	0.00270	5.98
125.100	0.00127	2.94
199.900	0.000572	1.38
279.800	0.000336	0.847
358.700	0.000189	0.495

[a]Artificial seawater, composition not specified but probably similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	(1) commercial, 99 + % pure

ESTIMATED ERROR:

Temperature ± 1 K

Solubility ± 10 relative %

REFERENCES:

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COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the system cyclohexane (1) and water (2) have been reported in the references listed in Table 1.

TABLE 1: Quantitatuve Solubility Studies of the Cyclohexane(1) - Water (2) System

Reference	T/K	Solubility	Method
Bennett and Philip (ref 1)	290	(1) in (2)	volumetric
Tarassenkow and Poloshinzewa (ref 2)	287-326	(2) in (1)	synthetic
Berkengeim (ref 3)	293-323	(2) in (1)	Karl Fischer
Black et al. (ref 4)	293	(2) in (1)	radiotracer
Durand (ref 5)	289	(1) in (2)	cloud point
McBain and Lissant (ref 6)	298	(1) in (2)	cloud point
Kudchadker and McKetta (ref 7)	311-411[a]	(1) in (2)	not specified
Guseva and Parnov (ref 9,10)	298-494	(1) in (2)	synthetic
Englin et al. (ref 11)	289-323	(2) in (1)	analytical
Zel'venskii et al. (ref 12)	293	(2) in (1)	radiotracer
Johnson et al. (ref 13)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 14)	298	(1) in (2)	GLC
Gregory et al. (ref 15)	298	(2) in (1)	Karl Fischer
Rebert and Hayworth (ref 8,16)	403-643[a]	mutual	synthetic
Burd and Braun (ref 17)	368-478[a]	(2) in (1)	GLC
Bröllos et al. (ref 18)	275-421[a]	mutual	synthetic
Roddy and Coleman (ref 19)	298	(2) in (1)	radiotracer
Roof (ref 20)	530	mutual	synthetic
Plenkina et al. (ref 21)	403-523	(2) in (1)	synthetic
Glasoe and Schultz (ref 22)	288-303	(2) in (1)	Karl Fischer
Pierotti and Liabastre (ref 23)	278-318	(1) in (2)	GLC
Leinonen and Mackay (ref 24)	298	(1) in (2)	GLC
Sultanov and Skripka (ref 25,32)	473-523[a]	(2) in (1)	not specified
Goldman (ref 26)	283-313	(2) in (1)	Karl Fischer
Mackay et al. (ref 27,28)	298	(1) in (2)	GLC
Budantseva et al. (ref 29)	293	mutual	GLC, Karl Fischer
Kirchnerova and Cave (ref 30)	298	(2) in (1)	Karl Fischer
Price (ref 31)	298	(1) in (2)	GLC

(Table 1 continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}: [110-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A. Australia. September 1986.

CRITICAL EVALUATION:

TABLE 1 (continued)

Reference	T/K	Solubility	Method
Korenman and Aref'eva (ref 33)	293,298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 35)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 36)	298	(1) in (2)	partition coefficient
Schwarz (ref 37)	297	(1) in (2)	chromatographic
Tsonopoulos and Wilson (ref 39)	313-482[a]	mutual	GLC, Karl Fischer

[a]Pressure also varied, see Table 4

Solubility data for cyclohexane in water may also be calculated from the calorimetric data of Gill *et al.* (ref 40) and quantitative solubility data for the cyclohexane-heavy water (D_2O) system are given in the publications of Guseva and Parnov (ref 9) and Backx and Goldman (ref 38).

Apart from the paper by Roof (ref 20), which did not contain sufficient information to justify compilation, the original data in all the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation. The datum of Krzyzanowska and Szeliga (ref 35) does not appear to be indendent of that of Price (ref 31) and so has been excluded from this Evaluation.

Despite the large number of investigations of this system (Table 1), the mutual solubilities are poorly characterised and warrant thorough reinvestigation over the entire liquid range. No data have been "Recommended".

In the Tables which follow values which have been obtained by the Evaluator by graphical interpolation of the original data are indicated by an asterisk (*). "Best" values were obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as convenient representation of the spread of reported values rather than error limits.

For convenience, further discussion of this system will be divided into three sections.

| COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

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

Most of the available data for the solubility of cyclohexane in water are summarized in Table 2 below.

In preparing Table 2 below the data of Mackay *et al.* (ref 27) were excluded as the temperature was not specified; anyway, these data are probably superceded by later measurements from the same laboratory (ref 28). The various data reported at high temperature have also been excluded as they are discussed in detail in section 3 below. The datum of Schwarz (ref 37) at 296.7K, although in reasonable agreement with other values, has been excluded for representational convenience.

At 298K, the only temperature where sufficient data have been obtained to enable meaningful evaluation to be made, the approximate values of Guseva and Parnov (ref 9,10) and Korenman and Aref'eva are rejected as is the datum of Pierotti and Liabastre (ref 23) which is markedly higher than all other values. All other data are included in Table 2.

At other temperatures the data are much too scattered to enable a satisfactory evaluation to be made. This can be clearly seen from Figure 1 which plots all the available data. Thus no "Best" values have been calculated in Table 2 other than at 298K. Clearly, this system requires a thorough reinvestigation over the whole temperature range.

TABLE 2: Solubility of Cyclohexane (1) in Water (2)

Solubility values

T/K	Reported values 10^3 g(1)/100 g sln	"Best" value ($\pm \sigma_n$)[a] 10^3 g(1)/100 g sln	$10^5 x_1$
278	8.19 (ref 23)		
288	6.2[b] (ref 5), 8.87 (ref 23)		
293	7.0 (ref 29) 10 (ref 33)		
298	5.5 (ref 14), 5.67 (ref 24), 5.75 (ref 28), 6.65 (ref 31), 5.5 (ref 36)	5.8 ± 0.4	1.2
308	4.54[c] (ref 7), 8.88 (ref 23)		
318	9.13 (ref 23), 7.14[*] (ref 39)		
323	7.55 (ref 39)		
329	17 (ref 9,10)		
343	10.1 (ref 39)		
344	2.7 (ref 7)		

a Best values not calculated except at 298 K (see text)
b Refers to 289K
c Refers to 310K

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)
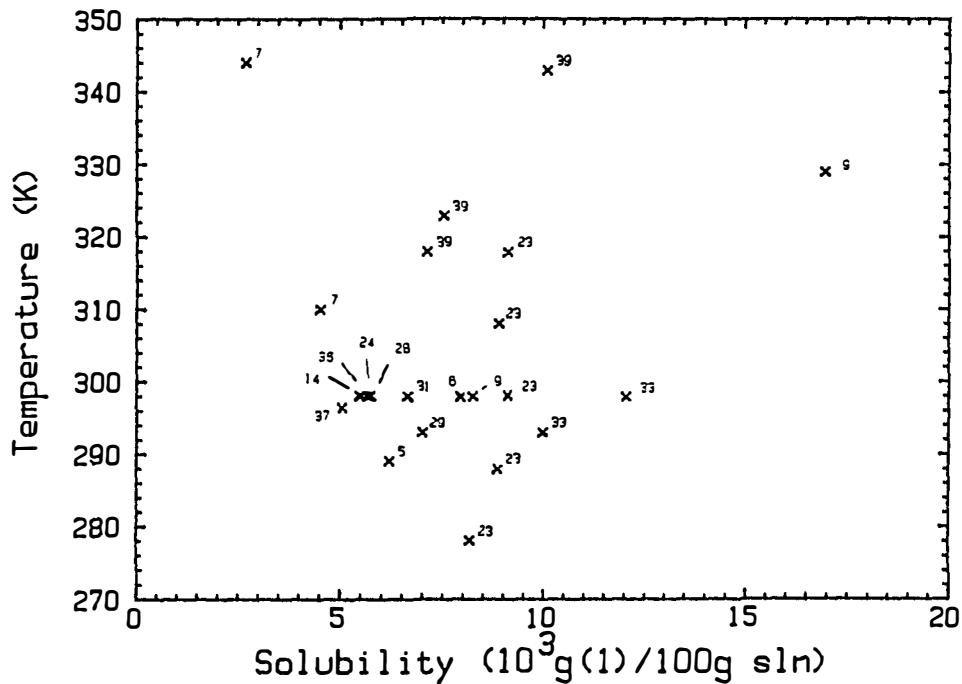
FIGURE 1. Solubility data for cyclohexane (1) in water. Numbers refer to the reference list. No line of best fit plotted because of scatter in data.

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

There are more solubility data for the hydrocarbon-rich phase than for the water-rich phase. Although the values of Tarassenkow and Poloshinzewa (ref 2) and Englin *et al.* (ref 11) are in good agreement over a wide temperature range, they are approximately twice as large as those reported by Goldman (ref 26) which in turn are close to those of most other studies (see Table 3). It should also be noted that the solubility data reported in ref 2 and ref 11 for a number of well-defined hydrocarbon-water systems are significantly higher than "Recommended" values. Nevertheless, there are insufficient independent data at present to justify exclusion of any values and thus all results are included in Table 3. In view of the lack of agreement between the various studies, the averaged "Best" values should be regarded as very tentative.

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

TABLE 3: Solubility of Water (2) in Cyclohexane (1)

T/K	Solubility values		
	Reported values $10^3 g(2)/100g$ sln	"Best" values ($\pm \sigma_n$) $10^3 g(2)/100g$ sln	$10^4 x_2$
283	4* (ref 2), 6.7 (ref 11), 3.4 (ref 2)	5 ± 1	2.3
293	9* (ref 2), 8.7 (ref 3), 10 (ref 4), 12.2 (ref 11), 9.8 (ref 12), 5.9 (ref 26), 10.1 (ref 29)	9 ± 2	4.2
298	13* (ref 2), 5.6 (ref 13), 6.9 (ref 15), 8.0 (ref 19), 7.4 (ref 22), 7.0 (ref 26), 7.0 (ref 30)	8 ± 2	3.7
303	17* (ref 2), 19.4 (ref 11), 8.7 (ref 22), 9.6 (ref 26)	14 ± 5	6.5
313	31* (ref 2), 31.7 (ref 11), 13.1 (ref 26), 13.3 (ref 39)	24 ± 8	12
323	46* (ref 2), 15 (ref 3), 49 (ref 11), 19.4* (ref 39)	32 ± 15	17

The data in Table 3 are also plotted in Figure 2. This plot shows that the temperature dependence of the solubility observed by Goldman (ref 26) and Glasoe and Schultz (ref 22) is much less than that of ref 2 and ref 11.
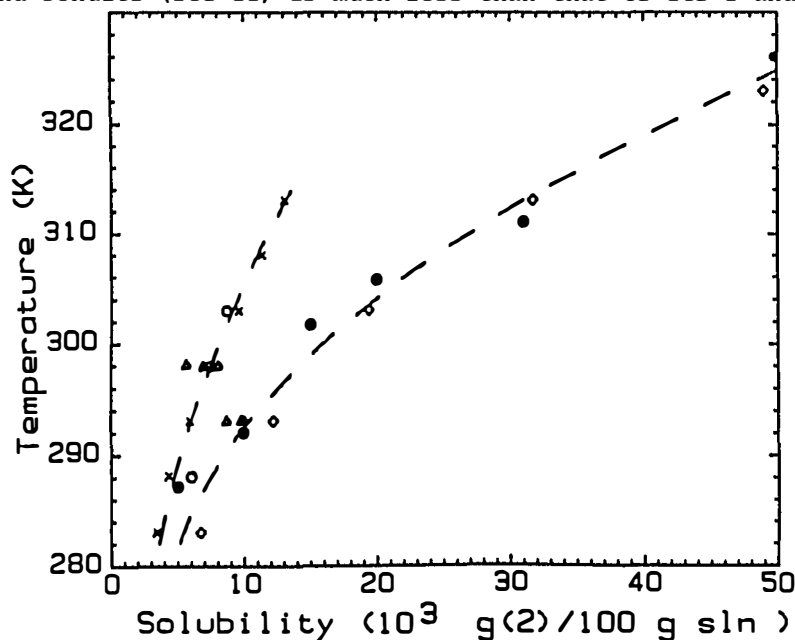
FIGURE 2. Solubility of water in cyclohexane: ref 2 (●); ref 11 (◇); ref 22 (○); ref 26 (x); other data (Δ). Full lines not drawn through data Points because of poor agreement (see text).

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (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.
	September 1986.

CRITICAL EVALUATION: (continued)

3.   THE MUTUAL SOLUBILITIES OF CYCLOHEXANE (1) AND WATER (2) AT ELEVATED PRESSURES

To clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram. Cyclohexane + water exhibits type III phase behaviour (ref 41,42) and the projection is topographically similar to that of benzene + water.

Solubilities in the cyclohexane-water system have been studied at higher than atmospheric pressures in the publications listed in Table 4.

TABLE 4:   Solubility Studies of the Cyclohexane-Water
System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Kudchadker and McKetta (ref 7)	0.1-3	311-411	(1) in (2)
Guseva and Parnov (ref 9,10)	-[a]	298-493	(1) in (2)
Rebert and Hayworth (ref 8,16)	0.6-22.1	403-643	mutual
Burd and Braun (ref 17)	0.2-3	368-478	(2) in (1)
Bröllos et al. (ref 18)	19-174	275-421	mutual
Roof (ref 20)	-[b]	-[b]	-[b]
Plenkina et al. (ref 21)	-[a]	403-523	(2) in (1)
Sultanov and Skripka (ref 25,32)	3-79	473-523	(2) in (1)
Tsonopoulos and Wilson (ref 39)	0.3-3	313-482	mutual

a Along three phase line
b Critical point at unspecified composition

In view of the limited amount of data at high pressures and the differing conditions employed, no Critical Evaluation is possible at present. However, the solubilities of water in cyclohexane at $p \simeq 3$ MPa, T ≈ 473K reported by Burd and Braun (ref 17) and Sultanov and Skripka (ref 25,32) are in reasonable agreement (approximately 3.0 and 3.8 g(2)/100 g sln respectively) but differ significantly from that reported by Tsonopoulos and Wilson (ref 39), (1.7 g(2)/100 g sln). Similarly, the atmospheric pressure data of Kudchadker and McKetta (ref 7) are only in fair agreement with comparable data (Table 3). Their conclusion that the solubility of cyclohexane in water increases linearly with pressure at a given temperature is inconsistent with the results for numerous hydrocarbon-water systems as noted by Guseva and Parnov (ref 9,10).

COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (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. September 1986.

CRITICAL EVALUATION: (continued)

The temperature and pressure of the critical end point have been determined by Rebert and Hayworth (ref 8,16) and by Roof (ref 20). The values are in good agreement.

Reference	T/K	p/MPa
Rebert and Hayworth (ref 8,16)	528.9	8.019
Roof (ref 20)	529.9	8.039

Bröllos *et al.* (ref 18) have reported detailed measurements in the high pressure region between the critical temperatures of the pure components. These data are for the two phase-one phase boundary and at most pressures and temperatures studied the phases are at liquid-like densities. These data are probably reliable as they were determined using a reliable, well-tested experimental method. However, in the absence of confirmatory studies no Critical Evaluation is possible.

The interested user is referred to the original measurements compiled in the data sheets following this Critical Evaluation for experimental values.

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COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [1100-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

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COMPONENTS:	EVALUATOR:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. September 1986.

CRITICAL EVALUATION: (continued)

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Tarassenkow, D.N.; Poloshinzewa, E.N. *Ber. Dtsch. Chem. Ges.* <u>1932</u>, *65B*, 184-6.

VARIABLES:	PREPARED BY:
Temperature: 14-53°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in cyclohexane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
14	0.005	2.3
19	0.010	4.7
28.5	0.015	7.0
32.5	0.020	9.3
38	0.031	14.5
53	0.050	23.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
No details were reported in the paper.	(1) Kahlbaum; dried over calcium chloride and twice distilled over Na-K. (2) not specified.

ESTIMATED ERROR:

soly. ± 0.01%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Berkengeim, T.I. *Zavod. Lab.* <u>1941</u>, *41*, 592-4.

VARIABLES:	PREPARED BY:
Temperature: 20 and 50°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of Water in Cyclohexane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
20	0.0087	4.1
50	0.015	7.0

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (2) in (1) was determined by the Karl Fischer reagent method.	(1) source not specified; CP reagent; b.p. 80°C; used as received. (2) not specified.

	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.
VARIABLES: One temperature: 20°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 20°C and at a total saturation pressure of 1 atm was reported to be 0.010 g(2)/100 g(1). The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 0.010 g(2)/100 g sln and 4.7×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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.* <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7734-18-5]	Durand, R. *C.R. Hebd. Seances Acad. Sci.* <u>1948</u>, *226*, 409-10.
VARIABLES:	PREPARED BY:
One temperature: 16°C	M. C. Haulait-Firson

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 16°C was reported to be 0.08 cm^3(1)/dm^3(2).

With the assumption of a solution density of 1.00 g cm^{-3} and a density value of 0.782 g cm^{-3} for cyclohexane at 16°C (ref 2), the corresponding mass percent is 0.0062 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.3 x 10^{-5} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The thermostatic method described in ref 1 was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.	(1) not specified (2) distilled
	ESTIMATED ERROR: soly. ± 0.005 cm^3(1)/dm^3(2)
	REFERENCES: 1. Durand, R. *C.R. Hebd. Seances Acad. Sci.* <u>1946</u>, *223*, 898. 2. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier. 1950.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	McBain, J.W.; Lissant, K.J. *J. Phys. Colloid. Chem.* <u>1951</u>, *55*, 655-62.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

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

With the assumption of a solution density of 1.00 g cm^{-3}, the corre-
sponding mass percent is 0.008 g(1)/100 g sln and the corresponding
mole fraction, x_1, is 1.7×10^{-5} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) was pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.	(1) C.P. grade. (2) distilled and boiled to remove CO_2.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Kudchadker, A.P.; McKetta, J.J. *A.I.Ch.E.J.* <u>1961</u>, *7*, 707.

VARIABLES:	PREPARED BY:
Temperature: 100-280°F Pressure: 14.7-450 psia	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexane in water. Smoothed data

		t = 100°F (310.93 K)		t = 160°F (344.26 K)	
p/psia	p/MPa (compiler)	$10^5 x_1$	g(1)/100 g sln (compiler)	$10^5 x_1$	g(1)/100 g sln (compiler)
14.7	0.101	0.97	0.00454	0.58	0.00271
20.0	0.138	1.34	0.00626	1.00	0.00468
30.0	0.207	2.03	0.00949	1.60	0.00748
40.0	0.276	2.72	0.01272	2.20	0.01029
50.0	0.345	3.41	0.01594	2.93	0.01323
60.0	0.414	4.10	0.01917	3.45	0.01613
80.0	0.552	5.48	0.02562	4.71	0.02202
100.0	0.689	6.85	0.03202	5.92	0.02767
120.0	0.827	8.22	0.03842	7.18	0.03356
140.0	0.965	9.60	0.04487	8.43	0.03940
160.0	1.103	11.03	0.05155	9.71	0.04538
180.0	1.241	12.04	0.05627	10.92	0.05104
200.0	1.379	13.8	0.06449	12.28	0.05739
250.0	1.724	17.08	0.07981	15.41	0.07201
300.0	2.068	20.2	0.09438	18.24	0.08522
350.0	2.413	23.11	0.10796	21.0	0.09811
400.0	2.758	25.84	0.12070	23.61	0.11029
450.0	3.103	28.35	0.13241	25.98	0.12135

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experimental technique and the analytical procedure are described in detail in ref 1. No more details are given in the paper.	(1) pure grade stock; purity of about 99.6% (gas chromatography) (2) distilled; boiled to remove any dissolved gases.
	ESTIMATED ERROR: not specified.
	REFERENCES: 1. Davis, J.E. M.S. Thesis, The University of Texas, Austin, 1959.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7]	Kudchadker, A.P.; McKetta, J.J.
(2) Water; H_2O; [7732-18-5]	*A.I.Ch.E.J.* <u>1961</u>, *7*, 707.

Solubility of cyclohexane in water.   Smoothed data

		t = 220°F (377.59 K)		*t* = 280°F (410.93 K)	
p/psia	p/MPa (compiler)	$10^5 x_1$	g(1)/100 g sln (compiler)	$10^5 x_1$	g(1)/100 g sln (compiler)
14.7	0.101				
20.0	0.138				
30.0	0.207	0.72	0.00337		
40.0	0.276	1.32	0.00617		
50.0	0.345	1.92	0.00898		
60.0	0.414	2.51	0.01173	0.70	0.00327
80.0	0.552	3.70	0.01730	1.91	0.00893
100.0	0.689	4.89	0.02286	3.13	0.01463
120.0	0.827	6.05	0.02828	4.40	0.02057
140.0	0.965	7.27	0.03398	5.62	0.02627
160.0	1.103	8.48	0.03964	6.82	0.03188
180.0	1.241	9.69	0.04529	7.95	0.03716
200.0	1.379	10.8	0.05048	9.08	0.04244
250.0	1.724	13.92	0.06505	12.1	0.05655
300.0	2.068	16.68	0.07794	14.6	0.06823
350.0	2.413	19.2	0.08971		
400.0	2.758	21.52	0.10054		
450.0	3.103	23.46	0.10959		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Zh. Fiz. Khim.* <u>1963</u>, *37*, 2763.
VARIABLES:	PREPARED BY:
Temperature: 25-220.5°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of cyclohexane in water

t/°C	g(1)/100 g(2)	g(1)/100 g sln	$10^4 x_1$ (compiler)
25	0.008	0.008	0.17
56	0.017	0.017	0.36
94	0.028	0.028	0.60
127	0.0517	0.0517	1.11
162	0.146	0.146	3.13
220.5	1.785	1.784	38.72

The same data are reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass ampules at pressures less than 17 kg/cm². No more details were reported in the paper.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES: 1. Guseva, A.N.; Parnov, E.I. *Radiokhimiya* <u>1963</u>, *5*, 507-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (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: 10-50°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in cyclohexane

t/°C	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.0067	3.1
20	0.0122	5.70
30	0.0194	9.06
40	0.0317	14.8
50	0.0490	22.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water, H_2O; [7732-18-5]	Zel'venskii, Ya.D; Efremov, A.A.; Larin, G.M. *Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 3-7.
VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 20°C was reported to be
0.0098 g(2)/100 g sln.
The corresponding mole fraction, x_2, calculated by the compiler
is 4.6×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.	(1) source not specified; pure grade; shaken with conc. H_2SO_4 + HNO_3; washed with water, dried over sodium, and distilled; purity not specified. b.p. 80.82°C. (2) source not specified; commercial; 1 Ci/mL HTO used as received.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Johnson, J.R.; Christian, S.D.; Affsprung, H.E. *J. Chem. Soc.* A <u>1966</u>, 77-8.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be 0.0024 mol(2) dm^{-3} sln.

With the assumption of a solution density of 0.7739 g cm^{-3} (density value of pure cyclohexane reported in ref 2), the corresponding mass percent is 0.0056 g(2)/100 g sln and the corresponding mole fraction, x_2, is 2.6×10^{-4} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solute isopiestic apparatus described in ref 1 was used. Samples were equilibrated in constant-temperature water-baths. Water solubilities were determined using the Beckman Model KF-3 Aqua-meter.	(1) source not specified; certified or reagent grade; distilled through a 30-plate oldershaw column. (2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. ± 0.0003 mol(2) dm^{-3} sln
     (type of error not specified)

REFERENCES:

1. Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Worley, J.D. *J. Chem. Educ.* <u>1963</u>, *40*, 419.
2. Goldman, S. *Can. J. Chem.* <u>1974</u>, *52*, 1668.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported to be 55 mg (1)/kg sln.

The corresponding mole fraction, x_1, calculated by the compiler, is 1.18×10^{-5}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.

ESTIMATED ERROR:
temp. ± 1.5 K   soly. 2.3 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092.

2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Gregory, M.D.; Christian, S.D.; Affsprung, H.E. *J. Phys. Chem.* <u>1967</u>, *71*, 2283-9.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be
0.00297 mol(2)dm^{-3} sln.

With the assumption of a solution density of 0.7739 g cm^{-3} (density
value of pure cyclohexane reported in ref 2), the corresponding mass
percent is 0.0069 g(2)/100 g sln and the corresponding mole fraction,
x_2, is 3.2 x 10^{-4} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubility of (2) in (1) was ob-tained using the solute isopiestic method described in ref 1. The samples were titrated by the Karl Fischer method using a Beckman KF-3 aquameter. The Karl Fisher reagent was standardized alternatively by titrating weighed amounts of sodium tartrate dihydrate or by titrating a 25° water-saturated benzene solu-tion.	(1) source not specified; reagent grade; fractionally distilled using a 30-plate oldershaw column. (2) not specified.

	ESTIMATED ERROR:
	temp. ± 0.1 K

	REFERENCES:
	1. Christian, S.D.; Affsprung, H.E.; Johnson, J.R.; Worley, J.D. *J. Chem. Educ.* <u>1963</u>, *40*, 419. 2. Goldman, S. *Can. J. Chem.* <u>1974</u>, *52*, 1668.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Cyclohexane; C_6H_{12}; [110-82-7] 2. Water; H_2O; [7732-18-5]	Rebert, C. J.; Hayworth, K. E. *Am. Inst. Chem. Engnrs. J.* <u>1967</u>, *13*, 118-121.

VARIABLES:	PREPARED BY:
Pressure and temperature along one phase-two phase boundary.	C. L. Young

EXPERIMENTAL VALUES:

Smoothed data

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{12}}$
593	320	11.43	1657	2.7	0.0059
603	330	13.06	1894		
613	340	14.92	2164		
623	350	16.86	2445		
633	360	19.21	2785		
643	370	21.83	3165		
643.8[a]	370.6	22.14	3210		
643	320	22.06	3199		
633	360	20.07	2910		
623	350	18.25	2646		
613	340	16.65	2414		
603	330	15.23	2209		
593	320	14.17	2054		
583	310	13.39	1942		
580	307	13.24	1920		
577	304	13.21	1916		
575	302	13.28	1925		
573	300	13.69	1985		
568	295	15.88	2303		
565	292	17.52	2540		
563	290	18.63	2702		
603	330	13.46	1952		
613	340	15.44	2239	9.0	0.021
623	350	17.70	2566		

(cont.)

AUXILIARY INFORMATION

METHOD APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Samples of mixtures of known composition confined over mercury. Samples heated in a vapor bath and the pressure-temperature phase boundaries determined by direct observation of appearance or disappearance of a phase. Apparatus similar to that described in ref. (1).	1. No details given.

ESTIMATED ERROR:
$\delta T/K = \pm 0.05$
$\delta p/psi = \pm 1.$

REFERENCES:
1. Rebert, C. J.; Kay, W. B.
   Am. Inst. Chem. Engnrs. J.
   <u>1959</u>, *5*, 285.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Cyclohexane; C_6H_{12}; [110-82-7]	Rebert, C. J. ; Hayworth, K. E.
2. Water; H_2O; [7732-18-5]	*Am. Inst. Chem. Engnrs. J.*
	<u>1967</u>, *13*, 118-121.

EXPERIMENTAL VALUES:

Smoothed data

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{12}}$
633	360	20.61	2989	9.0	0.021
635	362	21.38	3100		
636.5	363.3	21.94	3182		
635	362	22.32	3236		
633	360	22.45	3255		
632.6[a]	359.4	22.49	3261		
632	359	22.51	3264		
631	358	22.54	3269		
629	356	22.62	3280		
627	354	22.71	3294		
625	352	22.81	3308		
623	350	22.96	3329		
621	348	23.16	3358		
619	346	23.48	3405		
507	235	3.68	533	33.3	0.0966
517	245	4.36	632		
527	255	5.18	751		
537	265	6.10	885		
547	275	7.12	1032		
557	285	8.25	1196		
567	295	9.57	1388		
573	300	10.30	1494		
578	305	11.07	1605		
583	310	11.96	1734		
588	315	12.87	1866		
593	320	13.79	2000		
598	325	14.96	2169		
603	330	16.13	2339		
608	335	17.50	2538		
613	340	19.07	2765		
493	220	3.68	533	60.0	0.0243
503	230	4.47	648		
513	240	5.35	776		
523	250	6.30	914		
533	260	7.45	1081	94.8	0.0796
543	270	8.78	1273		
553	280	10.29	1492		
563	290	12.17	1764		
573	300	14.32	2076		
583	310	17.79	2580		
493	220	2.42	351		
503	230	2.88	417		
513	240	3.42	496		
523	250	4.09	593		
533	260	4.86	705		
535	262	5.06	734		
537	264	5.28	765		
539	266	5.54	803		
542.1	268.9	6.25	906		
541	268	6.60	957		
540.4	267.2	6.73	976		
540	267	6.76	980		
536	263	7.06	1024		
534	261	7.08	1027		
533	260	7.06	1024		
528	255	6.93	1005		
523	250	6.76	980		
518	245	6.56	951		
516.4[b]	243.2	6.48	939		

(cont.)

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Cyclohexane; C_6H_{12}; [110-82-7]	Rebert, C. J.; Hayworth, K. E.
2. Water; H_2O; [7732-18-5]	*Am. Inst. Chem. Engnrs. J.*
	1967, *13*, 118-121.

EXPERIMENTAL VALUES:

Smoothed data

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{12}}$

Three phase equilibrium locus

T/K	T/°C	P/MPa	p/psi
403	130	0.66	95
413	140	0.86	124
423	150	1.08	156
433	160	1.32	192
443	170	1.63	237
453	180	2.01	291
463	190	2.46	357
473	200	2.99	433
483	210	3.58	519
493	220	4.32	627
503	230	5.18	751
508	235	5.64	818
513	240	6.14	890
518	245	6.68	968
523	250	7.28	1055
528	255	7.92	1148
528.9	255.7	8.01	1162

[a] Critical point.

[b] Three-phase point.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Burd, S.D.; Braun, W.G. *Proc. Div. Refining, Am. Petrol.* *Inst.* 1968, *48*, 464-76.
VARIABLES: Temperature and pressure	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Hydrocarbon-rich liquid phase composition for the three-phase conditions.

p/psia	p/MPa (compiler)	t/°F	T/K (compiler)	g(2)/100 g sln	x_2 (compiler)
25	0.172	202	367.59	0.22	0.0102
50	0.345	241	389.26	0.46	0.0211
100	0.689	284	413.15	0.82	0.0372
150	1.034	312	428.70	1.20	0.0537
200	1.379	333	440.37	1.58	0.0698
250	1.724	350	449.81	1.93	0.0842
300	2.068	364	457.60	2.25	0.0971
350	2.413	377	464.82	2.60	0.1109
400	2.758	388	470.93	3.00	0.1262
24	0.165	200	366.48	0.22	0.0102
59	0.407	250	394.26	0.49	0.0225
127	0.876	300	422.04	1.03	0.0464
250	1.724	350	450.82	1.90	0.0830
450	3.103	400	477.60	3.70	0.1520

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The vapor and liquid phase composi-tions have been determined for the (1)-(2) system in the two-phase hydrocarbon-rich liquid region. Equilibrium points were obtained by incremental addition of water followed by stirring, settling, sampling and chromatographic analy-sis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. Many de-tails are given in the paper.	(1) Phillips Petroleum Company; 99.5% purity. (2) laboratory distilled.
	ESTIMATED ERROR: soly. ± 0.004 weight fraction of the (2) present.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Brollos, K.; Peter, K.; Schneider, G. M. *Ber. Bunsenges. Phys. Chem.* 1970, 74, 682-6.

VARIABLES:	PREPARED BY:
Pressure and temperature on one phase-two phase boundary.	C. L. Young

EXPERIMENTAL VALUES:

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
379.8	1742	0.100	34.1
369.0	1403		
363.0	1200		
360.1	1000		
351.5	798		
343.5	595		
333.7	395		
329.2	328		
330.0	293		
333.0	271		
334.2	245		
338.0	217		
392.2	1600	0.150	45.2
384.0	1400		
376.5	1202		
369.2	1000		
361.2	800		
351.0	600		
346.5	500		
340.0	394		
338.0	347		
339.0	299		

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measurements were made in a steel optical cell within an aluminum block furnace. The cell contents were stirred magnetically. Pressure was measured using a movable piston and Bourdon gauge. Temperature was measured with a steel-sheathed thermocouple. Components were charged into the cell and the transition from one phase to two phases was observed visually.	1. Merck sample purity 99.9 mole per cent. 2. Twice distilled.

ESTIMATED ERROR:

δT/K = ±0.1
$\delta P/P$ = ±0.01
(estimated by compiler)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7]	Brollos, K.; Peter, K.; Schneider, G. M.
(2) Water; H_2O; [7732-18-5]	*Ber. Bunsenges. Phys. Chem.* <u>1970</u>, *74*, 682-6.

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
340.5	250	0.150	45.2
357.7	222		
403.5	1610	0.200	53.9
393.9	1408		
387.0	1204		
378.7	1002		
369.0	800		
359.5	600		
352.2	500		
347.0	416		
343.0	328		
342.0	298		
345.0	246		
355.0	223		
412.4	1600	0.298	66.5
404.7	1400		
396.2	1200		
387.1	1004		
375.3	800		
363.8	600		
360.4	550		
349.2	398		
346.2	339		
346.5	237		
349.5	224		
352.7	214		
414.9	1600	0.400	75.7
406.5	1398		
399.2	1200		
390.1	995		
378.0	800		
364.3	600		
355.6	465		
347.6	352		
345.0	295		
342.0	230		
335.0	195		
421.5	1718	0.500	82.4
419.0	1645		
416.5	1584		
408.0	1406		
399.0	1195		
388.9	1004		
376.0	789		
364.0	600		
350.0	460		
340.1	375		
343.0	330		
338.5	250		
330.0	200		
413.0	1603	0.600	87.5
405.4	1405		
395.8	1200		
386.4	1000		
375.3	800		
362.0	595		
345.7	395		
336.2	319		
333.4	290		

Values of pressure and temperature on the one phase-two phase boundary

T/K	p/bar	x_1	g (1)/100 g soln
329.4	261	0.600	87.5
326.5	243		
323.1	220		
318.5	205		
406.7	1600	0.700	91.6
399.0	1405		
389.1	1200		
380.5	1000		
367.2	800		
351.1	588		
332.5	400		
325.0	342		
314.0	299		
300.5	250		
395.4	1605	0.800	96.9
387.1	1403		
377.6	1200		
367.2	1005		
353.9	800		
337.5	600		
316.5	400		
305.0	295		
295.1	244		
275.2	200		

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Roddy, J.W.; Coleman, C.F. *Talanta* <u>1968</u>, *15*, 1281-6.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be 0.00345 mol(2) dm^{-3} sln corresponding to a mole fraction, x_2, of 3.75×10^{-4}. The corresponding mass percent value calculated by the compiler is 0.0080 g(2)/100 g sln.

The compiler's calculation assumes a solution density of 0.7739 g mL^{-1} (density of cyclohexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A method of gravimetric absorption monitored by tritium tracer was used. (1) was equilibrated with a slight excess of tritiated water by shaking over a period of at least 8 hr in a thermostat. The phases were allowed to separate for at least 16 hr and then were sampled for tritium analysis. Most of the (1) phase was weighed into a boiling flask of a closed distillation system and then distilled through a magnesium perchlorate weighing tube. The magnesium perchlorate was then dissolved for measurement of its tritium content by liquid scintillation counting with a Packard Tri-Carb Scintillation Spectrometer.	(1) source not specified; spectral-grade reagent. (2) tritiated water at 5 Ci/mL; New England Nuclear Corp.; diluted to about 1 mCi/mL.

ESTIMATED ERROR:
soly. better than 1% (type of error not specified)

REFERENCES:
1. Goldman, S. *Can. J. Chem.*, <u>1974</u>, *52*, 1968.

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) Cyclohexane; C_6H_{12}; [110-82-7]
 	
(2) Water; H_2O; [7732-18-5]
	Plenkina, R.M.; Pryanikova, R.O.;
	   Efremova, G.D.
	
	Zh. Fiz. Khim. <u>1971</u>, *45*, 2389
	   <u>Deposited doc.</u> 1971,
	   VINITI 3028-71.

VARIABLES:
 	
  Temperature: 130-250°C
	PREPARED BY:
	
	  A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in cyclohexane

$t/°C$	x_2	g(2)/100 g sln (compiler)
130	0.036	0.79
163.0	0.093	2.15
188.0	0.130	3.10
200.9	0.154	3.75
213.5	0.193	4.87
219.0	0.216	5.52
232.0	0.265	7.16
244.0	0.322	9.23
250.0	0.350	10.33

AUXILIARY INFORMATION

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

The solubility of (2) in (1) was
determined in sealed glass tubes.
	(1) source not specified; CP
	   reagent; crystallized several
	   times; m.p. 6.50°C.
	
	(2) distilled.

	ESTIMATED ERROR: temp. ± 0.5 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Glasoe, P.K.; Schultz, S.D. *J. Chem. Eng. Data* <u>1972</u>, *17*, 66-8.

VARIABLES:	PREPARED BY:
Temperature: 15-30°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in cyclohexane

$t/°C$	$mol(2)dm^{-3}$ sln	g(2)/100 g sln (compiler)	$10^4 x_2$ (compiler)
15	0.0026 ± 0.0001	0.0060[a]	2.8
25	0.0032 ± 0.0002	0.0074[a]	3.5
30	0.0037 ± 0.0002	0.0087[a]	4.1

[a]calculated with the assumption of a solution density of 0.7831, 0.7739 and 0.7692 g cm^{-3} at respectively 15, 25 and 30°C; these values are the density values of pure cyclohexane at these temperatures (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was saturated with (2) by allowing it to stand in contact with (2) in a closed pyrex storage bottle protected from atmospheric moisture and placed in a constant temperature water bath. The concentration of (2) in (1) was determined by the Karl Fischer method using a conventional "dead-stop" end-point apparatus. The Karl Fischer reagent was standardized using standard sodium tartrate.	(1) source not specified; reagent grade; purified by distillation and dried over molecular sieve. (2) distilled in a pyrex system.

ESTIMATED ERROR:
soly.: see above (type of error not specified.

REFERENCES:
1. Timmermans, J. *Physico-chemical constants of pure organic compounds* Elsevier, <u>1950</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions" U.S. Nat. Tech. Inform. Serv., PB Rep., <u>1972</u>, No. 21163, 113 pp.

VARIABLES:	PREPARED BY:
Temperature: 278.26-318.36 K	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexane in water

$T/$ K	g(1)/100 g sln	$10^3 x_1$
278.26	0.008193 ± 0.00017	0.01837
288.36	0.008870 ± 0.00025	0.01991
298.26	0.008884 ± 0.00024	0.01998
308.36	0.008884 ± 0.00025	0.02004
318.36	0.009132 ± 0.00025	0.02068

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in a rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Fisher Scientific Co.; certified grade; used as received. (2) laboratory distilled water.

	ESTIMATED ERROR:
	soly.: standard deviation from at least 15 measurements are given above.

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12} [110-82-7] (2) Water; H_2O; [7732-18-5]	Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* <u>1973</u>, *51*, 230-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported to be 56.7 mg(1)dm^{-3} sln.

With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.00567 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.21 x 10^{-5} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was equilibrated for at least 12 hrs in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 hrs and the aqueous phase was tested (Tyndall effect). Both phases were analysed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analysed by GLC. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.	(1) Phillips Petroleum Co.; research grade; purity 99%+; used without further purification. (2) doubly distilled.

ESTIMATED ERROR:
temp. ± 0.1 K   soly. ± 1 mg(1)dm^{-3} sln

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Goldman, S. *Can. J. Chem.* <u>1974</u>, *52*, 1668-80.

VARIABLES:	PREPARED BY:
Temperature: 10-40°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in cyclohexane

t/°C	mol(2)dm^{-3} sln	g(2)/100 g sln (compiler)	$10^4 x_2$ (compiler)
10	0.00147	0.0034[a]	1.6
15	0.00185	0.0043[a]	2.0
20	0.00255	0.0059[a]	2.8
25	0.00301	0.0070[a]	3.3
30	0.00410	0.0096[a]	4.5
35	0.00485	0.0114[a]	5.3
40	0.00552	0.0131[a]	6.1

[a] calculated with the assumption of a solution density of 0.7878, 0.7831, 0.7785, 0.7739, 0.7692, 0.7643 and 0.7595 g cm^{-3} at respectively 10, 15, 20, 25, 30, 35 and 45°C; these values are the density values of pure cyclohexane at these temperatures (ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(1) was equilibrated with an excess of (2) in 175 mL bottles fitted with Bakelite screw caps. The bottles immersed in a water-bath were given end-over-end rotation at 20 r.p.m. After equilibration, aliquots (5 mL ± 0.2%) were taken with calibrated Hamilton syringes and injected into the titration vessel. Analyses were performed with an Aquatest II automatic Karl Fischer Titrator.	(1) certified grade; washed with water, dried with silica gel, and distilled. d_4^{25} 0.77390 ± 0.00002 (2) distilled.

ESTIMATED ERROR:

temp. ± 0.02 K
soly. ± 0.00024 (mean of std. dev.)

REFERENCES:

1. Timmermans, J. *Physico-chemical constants of pure organic compounds* Elsevier, <u>1950</u>.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.J.; Wolkoff, A.W. "Water Quality Parameters" Symp. 1973, ASTM Spec. Tech. Publ. <u>1975</u>, *573*, 251-8.

VARIABLES:	PREPARED BY:
not specified	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported three different values for the solubility of cyclohexane in water: 55.8, 50.2 and 61.7 $mg(1)dm^{-3}$ sln. Using the mean value and assuming a solution density of 1.00 g mL^{-1}, the corresponding mass percent, calculated by the compiler, is 0.0056 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.2 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(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 equili-brations it is possible to calculate the amount of (1) in the original sample.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 10% (compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* <u>1975</u>, *53*, 239-41.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported to be 0.0575 g(1)dm^{-3} sln.

With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.00575 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.23 x 10^{-5} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined using a vapor phase extraction technique followed by gas chromatographic analysis. Equilibration apparatus and procedure are given in detail in the paper. The gas chromatograph was a Hewlett-Packard Model equipped with a hydrogen flame-ionization detector.	(1) Phillips Petroleum Co.; research grade (>99.9%); used as received. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 0.1 K soly. ± 0.0073 g(1)dm^{-3} sln
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* <u>1976</u>, *50*, 1344. <u>Deposited doc.</u> 1976, VINITI 438-76.
VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 20°C was reported to be $x_1 = 1.5 \times 10^{-5}$.
The corresponding mass percent calculated by the compiler is
0.0070 g(1)/100 g sln.

The solubility of water in cyclohexane at 20°C was reported to be $x_2 = 4.7 \times 10^{-4}$.
The corresponding mass percent calculated by the compiler is
0.0101 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.	(1) source not specified; pure or analytical reagent grade; purity <99.9%. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Kirchnerova, J.; Cave, G.C.B. *Can. J. Chem.* <u>1976</u>, *54*, 3909-16.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in cyclohexane at 25°C was reported to be
0.0030 mol(2)/dm^3 sln.

With the assumption of a solution density of 0.7739 g cm^{-3} (density
value of pure cyclohexane reported in ref 1, the corresponding mass
percent is 0.0070 g(2)/100 g sln and the corresponding mole fraction,
x_2, is 3.3 x 10^{-4} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The Karl Fischer dead-stop back-titration method was used. 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 tube rested against the upper inside wall of the vessel. The vessel was then stoppered, placed inside a plastic bag and submerged in a water thermostat. Trials had shown that the concentration of (2) in (1) became constant within 2 days. 10 mL of (1) saturated with (2) were transferred to the titration vessel for water determination. Apparatus is described in the paper.	(1) Fisher C-555; purified by double crystallization; purity 99.6% (gas chromatographic analysis); d_4^{25} 0.7734 ± 0.0001 (2) distilled and de-ionized
	ESTIMATED ERROR: temp. ± 0.1 K soly. ± 0.0002 mol(2)/dm^3 sln (std. dev. from 5 determinations)
	REFERENCES: 1. Goldman, S. *Can. J. Chem.* <u>1974</u>, *52*, 1668.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C and at system pressure was reported to be 66.5 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00665 g(1)/100 g sln and 1.423 x 10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.8 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12} [110-82-7] (2) Water; H_2O; [7732-18-5]	Skripka, V.G. *Tr. Vses. Neftegazov. Nauch. Issled. Inst.* <u>1976</u>, *61*, 139-51. Sultanov, R.G.; Skripka, V.G. *Zh. Fiz. Khim.* <u>1973</u>, *47*, 1035.
VARIABLES: Temperature: 200-250°C Pressure: 2.8-78.5 MPa	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in cyclohexane

$t/°C$	p/kg cm^{-2}	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
200	29	2.8	0.156	3.81
	50	4.9	0.091	2.10
	100	9.8	0.052	1.16
	150	14.7	0.046	1.02
	200	19.6	0.043	0.95
	300	29.4	0.042	0.93
	400	39.2	0.042	0.93
	500	49.0	0.042	0.93
	600	58.8	0.042	0.93
	700	68.6	0.042	0.93
	800	78.5	0.041	0.91
225	46.2	4.5	0.230	6.01
	50	4.9	0.209	5.35
	100	9.8	0.128	3.05
	150	14.7	0.100	2.32
	200	19.6	0.087	2.00
	300	29.4	0.084	1.92
	400	39.2	0.080	1.83
	500	49.0	0.076	1.73
	600	58.8	0.072	1.63
	700	68.6	0.068	1.54
	800	78.5	0.055	1.23

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experimental technique was described in ref 1. No details reported in the paper.	(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.* <u>1971</u>, *4*, 6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7]	Skripka, V.G.
	Tr. Vses. Neftegazov. Nauch. Issled. Inst. 1967, *61*, 139-51.
(2) Water; H_2O; [7732-18-5]	
	Sultanov, R.G.; Skripka, V.G.
	Zh. Fiz. Khim. 1973, *47*, 1035.

$t/°C$	$p/\text{kg cm}^{-2}$	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
250	70	6.9	0.345	10.13
	100	9.8	0.232	6.07
	150	14.7	0.182	4.55
	200	19.6	0.165	4.06
	300	29.4	0.145	3.50
	400	39.2	0.131	3.13
	500	49.0	0.122	2.89
	600	58.8	0.114	2.68
	700	68.6	0.106	2.47
	800	78.5	0.100	2.32

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. *87*:87654

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 20°C was reported to .
be 0.10 g(1)mL(2).
The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.010 g(1)/100 g sln and 2.1 x 10^{-5}.
The compiler's calculations assume a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* <u>1978</u>, *51*, 957-8.

VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported to be 0.12 $g(1)dm^{-3}$ sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.012 g(1)/100 g sln and 2.6 x 10^{-5}.

The compilers calculations assume a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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).	(1) not specified. (2) not specified.

ESTIMATED ERROR:
soly. ± 0.01 $g(1)dm^{-3}$ sln (standard deviation from 6 determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water at 25°C was reported
to be 66.5 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 0.00665 g(1)/100 g sln and 1.423×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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 at 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. 1.3 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of cyclohexane between the gas and aqueous phase. $\alpha = 8.0 \pm 02$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 97.58$ mm of Hg and $\log C_g = \log p - 4.269 = -2.28$ expressed in moles per liter. Therefore $C_s = 6.56 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0055 g(1)/100 g sln and the corresponding mole fraction, x_1, is 1.2×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.	(1) not specified. (2) not specified.

	ESTIMATED ERROR:
	soly. ± 10% (estimated by the compiler)

	REFERENCES:
	1. Hine, J.; Mooker, P.K. *J. Org. Chem.* <u>1975</u>, *4*, 292.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *Anal. Chem.*, <u>1980</u>, *52*, 10-15.
VARIABLES:	PREPARED BY:
One temperature: 23.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of cyclohexane in water at 23.5°C was reported to be .
0.0052 ± 0.0002 g(1)/100 g sln.

The corresponding mole fraction, x_1 was calculated by the compiler
to be 1.1×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.	(1) 99.9% purity used without further purification (2) distilled
	ESTIMATED ERROR: temp. ± 1.5°C soly. 4% (average std. dev.)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Water; H_2O; [7732-18-5]	Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* <u>1983</u>, *29*, 990-9.

VARIABLES:	PREPARED BY:
Temperature: 313-482 K Pressure: 0.03-3.0 MPa	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of cyclohexane in water

T/K	p / MPa	$10^4 \, x_1$	10^2 g(1)/100 g sln (compiler)
313.15	0.03151	0.156^b	0.728
373.15	0.2723	0.379^b	1.77
422.04	$-^a$	1.03	4.81
423.15	1.0032	1.30	6.07
473.15	2.965	3.92	18.3
482.21	$-^a$	4.93	23.0

a Not specified.

b Other data presented but rejected by the authors.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
All experimental details are given in an Appendix deposited in a Documentation Centre rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, whilst that of (2) in (1) was measured by Karl Fischer titration.	(1) No details given (2) No details given

ESTIMATED ERROR:
soly. ± 5% relative; repeatability of replicate analyses.
temp. not stated.
press. ± 1%; type of error not stated.

REFERENCES:

(1) Cyclohexane; C_6H_{12}; [110-82-7]
(2) Water; H_2O; [7732-18-5]

(continued)

The solubility of water in cyclohexane

T/K	p^{a}/MPa	$10^3\ x_2$	g(2)/100 g sln (compiler)
313.15	0.03151	0.887,0.924,1.13	0.021^{a}
373.15	0.2723	4.35, 5.12	0.10^{a}
423.15	1.0082	20.4,24.0	0.47^{a}
473.15	2.965	79.3	1.81

a Average value.

The three phase critical point was reported to be 529.4 K, 8.025 MPa and $x_1 = 1.748 \times 10^{-3}$ (0.82 g(1)/100 g sln, compiler).

The authors also report equations fitted to their own and literature data over the range 273-529 K, *viz.*

$$\ln x_1 = -209.11689 + 8325.49/T + 29.8231 \ln T$$

$$\ln x_2 = -62.7645 - 654.027/T + 9.99967 \ln T$$

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7]	Guseva, A.N.; Parnov, E.I.
(2) Deuterium oxide; (heavy water); D_2O; [7789-20-0]	*Radiokhimiya* <u>1963</u>, *5*, 507-9.

VARIABLES:	PREPARED BY:
Temperature: 71-179.5°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of cyclohexane in deuterium oxide

$t/°C$	$10^4 x_1$	g(1)/100 g sln (compiler)
71	0.331	0.0139
143	1.48	0.0622
168	3.2	0.134
179.5	4.47	0.188

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes.	(1) not specified. (2) distilled.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cyclohexane; C_6H_{12}; [110-82-7] (2) Deuterium oxide (heavy water); D_2O; [7789-20-0]	Backx, P.; Goldman, S. *J. Phys. Chem.* <u>1981</u>, *85*, 2975-9.

VARIABLES:	PREPARED BY:
Temperature: 283-313 K	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of deuterium oxide in cyclohexane

T/K	$10^4 x_2$	std. dev.	10^4 g(2)/100 g sln (compiler)
283	1.57	0.08	0.374
288	1.81	0.10	0.431
293	2.42	0.10	0.576
298	2.80	0.11	0.666
303	3.61	0.24	0.859
308	4.64	0.56	1.104
313	5.35	0.24	1.274

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a 175-ml milk-dilution bottle fitted with a Bakelite screw cap and a Teflon insert and rotated end-over-end, (1) was equilibrated with an excess of (2), sampled with Hamilton syringes and titrated in an Aquatest II automatic Karl Fischer Titrator.	(1) certified grade; washed with water, dried with silica gel, and distilled; d^{25} 0.77390. (2) obtained from the manufacturer; minimum isotopic purity of 99.7 atom % D.
	ESTIMATED ERROR: Temp. ± 0.01 K Std. dev. of soly calcd from 18-32 determinations reported above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethyl-1-butene; C_6H_{12}; [563-78-0] (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:
One temperature: 30°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in 2,3-dimethyl-1-butene at 30°C was reported to be 0.0459 g(2)/100 g sln.

The corresponding whole fraction, x_2 calculated by the compilers is 2.14×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methyl-1-pentene; C_6H_{12}; [763-29-1] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 2-methyl-1-pentene in water at 25°C was reported to be 78 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0078 g(1)/100 g sln and 1.7×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.

ESTIMATED ERROR:
temp. ± 1.5 K   soly. 3.2 g(1)/10^6 g(2)   (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 4-Methyl-1-pentene; C_6H_{12}; [691-37-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 4-methyl-1-pentene in water at 25°C was reported to be 48 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0048 g(1)/100 g sln and 1.0×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 chromato- graphed in conjunction with a flame- ionization detector.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 2.6 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland. G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 1-hexene (1) and Water (2) have been reported in the publications listed in Table 1.

TABLE 1:   Quantitative Solubility Studies of

the 1-Hexene (1) - Water (2) System

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	303	(2) in (1)	analytical
McAuliffe (ref 2)	298	(1) in (2)	GLC
Leinonen and Mackay (ref 3)	298	(1) in (2)	GLC
Budantseva *et al.* (ref 4)	293	mutual	GLC, Karl Fischer

Solubilities of 1-hexene in dilute aqueous HNO_3 solutions have also been reported (ref 5) but will not be considered in this Evaluation.

The original data in all of these publications (ref 1-5) 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 1-HEXENE (1) IN WATER (2)

The solubility data for 1-hexene in water are given in Table 2.

TABLE 2:   Recommended (R) and Tentative

Values of the Solubility of 1-Hexene (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	$10^5 x_1$
293	5 (ref 4)	1	1
298	5.0 (ref 2), 5.54 (ref 3)	5.3 ± 0.3 (R)	1.14 (R)

[a]"Best" values obtained by averaging where possible; σ_n has no statistical significance.

COMPONENTS:	EVALUATOR:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	A. Maczynski, Institute of Physical Chemistry, Polish Academy of Sciences, Warszawa, Poland.
	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia November 1984

CRITICAL EVALUATION: (continued)

2.   THE SOLUBILITY OF WATER (2) IN 1-HEXENE (1)

The solubility data for water in 1-hexene are listed in Table 3. As data have not been obtained under comparable conditions they must be classified as "Tentative". However, it can be noted that in (other) well characterised systems the data of Englin *et al.* (ref 1) at $T<300K$ are usually close to "Recommended" values. The data of Budantseva *et al.* (ref 4) on the other hand an often high.

TABLE 3:   Tentative values of the Solubility
of Water (2) in 1-Hexene (1)

T/K	Solubility values	
	g(2)/100g sln	$10^3 x_2$
293	0.029 (ref 4)	1.4
303	0.048 (ref 1)	2.2

REFERENCES

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

2.   McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

3.   Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* 1973, *51*, 230-3.

4.   Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* 1976, *50*, 1344; Deposited doc., VINITI 438-76.

5.   Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* 1972, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* *10*, 42-6.
VARIABLES: One temperature: 30°C	PREPARED BY: <u>1965</u>, A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in 1-hexene at 30°C was reported to be 0.0477 g(2)/100 g sln.

The corresponding mole fraction, x_2, calculated by the compilers is 2.23×10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-hexene 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 9.2×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.2 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 1-hexene in water was reported to be 7.781×10^{-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, 0.00654 g(1)/100 g sln and 1.40×10^{-5}.

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

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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Matheson, Coleman and Bell; 99% (2) Not specified
	ESTIMATED ERROR: Temp. ± 0.05 K Soly. not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Hexene; C_6H_{12}; [592-41-6] (2) Water; H_2O; [7732-18-5]	Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* <u>1973</u>, *51*, 230-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-hexene in water at 25°C was reported to be 55.4 mg(1) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.00554 g(1)/100 g sln and 1.18×10^{-5}.

The compiler's calculation assumes a solution density of 1.00 g mL^{-1}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was equilibrated at 25 ± 0.1°C for a minimum of 12 hrs in a 200-mL Teflon-stoppered vessel (25 cm long and 3.5 cm across) with gentle shaking, allowed to settle for 6 hrs and tested for the absence of emulsion (Tyndall effect). The aqueous and organic phases were analyzed by glc (with internal standardization) on a Hewlett-Packard Model 700 instrument equipped with a 15% SE-30 on 60/80 mesh acid-washed $(CH3)_2Cl_2Si$-treated Chromosorb P column (steel capillary 10 ft x 0.125 inch). The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analyzed by glc.	(1) Phillips Petroleum Co. research grade, 99+ mole%; used as received. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1 K soly. 30 mg(1) dm^{-3} (two standard deviations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) 1-Hexene; C_6H_{12}; [592-41-6]
 	
(2) Water; H_2O; [7732-18-5]
	Budantseva, L.S.; Lesteva, T.M.;
	  Nemstov, M.S.
	
	Zh. Fiz. Khim. <u>1976</u>, *50*, 1344.
	  Deposited doc. <u>1976</u>,
	  VINITI 438-76.

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of 1-hexene in water at 20°C was reported to
be $x_1 = 1 \times 10^{-5}$.

The corresponding mass percent calculated by the compiler is
0.005 g(1)/100 g sln.

The solubility of water in 1-hexene at 20°C was reported to
be $x_2 = 0.0016$.

The corresponding mass percent calculated by the compiler is
0.029 g(2)/100 g sln.

AUXILIARY INFORMATION

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

The solubility of (1) in (2) was de-
termined by glc. The solubility of
(2) in (1) was determined by Karl
Fischer reagent method.
	(1) source not specified; pure
	   or analytical reagent grade;
	   purity <99.9%.
	
	(2) not specified.

	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Hexene; C_6H_{12}; [592-43-8] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9.
VARIABLES: Temperature: 20-30°C	PREPARED BY: M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of 2-hexene 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)	10^5 x_1 (compiler)
20	8.75 ± 0.21	7.4	1.6
25	7.99 ± 0.23	6.7	1.4
30	6.60 ± 0.26	5.5	1.2

a   Uncertainties stated to be "standard deviations from means".
b   Assuming a solution density of 1.00 g mL^{-1} at all temperatures.

<u>Compiler's note</u>: 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^{-1} HCl.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Prepared by dehydration of 2-hexanol 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:	EVALUATOR:
(1) 2,2-Dimethylbutane; C_6H_{14}; [75-83-2]	M.C. Haulait-Pirson, Department of Chemistry, University of Leuven, Belgium.
(2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984

CRITICAL EVALUATION:

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

TABLE 1: Quantitative Solubility Studies of the
2,2-Dimethylbutane (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
Price (ref 3)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 4)	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. THE SOLUBILITY OF 2,2-DIMETHYLBUTANE (1) IN WATER (2)

The solubility data for 2,2-dimethylbutane in water are listed in Table 2. The datum of Krzyzanowska and Szeliga (ref 4) has been excluded from this evaluation as it does not appear to be independent of that of Price (ref 3). The agreement between the other reported values at 298K (ref 1, 2, 3) is only fair (± 10% relative) and the average "best" value can only be regarded as tentative at this stage. It should also be noted that the increase in solubility as the temperature goes from 298K to 273K reported by Polak and Lu (ref 2) is larger than typically observed in hydrocarbon-water systems (e.g. benzene in water).

TABLE 2: Tentative Values of the Solubility
of 2,2-Dimethylbutane (1) in Water (2)

T/K	Solubility values		
	Reported values 10^3 g(1)/100g sln	"Best" values (± σ_n)[a] 10^3 g(1)/100g sln	$10^6 x_1$
273	3.94 (ref 2)	3.9	8.2
298	1.84 (ref 1), 2.38 (ref 2), 2.11 (ref 3)	2.1 ± 0.2	4.4

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

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COMPONENTS:	EVALUATOR:
(1) 2,2-Dimethylbutane; C_6H_{14}; [75-83-2] (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. November 1984

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2,2-DIMETHYLBUTANE (1)

The solubility of water in 2,2-dimethylbutane has been reported in only one publication (ref 2), and thus no Critical Evaluation can be made. However, the data of Polak and Lu are generally in good agreement with "Recommended" values in well characterized systems. The interested user is referred to the appropriate data sheet for solubility values.

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

2. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

4. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *34*, 413-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylbutane; C_6H_{14}; [75-83-5] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2-dimethylbutane in water at 25°C was reported to
be 18.4 mg (1)/kg sln (0.00184 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler,
is 3.85×10^{-6}.
The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.3 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylbutane; C_6H_{14}; [75-83-2] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2,2-dimethylbutane in water

$t/$°C	mg(1)/kg sln	x_1 (compiler)
0^a	39.4^c	8.23×10^{-6}
25^b	23.8^c	4.97×10^{-6}

Solubility of water in 2,2-dimethylbutane

$t/$°C	mg(2)/kg sln	x_2 (compiler)
0^a	32^d	1.53×10^{-4}
25^b	84^e	4.02×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

ESTIMATED ERROR:
temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%;   e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylbutane; C_6H_{14}; [75-83-2] (2) Water, H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2-dimethylbutane in water at 25°C and at system pressure was reported to be 21.1 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00212 g(1)/100 g sln and 4.43 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.3 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylbutane; C_6H_{14}; [75-83-2] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,2-dimethylbutane in water at 25°C was reported to be 21.20 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00212 g(1)/100 g sln and 4.43×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 1.2 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (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. November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 2,3-dimethylbutane (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the
2,3-Dimethylbutane (1) - Water (2) System

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	273-323	(2) in (1)	analytical
Polak and Lu (ref 2)	273,298	mutual	GLC, Karl Fischer
Price (ref 3)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 4)	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.   THE SOLUBILITY OF 2,3-DIMETHYLBUTANE (1) IN WATER (2)

The solubility data for 2,3-dimethylbutane in water (ref 2, 3) are listed in Table 2 and plotted in Figure 1. The datum of Krzyzanowska and Szeliga (ref 4) has been excluded from this Evaluation as it does not appear to be independent of that of Price (ref 3).

At 298K, where comparison is possible, agreement between the reported values is only fair. At other temperatures only the values of Price (ref 3) are available. Thus all values are classified as Tentative. It should be noted firstly that the increase in solubility at lower temperatures reported by Polak and Lu (ref 2) is larger than is usually observed in hydrocarbon-water systems (e.g. benzene in water), and secondly the values of Price (ref 3) are usually reliable over the entire temperature range studied.

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (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. November 1984

CRITICAL EVALUATION: (continued)

TABLE 2: Tentative Values for the Solubility 2,3-Dimethylbutane (1) in Water (2)

T/K	Reported values[a] 10^3g(1)/100g sln	"Best" values ($\pm \sigma_n$)[b] 10^3g(1)/100g sln	$10^6 x_1$
273	3.29 (ref 2)	3.3	6.9
298	2.25 (ref 2), 1.91 (ref 3)	2.1 $\pm$ 0.2	4.4
303	1.9* (ref 3)	1.9	4.0
313	1.9* (ref 3)	1.9	4.0
323	2.1* (ref 3)	2.1	4.4
343	2.8* (ref 3)	2.8	5.9
363	3.5* (ref 3)	3.5	7.3
383	4.6* (ref 3)	4.6	9.6
403	7.5* (ref 3)	7.5	16
423	18* (ref 3)	18	38

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

[b] Obtained by averaging where appropriate, σ_n has no statistical significance.
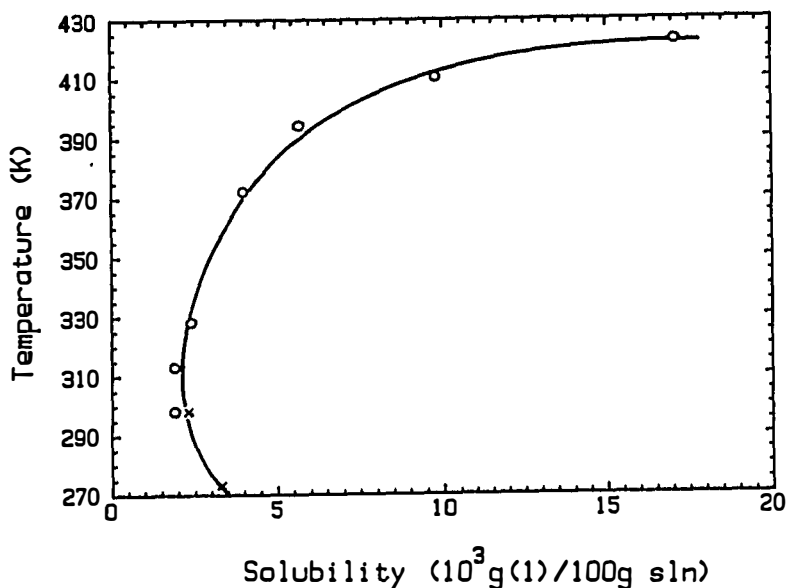
FIGURE 1. Solubility of 2,3-dimethylbutane in water: ref 2 (x); ref 3 (O).

COMPONENTS:	EVALUATOR:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (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. November 1984

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) IN 2,3-DIMETHYLBUTANE (1)

The reported solubility data for water in 2,3-dimethylbutane (ref 1, 2) are listed in Table 3. There are insufficient data to warrant plotting.

Agreement between the values at 273K is excellent but at 298K the datum of Englin *et al.* (ref 1) is about 50% (relative) higher than that of Polak and Lu (ref 2). In well characterized systems (e.g. water in benzene) the data of Englin *et al.* are generally satisfactory at $T < 300K$ but are markedly higher than "Recommended" values at higher temperatures. The value of Polak and Lu (ref 2) is therefore preferred at 298K and at higher temperatures the data of Englin *et al.* should be regarded only as order of magnitude values.

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

T/K	Solubility values		
	Reported values 10^3g(2)/100g sln	"Best" values 10^3g(2)/100g sln	$10^4 x_2$
273	2.9 (ref 1), 3.0 (ref 2)	3.0 (*R*)	1.43 (*R*)
283	5.8 (ref 1)	5.8	2.8
293	11.0 (ref 1)	11	5
298	15^a (ref 1), 9.0 (ref 2)	9	4
303	19.2 (ref 1)	20^b	10^b
313	32.3 (ref 1)	30^b	14^b
323	51.6 (ref 1)	50^b	24^b

[a] Graphically interpolated by the Evaluator; datum of Polak and Lu (ref 2) preferred, see text.

[b] Order-of-magnitude values only, see text.

REFERENCES

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

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

3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* **1976**, *60*, 213-44.

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (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: 0-50°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2,3-dimethylbutane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0029	1.4
10	0.0058	2.8
20	0.0110	5.26
30	0.0192	9.18
40	0.0323	15.4
50	0.0516	24.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* 1973, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2,3-dimethylbutane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	32.9^c	6.87×10^{-6}
25^b	22.5^c	4.70×10^{-6}

Solubility of water in 2,3-dimethylbutane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	30^d	1.43×10^{-4}
25^b	90^e	4.30×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION	

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

ESTIMATED ERROR:

temp. a) ± 0.02 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
      e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of 2,3-dimethylbutane in water at system pressure

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	19.1 ± 0.2	0.00191	3.99
40.1	19.2 ± 0.5	0.00192	4.01
55.1	23.7 ± 1.1	0.00237	4.95
99.1	40.1 ± 1.2	0.00401	8.38
121.3	56.8 ± 3.5	0.00568	11.87
137.3	97.9 ± 2.3	0.00979	20.46
149.5	171.0 ± 5.0	0.01710	35.75

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

	ESTIMATED ERROR: temp. ± 1 K soly. range of values given above
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylbutane; C_6H_{14}; [79-29-8] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3-dimetylbutane in water at 25°C was reported to be 19.10 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00191 g(1)/100 g sln and 3.99×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 0.48 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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. November 1984

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Connolly (ref 1)	573-628[a]	(1) in (2)	cloud-point
McAuliffe (ref 2)	298	(1) in (2)	GLC
Leinonen and Mackay (ref 3)	298	(1) in (2)	GLC
Polak and Lu (ref 4)	273,298	mutual	GLC, Karl Fischer
Price (ref 5)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 6)	298	(1) in (2)	GLC

[a] At elevated pressures, p = 14-70 MPa

The original data in all of these publications are compiled in the data sheets immediately following this Critical Evaluation.

Connolly (ref 1) has reported solubilities of (1) in (2) at elevated pressures (Table 1) and determined an upper critical solution temperature of 625K at 31 MPa. However, as no other data are available under comparable conditions, no critical evaluation of his results can be made. The interested user is referred to the relevant Data Sheets for experimental values. For convenience, further discussion of this system will be divided into two parts.

1.   SOLUBILITY OF 2-METHYLPENTANE (1) IN WATER (2)

The solubility data for 2-methylpentane in water are listed in Table 2 and plotted in Figure 1 with the exceptions noted below.

The datum of Krzyzanowska and Szeliga (ref 6) has been excluded because it does not appear to be independent of that of Price (ref 5). The data of Connolly (ref 1) have already been discussed above.

The datum of Polak and Lu (ref 4) at 298K is somewhat higher than those reported by others (ref 2, 3, 5). Also their value at 273K, as with other hydrocarbons investigated by these authors, shows an unusually large increase over the value at 298K. Their data are therefore rejected.

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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. November 1984

CRITICAL EVALUATION: (continued)

At temperatures other than 298K only the data of Price (ref 5) are available and thus must be considered "Tentative".

TABLE 2: Recommended (R) and Tentative
Values for the Solubility of 2-Methylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values[a] $10^3 g(1)/100g$ sln	"Best" values ($\pm \sigma_n$)[b] $10^3 g(1)/100g$ sln	$10^6 x_1$
298	1.38 (ref 2), 1.42 (ref 3), 1.30 (ref 5)	1.37 ± 0.05 (R)	2.87 (R)
303	1.3* (ref 5)	1.3	2.7
313	1.4* (ref 5)	1.4	2.9
323	1.5* (ref 5)	1.5	3.1
343	1.7* (ref 5)	1.7	3.6
363	2.3* (ref 5)	2.3	4.8
383	3.6* (ref 5)	3.6	7.5
403	6.8* (ref 5)	6.8	14
423	11.6* (ref 5)	12	25

[a] Values marked with an asterisk (*) obtained by graphical interpolation of original measurements by the Evaluators.

[b] "Best" values obtained by averaging where appropriate; σ_n has no statistical significance.

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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. November 1984

CRITICAL EVALUATION: (continued)

FIGURE 1.   Solubility of 2-methylpentane in water: ref 5 (o); average of ref 2, 3 and 5 (•).

2.   THE SOLUBILITY OF WATER (2) IN 2-METHYLPENTANE

The solubility of water in 2-methylpentane has been reported only by Polak and Lu (ref 4) and thus no Critical Evaluation can be made. However, it can be noted that the data of these authors are generally close to "Recommended" values in well characterized systems. The interested user is referred to the appropriate data sheet for solubility values.

COMPONENTS:	EVALUATOR:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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. November 1984

CRITICAL EVALUATION: (continued)

REFERENCES

1. Connolly, J.F. *J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

2. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

3. Leinonen, P.K.; Mackay, D. *Can. J. Chem. Eng.* <u>1973</u>, *51*, 230-3.

4. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

5. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

6. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *34*, 413-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Connolly, J.F. *J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

VARIABLES:	PREPARED BY:
Temperature: 300-355°C Pressure: 140-700 atm	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2-methylpentane in water

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
300	140	14.18	1.1	0.0023
	275	27.86	1.3	0.0027
	475	48.12	1.3	0.0027
	700	70.91	1.3	0.0027
330	160	16.21	1.8	0.0038
	185	18.74	2.7	0.0058
	215	21.78	3.9	0.0084
	245	24.82	4.0	0.0086
	300	30.39	4.2	0.0091
	410	41.53	4.1	0.0089
	500	50.65	3.7	0.0080
340	210	21.27	4.5	0.0097
	235	23.80	5.4	0.0118
	265	26.84	6.3	0.0138
	300	30.39	6.9	0.0152
	370	37.48	6.4	0.0140
	485	49.13	5.3	0.0116

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.	(1) Phillips reagent grade; better than 99.8%; used as received. (2) distilled and deaerated.
	ESTIMATED ERROR: temp. ± 0.02 K press. ± 2 atm (accuracy)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5]	Connolly, J.F.
(2) Water, H_2O; [7732-18-5]	*J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
350	230	23.30	7.1	0.0157
	240	24.31	8.2	0.0183
	260	26.34	10.4	0.0237
	275	27.86	11.6	0.0267
	290	29.38	12.5	0:0290
	310	31.40	12.8	0.0297
	335	33.94	12.5	0.0290
	365	36.97	11.6	0.0267
	405	41.03	10.5	0.0239
355	245	24.82	13.0	0.0303
	245	24.82	14.9	0.0353
	250	25.32	17.4	0.0421
	250	25.32	21.0	0.0526
	385	39.00	37.4	0.1109
	380	38.49	35.1	0.1015
	380	38.49	32.8	0.0925
	380	38.49	30.2	0.0829
	380	38.49	27.4	0.0731
	380	38.49	24.3	0.0628
	385	39.00	21.0	0.0526
	385	39.00	17.3	0.0419

COMMENTS AND ADDITIONAL DATA:

Upper critical solution temperature: 352°C at p = 310 atm.

The uncertainty in the CST is about 2°C and that of the corresponding pressure about 10 atm.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylpentane in water at 25°C was reported to
be 13.8 mg (1)/kg sln (0.00138 g(1)/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler,
is 2.88×10^{-6}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 0.9 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* <u>1973</u>, *51*, 230-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylpentane in water at 25°C was reported to be 14.2 mg(1)dm^{-3} sln.

With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.00142 g(1)/100 g sln and the corresponding mole fraction, x_1, is 3.0×10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was equilibrated for at least 12 hrs in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 hrs and the aqueous phase was tested (Tyndall effect). Both phases were analysed by the gas chromatographic technique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analysed by GLC. The instrument was a Hewlett-Packard model equipped with a flame ionization detector.	(1) Phillips Petroleum Co.; research grade; purity 99%+; used without further purification. (2) doubly distilled.
	ESTIMATED ERROR: temp. ± 0.1 K soly. ± 1 mg(1)dm^{-3} sln
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2-methylpentane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	19.45^c	4.06×10^{-6}
25^b	15.7^c	3.28×10^{-6}

Solubility of water in 2-methylpentane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	29^d	1.39×10^{-4}
25^b	90^e	4.31×10^{-4}

$a-e$ see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

	ESTIMATED ERROR:
	temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%; e) ± 3.1% (mean)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.
VARIABLES:	PREPARED BY:
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of 2-methylpentane in water at system pressure

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	13.0 ± 0.2	0.00130	2.72
40.1	13.8 ± 0.2	0.00138	2.88
55.7	15.7 ± 0.9	0.00157	3.28
99.1	27.1 ± 0.9	0.00271	5.67
118.0	44.9 ± 2.9	0.00449	9.39
137.3	86.8 ± 1.6	0.00868	18.15
149.5	113.0 ± 7.0	0.01130	23.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.
	ESTIMATED ERROR:
	temp. ± 1 K soly. range of values given above
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylpentane; C_6H_{14}; [107-83-5] (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 2-methylpentane in water at 25°C was reported to be 13.00 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.0013 g(1)/100 g sln and 2.72×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 0.4 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (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. November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 3-methylpentane (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the
3-Methylpentane (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
Price (ref 3)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 4)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 5)	298	(1) in (2)	partition coefficient

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 3-METHYLPENTANE (1) IN WATER (2)

Of the data reported for the solubility of 3-methylpentane in water (Table 1), the datum of Krzyzanowska and Szeliga (ref 4) has been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 3). The 298K datum of Polak and Lu (ref 2) is much higher (ca. 30% relative) than all other reported values (ref 1, 3, 5). Furthermore, the value at 273K, as with other hydrocarbons investigated by these authors, shows an unusually large increase over the value at 298K. Thus the data of Polak and Lu (ref 2) are rejected. All the remaining data (all at 298K) are listed in Table 2).

TABLE 2: Recommended (R) Value for the Solubility
of 3-Methylpentane (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	$10^5 x_1$
298	1.28 (ref 1), 1.31 (ref 3), 1.29 (ref 5)	1.29 ± 0.01 (R)	2.70 (R)

^{a}"Best" values obtained by averaging; σ_n has no statistical significance.

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COMPONENTS:	EVALUATOR:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (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. November 1984

CRITICAL EVALUATION: (continued)

2. THE SOLUBILITY OF WATER (2) in 3-METHYLPENTANE (1)

The solubility of water in 3-methylpentane has been reported only by Polak and Lu (ref 2) and thus no Critical Evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it can be noted that the data of Polak and Lu are generally close to "Recommended" values in well characterized systems.

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

2. Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

3. Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

4. Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *34*, 413-7.

5. Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES:	**PREPARED BY:**
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylpentane in water at 25°C was reported to
be 12.8 mg (1)/kg sln (0.00128 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler,
is 2.68×10^{-6}.
The same value is also reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 frac-tionator of the gas chromatograph. A hydrogen-flame ionization detector was used. Many details are given in the paper.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 0.6 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* **1973**, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 3-methylpentane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0^a	21.5^c	4.49×10^{-6}
25^b	17.9^c	3.74×10^{-6}

Solubility of water in 3-methylpentane

t/°C	mg(2)/kg sln	x_2 (compiler)
0^a	23^d	1.10×10^{-4}
25^b	94^e	4.50×10^{-4}

$a-e$ see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.
	ESTIMATED ERROR: temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%; e) ± 3.1% (mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylpentane in water at 25°C and at system pressure was reported to be 13.1 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.00131 g(1)/100 g sln and 2.74 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1 K soly. ± 0.4 mg(1)/kg(2)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylpentane in water at 25°C was reported to be 13.10 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated by compiler are 0.00131 g(1)/100 g sln and 2.74×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 0.4 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylpentane; C_6H_{14}; [96-14-0] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of 3-methylpentane between the gas and aqueous phase. $\alpha = 68 \pm 4$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 189.8$ mm of Hg and $\log C_g = \log p - 4.269 = -1.99$ expressed in moles per liter. Therefore $C_s = 1.50 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0013 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.7×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	soly. ± 10% (estimated by the compiler)
	REFERENCES:
	1. Hine, J.; Mooker, P.K. *J. Org. Chem.* <u>1975</u>, *4*, 292.

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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 system hexane (1) and water (2) have been reported in the publications listed in Table 1.

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

Reference	T/K	Solubility	Method
Herz (ref 1)	295	(1) in (2)	densimetric
Fühner (ref 3)	289	(1) in (2)	titration
Milligan (ref 4)	298	(1) in (2)	partition coefficient
Bennett and Philip (ref 5)	290	(1) in (2)	volumetric
Booth and Everson (ref 6)	298	(1) in (2)	residue volume
Gester (ref 7)	298-328	(2) in (1)	Karl Fischer
Black et al. (ref 8)	293	(2) in (1)	radiotracer
Durand (ref 9)	289	(1) in (2)	cloud point
McBain and Lissant (ref 10)	298	(1) in (2)	cloud point
McCants et al. (ref 11,12)	311	mutual	cloud point
Kudchadker and McKetta (ref 13)	311-411[a]	(1) in (2)	not specified
Englin et al. (ref 14)	293-313	(2) in (1)	analytical
Zel'venskii et al. (ref 15)	293	(2) in (1)	radiotracer
Barone et al. (ref 16)	298	(1) in (2)	GLC
McAuliffe (ref 17)	298	(1) in (2)	GLC
Burd and Braun (ref 18)	355-478[a]	(2) in (1)	GLC
Nelson and DeLigny (ref 19)	277-328	(1) in (2)	GLC
Roddy and Coleman (ref 20)	298	(2) in (1)	GLC
Benkovski et al. (ref 21)	303	(2) in (1)	Karl Fischer
Krasnoshchekova and Gubergrits (ref 22)	298	(1) in (2)	GLC
Skripka et al. (ref 23, 28, 30)	473,493[a]	(2) in (1)	vap.liq. equilibrium
Leinonen and MacKay (ref 24)	298	(1) in (2)	GLC
Polak and Lu (ref 25)	273,298	(1) in (2)	GLC
Mackay et al. (ref 26)	unspecified	(1) in (2)	GLC
Budantseva et al. (ref 27)	293	mutual	GLC
Price (ref 29)	298-425	(1) in (2)	GLC

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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 1 (continued)

Reference	T/K	Solubility	Method
Korenman and Aref'eva (ref 31,34)	293,298	(1) in (2)	titration
Sugi and Katayama (ref 32)	298	(2) in (1)	Karl Fischer
Charykov et al. (ref 33)	293	(2) in (1)	Karl Fischer
Krzyzanowska and Szeliga (ref 35)	298	(1) in (2)	GLC
Aquan-Yuen et al. (ref 36)	298	(1) in (2)	GLC
Jonsson et al. (ref 38)	288-308	(1) in (2)	GLC
De Loos et al. (ref 39)	610-675[a]	mutual	synthetic
Tsonopoulos and Wilson (ref 40)	313-422[a]	mutual	GLC, Karl Fischer
Rebert and Hayworth (ref 41)	493-645[a]	(1) in (2)	synthetic

[a] Also studied at variable pressure, see Table 4.

Apart from the following exceptions, original data in all the references listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation. The work of Herz (ref 1) and Milligan (ref 4) have not been compiled because they employed petroleum fractions of unspecified composition rather than pure hexane. The work of Scheffer and Roof (ref 2,42; critical point data only), Bennett and Philip (ref 5; order of magnitude solubility only) and Gester (ref 7; graphical data only) did not contain sufficient information to justify compilation. Solubility data for hexane in water may also be obtained from the calorimetric data of Gill et al. (ref 37).

Despite the relatively large number of studies of the hexane-water system (Table 1) little information is available on the temperature dependence of the mutual solubilities of hexane and water. Even when comparable data are available, independently obtained values often differ by an order of magnitude. This system warrants thorough re-investigation at all temperatures.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation of the original measurements contained in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. Uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of reported values rather than as error limits.

For convenience, further discussion of this system will be divided into three parts.

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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)

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

The various data reported for the solubility of hexane in water are in poor agreement.

The value of Mackay *et al.* (ref 26) is rejected because the temperature was not specified. The data of Krzyzanowska and Szeliga (ref 35) have been excluded from consideration as they do not appear to be independent of those of Price (ref 29).

Of the remaining data, the results of Fühner (ref 3), Booth and Everson (ref 6, order of magnitude), Durand (ref 9), McBain and Lissant (ref 10), Kudchadker and McKetta (ref 13, atmospheric pressure data only), McCants *et al.* (ref 11,12) Barone *et al.* (ref 16), Nelson and De Ligny (ref 19) and Korenman and Aref'eva (ref 31,34) are markedly higher, sometimes by an order of magnitude, than other results and are therefore rejected. All other data are included in Table 2 on the next page.

At 298K, the temperature where there is a reasonable number of independent determinations (Table 2), the various values are in reasonable agreement although the uncertainty on the average result means that it can be considered as "Tentative" only. This is almost certainly a reflection of the difficulties of accurate analysis of the very low concentrations involved even when using modern techniques (it is interesting to note that all the data at 298K were obtained by GLC methods).

At other temperatures, the results of Price (ref 29) and Tsonopoulos and Wilson (ref 40) are in quite good agreement up to 353K but begin to diverge at higher temperatures (Table 2 and Figure 1). Application of the van't Hoff equation to a combination of both data sets (ref 29,40) yields values for $\Delta H^\infty_{sln} = 1.87$ kJ mol^{-1}, $\Delta C^\infty_{p,sln} = 296$ JK^{-1} mol^{-1} which are in relatively poor agreement with the calorimetric values of $\Delta H^\infty_{sln} = 0.0 \pm 0.2$ kJ mol^{-1} and $\Delta C^\infty_{p,sln} = 440 \pm 45$ JK^{-1} mol^{-1} reported by Gill *et al.* (ref 37). In view of the disparities at higher temperatures, the uncertainty in the 298K value, and the poor agreement with calorimetric data, none of averaged "Best" values have been Recommended.

Figure 1 plots a selection of the solubility data of hexane in water. As well as the values of Price (ref 29) and Tsonopoulos and Wilson (ref 40), referred to above, the rejected data of Nelson and De Ligny (ref 19) have also been included for comparison.

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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: Tentative Values of the Solubility of Hexane (1) in Water (2)

T/K	Reported values 10^3g(1)/100g sln	"Best" values ($\pm \sigma_n$)[a] 10^3g(1)/100g sln	$10^6 x_1$
273	1.65 (ref 25)	1.7	3.5
293	1.4 (ref 27), 1.03 (ref 38)	1.2 ± 0.2	2.5
298	0.95 (ref 17), 1.3 (ref 22), 1.2 (ref 24), 1.24 (ref 25) 0.95 (ref 29), 1.23 (ref 36) 1.01 (ref 38)	1.1 ± 0.1	2.3
303	0.97* (ref 29), 1.00 (ref 38)	0.99 ± 0.02	2.1
313	1.04* (ref 29), 1.15[b] (ref 40)	1.10 ± 0.06	2.3
323	1.17* (ref 29), 1.23[b] (ref 40)	1.20 ± 0.03	2.5
333	1.34* (ref 29), 1.38[b] (ref 40)	1.36 ± 0.02	2.8
343	1.54* (ref 29), 1.60[b] (ref 40)	1.57 ± 0.03	3.3
353	1.77* (ref 29), 1.93[b] (ref 40)	1.85 ± 0.08	3.9
373	2.28* (ref 29), 3.06[b] (ref 40)	2.7 ± 0.4	5.6
393	3.60* (ref 29), 5.36[b] (ref 40)	4.5 ± 0.9	9.4
413	6.5* (ref 29), 10.1[b] (ref 40)	8 ± 2	16

a No "Best" values Recommended because of uncertainties in data, see text.

b Calculated from the original authors' fitting equation over the range of their experimental data.
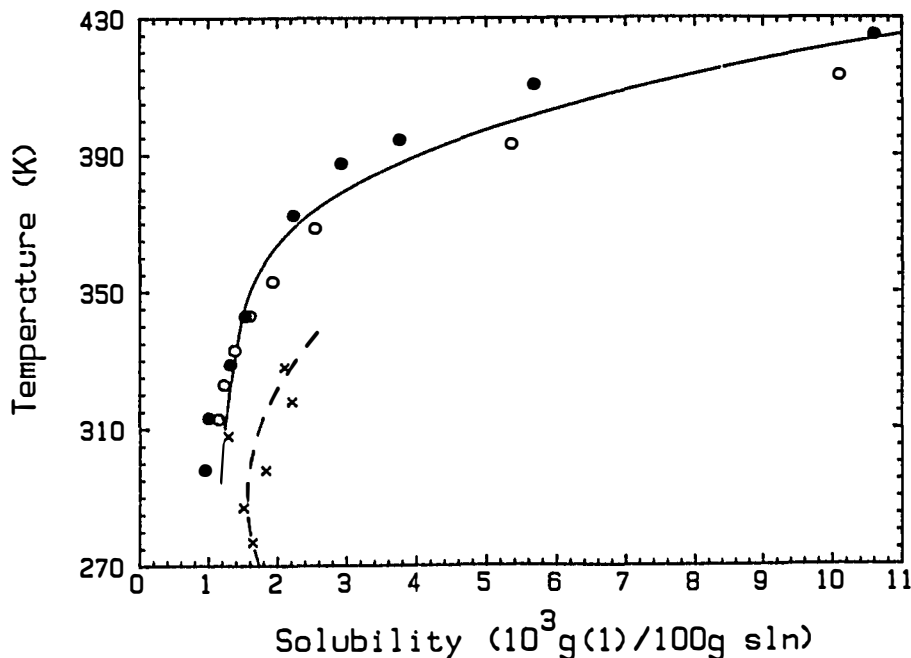
FIGURE 1. Solubility of hexane in water, selected data: ref 19 (x, rejected data); ref 29 (●); ref 40 (o).

(continued next page)

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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)

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

Solubility data for water in hexane are listed in Table 3, apart from the values of McCants *et al.* (ref 11,12), which are an order of magnitude higher than all other studies and have therefore been rejected.

In general, agreement amongst independently obtained values is poor (Table 3). This is probably a reflection of the difficulties of accurate analysis at these low concentrations. No data have been Recommended.

   TABLE 3:   Tentative Values of the Solubility of Water (2) in Hexane (1)

T/K	Solubility values		
	Reported values $10^2g(1)/100g$ sln	"Best" values ($\pm \sigma_n$) $10^2g(1)/100g$ sln	$10^4 x_2$
273	1.01 (ref 14), 0.28 (ref 25)	0.6 ± 0.4	2.9
293	1.11 (ref 8), 1.66 (ref 15) 0.77 (ref 27), 0.836 (ref 33)	1.1 ± 0.4	5.3
298	0.995 (ref 20), 0.90 (ref 25), 1.07 (ref 32)	0.98 ± 0.07	4.7
303	1.79 (ref 14), 0.51 (ref 21)	1.1 ± 0.6	5.3
313	3.17 (ref 14), 2.51[a] (ref 40)	2.8 ± 0.3	13
323	2.65[a] (ref 40)	2.7	13
333	3.88[a] (ref 40)	3.9	19
343	5.60[a] (ref 40)	5.6	27
353	7.95[a] (ref 40)	8.0	38

a Calculated from the original authors' fitting equation over the range of their experimental values.

Figure 2 plots all the available data for the solubility of water in hexane. The smooth curve which has been fitted to the "Best" values (Table 3) has the form s ($10^2g(1)/100g$ sln) = 86.5345 - 0.6183 T + 0.00113 T^2 with R^2 = 0.977 and σ = 0.446, 293 ≤ T ≤ 353 K.

Application of the van't Hoff equation to the "Best" values gives ΔH^∞_{sln} = 28.7 kJ mol^{-1} and $\Delta C^\infty_{p,sln}$ = 73 JK^{-1} mol^{-1} for the dissolution of water in hexane. These values are broadly similar to those reported for other hydrocarbons and suggests, despite the lack of agreement amongst the individual studies in Table 3, that the Tentative "Best" values are reasonably reliable.

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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)
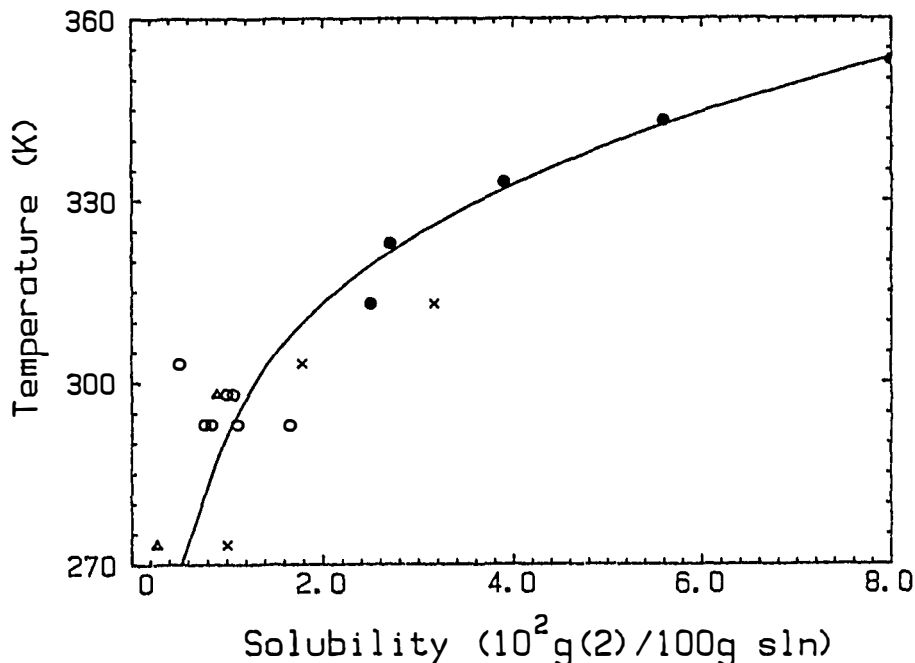
FIGURE 2. Solubility of water in hexane: ref 14 (x); ref 25 (Δ); ref 40 (●); other data (O). Line of best fit calculated for averaged "Best" values, see text.

3. MUTUAL SOLUBILITIES OF HEXANE (1) AND WATER (2) AT ELEVATED PRESSURES

This system exhibits the phenomenon of gas-gas immiscibility of the second kind and has type III phase behaviour (ref 43,44). In order to clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram. A schematic representation of this projection for water + hexane is given in Figure 3. There are two critical lines, one starting at the critical point of hexane and ending on a three phase line. It should be noted that the three phase line on a pressure-temperature projection corresponds to three lines on the pressure-temperature-composition diagram, representing the composition of gas, liquid 1 and liquid 2 in equilibrium. The second critical line starts at the critical point of water, moves to lower temperatures at high pressures, passes through a minimum in temperature and eventually goes to temperatures greater than that of the critical point of water (this behaviour is referred to as gas-gas immiscibility of the second kind).

In the region above the three phase line on the p, T projection there is no vapor phase but may be a maximum of two liquid phases. Whether there is (are) one or two liquid phases depends on the overall composition. To the

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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)

FIGURE 3: Pressure-temperature projection of the equilibrium-pressure-temperature-composition surface for the hexane-water system.

left of the critical line starting at the critical point of water it may be possible to have one or two phases present depending on the overall composition.

Solubility studies of the hexane-water system at pressures higher than atmospheric are listed in Table 4.

TABLE 4: Solubility Studies of the Hexane-Water System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Scheffer (ref 2)	5.274^b	495.2^b	$-^b$
Kudchadker and McKetta (ref 13)	0.2 - 3.6	311-411	(1) in (2)
Burd and Braun (ref 18)	0.2 - 3.2	355-478	(2) in (1)
Skripka et al. (ref 23,28,30)	2 - 79	473,493	(2) in (1)
Price (ref 29)	$-^a$	298-425	(1) in (2)
De Loos et al. (ref 39)	15 - 140	610-675	mutual
Tsonopoulos and Wilson (ref 40)	$-^a$	313-473	mutual
Rebert and Hayworth (ref 41)	4.6 - 22.2	493-645	(1) in (2)
Roof (ref 42)	5.295^b	495.2^b	$-^b$

a Along 3-phase equilibrium line.
b Critical point.

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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)

As can be seen from Table 4, virtually none of the solubility data at elevated pressures have been obtained under comparable conditions, thus precluding evaluation of their reliability. However, it should be noted that the atmospheric pressure data of Kudchadker and McKetta (ref 13) disagree markedly from other studies. Also, the interpolated values of Burd and Braun (ref 18) and Skripka *et al*. (ref 28) at ~ 473K and ~ 3.2 MPa are in poor agreement (~ 3.2 and ~ 1.8 g(2)/100g sln respectively).

Roof and Scheffer have measured the temperature and pressure at the critical end point. Their values are in reasonable agreement (Table 4).

De Loos *et al*. (ref 39) have studied the two phase-one phase boundaries near but to the left of the critical line starting at the critical point of water (refer to Figure 3). Although the absence of confirmatory studies precludes Critical Evaluation the results are consistent with the phase behaviour of other alkane + water systems.

The interested user is referred to the original measurements in the data sheets for further information, bearing in mind that all values should be regarded as very tentative.

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COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (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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ACKNOWLEDGEMENTS

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3]	Führer, H.
(2) Water; H_2O; [7732-18-5]	*Ber. Dtsch. Chem. Ges.* <u>1924</u>, 57, 510-5.

VARIABLES:	PREPARED BY:
One temperature: 15.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 15.5°C was reported to be 0.022 mL(1)/100 mL sln or 0.014 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compiler is 2.92×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; commercial grade; used as received. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.
VARIABLES:	PREPARED BY:
One temperature: 20°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 20°C and at a total
saturation pressure of 1 atm was reported to be 0.0111 g(2)/100 g(1).
The corresponding mass percent and mole fraction, x_2, calculated
by the compiler are 0.0111 g(2)/100 g sln and 5.3×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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:
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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; 110-54-3 (2) Water; H_2O; 7732-18-5]	Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* <u>1948</u>, *40*, 1491-3.

VARIABLES:	PREPARED BY:
One temperature: 25.0°C (298.2 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *n*-hexane in water at 25.0°C was reported to be <0.04 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:	SOURCE AND PURITY OF MATERIALS:
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 0.02 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.	1. "Highest grade commercial sample available"; no other details given. 2. Distilled.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Durand, R. *C.R. Hebd. Seances Acad. Sci.* <u>1948</u>, *226*, 409-10.
VARIABLES:	PREPARED BY:
One temperature: 16°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 16°C was reported to be
0.055 cm^3(1)/dm^3(2).

With the assumption of a solution density of 1.00 g cm^{-3} and a
density value of 0.6629 g cm^{-3} for hexane at 16°C (ref 2), the
corresponding mass percent is 0.0036 g(1)/100 g sln and the
corresponding mole fraction, x_1, is 7.5 x 10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The thermostatic method described in ref 1 was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.	(1) not specified. (2) distilled.
	ESTIMATED ERROR: soly. ± 0.005 cm^3(1)/dm^3(2).
	REFERENCES: 1. Durand, R. *C.R. Hebd. Seances Acad. Sci.* <u>1946</u>, *223*, 898-900. 2. Timmermans, J.; *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	McBain, J.W.; Lissant, K.J. *J. Phys. Colloid. Chem.* 1951, *55*, 655-62.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be
0.012 g(1)/100 mL sln.
With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.012 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.5 x 10^{-5} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) was pipetted into glass vials, following which, varying amounts of (1) were added to each bottle by direct weighing. The vials were shaken overnight. When two vials had been obtained, one clear and one with excess hydrocarbon and containing amounts differing by less than 1 mg, the two values were averaged and the mean taken as the amount solubilized.	(1) C.P. grade. (2) distilled and boiled to remove CO_2.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	McCants, J.F.; Jones, J.H.; Hopson, W.H. *Ind. Eng. Chem.* <u>1953</u>, *45*, 454-6.
VARIABLES:	PREPARED BY:
One temperature: 100°F (311 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *n*-hexane in water at 100°F (311 K) was reported to be <0.1 g(1)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is $< 2 \times 10^{-4}$.

The solubility of water in *n*-hexane at 100°F (311 K) was reported to be <0.1 g(2)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is $< 5 \times 10^{-3}$.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was essentially that of ref. 1 and involved titration of the second component to the cloud point, in a constant temperature bath.	1. Phillips; pure grade; used without further purification; n_D^{20} 1.3752. 2. Distilled.
	ESTIMATED ERROR:
	Not specified.
	REFERENCES:
	1. Washburn, E.R.; Hnizda, V.; Vold, R.D. *J. Am. Chem. Soc.* <u>1931</u>, *53*, 3232.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Jones, J.H.; McCants, J.F. *Ind. Eng. Chem.* <u>1954</u>, *46*, 1956-8.
VARIABLES:	PREPARED BY:
One temperature: 100°F	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 100°F (37.78°C) was reported to be 0.4 g(1)/100 g sln. The corresponding mole fraction, x_1, calculated by the compiler is 8.3×10^{-4}.

The solubility of water in hexane at 100°F (37.78°C) was reported to be 0.2 g(1)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler is 9.5×10^{-3}.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (2) in (1) was obtained by titrating (1), brought to 100°F. As the cloud point was approached, (2) was added dropwise and the flask agitated in the 100°F constant temperature bath. The solubility of (1) in (2) was determined by titrating (2) at 100°F with (1).	(1) Phillips; used as received; $n_D^{20} = 1.3745$ $d_4^{20} = 0.6607$ (2) distilled; $n_D^{20} = 1.3330$
	ESTIMATED ERROR:
	temp. ± 0.2°F
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Kudchadker, A.P.; McKetta, J.J. *Petrol. Refiner.* <u>1961</u>, *40*, 231-2.

VARIABLES:	PREPARED BY:
Temperature: 100-280°F Pressure: 24-525 psia	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of hexane in water

t/°F	T/ K (compiler)	p/psia	p/MPa (compiler)	$10^4 x_1$	g(1)/100 g sln (compiler)
100	310.94	24.8	0.171	0.2214	0.01060
		41.2	0.284	0.302	0.01446
		74.9	0.516	0.319	0.01527
		101.1	0.697	0.342	0.01637
		133.8	0.923	0.339	0.01623
		220.2	1.518	0.342	0.01637
		308.5	2.127	0.3398	0.01627
		422.5	2.913	0.3396	0.01626
		513.0	3.537	0.342	0.01637
160	344.27	45.2	0.312	0.398	0.01905
		75.3	0.519	0.541	0.02590
		112.6	0.776	0.644	0.03083
		172.2	1.187	0.6349	0.03039
		252.0	1.737	0.633	0.03030
		338.6	2.335	0.64	0.03063
		432.2	2.980	0.648	0.03102
		488.1	3.365	0.64	0.03063

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Apparatus for producing equilibrium conditions and analytical procedure are the same as described in ref 1. No more details are given in the paper.	(1) Phillips Petroleum Co.; certified purity of at least 99.0 mole percent; used as received. (2) distilled; boiled to remove any dissolved gases.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Davis, J.E. M.S. Thesis, The University of Texas, Austin, <u>1959</u>.

(1) Hexane; C_6H_{14}; [110-54-3]

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

Solubility of hexane in water

$t/°F$	T/K (compiler)	p/psia	p/MPa (compiler)	$10^4 x_1$	g(1)/100 g sln (compiler)
220	377.60	80.3	0.554	0.394	0.01886
		116.6	0.804	0.608	0.02910
		174.8	1.205	0.87	0.04164
		233.3	1.609	1.08	0.05169
		282.5	1.948	1.092	0.05226
		355.1	2.448	1.112	0.05322
		444.4	3.064	1.09	0.05217
		524.8	3.618	1.11	0.05312
280	410.94	98.2	0.677	0.272	0.01302
		137.5	0.948	0.475	0.02274
		205.0	1.413	0.826	0.03953
		268.8	1.853	1.155	0.05527
		353.9	2.440	1.478	0.07072
		392.2	2.704	1.588	0.07598
		435.0	2.999	1.685	0.08062
		506.5	3.492	1.772	0.08478

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane, C_6H_{14}; [110-54-3] (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: Temperature: 20-40°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in hexane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
20	0.0101	4.83
30	0.0179	8.56
40	0.0317	15.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) Hexane; C_6H_{14}; [110-54-3]
 	
(2) Water, H_2O; [7732-18-5]
	Zel'venskii, Ya.D; Efremov, A.A.;
	  Larin, G.M.
	
	Khim. Tekhnol. Topl. Masel <u>1965</u>,
	  10, 3-7.

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in hexane at 20°C was reported to be
0.0166 g(2)/100 g sln.
The corresponding mole fraction, x_2, calculated by the compiler
is 7.9×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.	(1) source not specified; pure grade; shaken with conc. H_2SO_4; washed with water, dried over sodium, and distilled; purity not specified. b.p. 68.81°C, m.p. -95.5°C. (2) source not specified; commercial; 1 Ci/mL HTO used as received.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Barone, G.; Crescenzi, V.; Pispisa, B.; Quadrifoglio, F. *J. Macromol. Chem.* <u>1966</u>, *1*, 761-71.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors report a value of 9.6×10^{-4} mol(1)/dm^3(2) for the solubility of hexane in water at 25°C. This value is the experimental one multiplied by $760/p$ where p is the partial pressure of (1) over (2). $p = 149$ mm Hg. The solubility at system pressure calculated by the compiler is 1.882×10^{-4} mol(1)/dm^3(2) and the corresponding mass percent and mole fraction, x_1, are 0.001621 g(1)/100 g sln and 3.385×10^{-6}.

The compiler's calculation assumes a solution density of 0.6629 g/mL (the density of hexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation was carried out by bubbling the vaporized (1) into the solution and letting an excess of the condensed (1) stand in contact with the aqueous phase for more than 12 hr at 25°C under gentle shaking. 0.20 mL samples of (2) saturated with (1) were taken with a calibrated syringe and injected into the chromatographic column packed with 15% of poly(propylene glycol) on chromosorb. A gas chromatography unit having a tungsten-wire katharometer as detector was employed. More details are given in the paper.	(1) RP product, C. Erba, Milan; chromatographically pure. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.02 K soly. ± 4% (type of error not specified).
	REFERENCES: 1. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 9.5 mg (1)/kg sln (0.00095 g(1)/100 g sln). The corresponding mole fraction, x_1, calculated by the compiler, is 1.99×10^{-6}. The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.3 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Burd, S.D.; Braun, W.G. *Proc. Div. Refining, Am. Petrol. Inst.* <u>1968</u>, *48*, 464-76.

VARIABLES:	PREPARED BY:
Temperature and pressure	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Hydrocarbon-rich liquid phase composition for the three-phase conditions.

p/psia	p/MPa (compiler)	t/°F	T/K (compiler)	g(2)/100 g sln	x_2 (compiler)
30	0.207	179	354.82	0.14	0.0067
60	0.414	223	379.26	0.32	0.0151
100	0.689	261	400.37	0.58	0.0272
150	1.034	292	417.59	0.91	0.0421
200	1.379	317	431.48	1.26	0.0575
250	1.724	337	442.59	1.62	0.0730
300	2.068	355	452.59	2.03	0.0902
350	2.413	369	460.37	2.35	0.1032
400	2.758	383	468.15	2.78	0.1294
42	0.290	200	366.48	0.21	0.0100
87	0.600	250	394.26	0.49	0.0230
165	1.138	300	422.04	1.03	0.0474
286	1.972	350	449.82	1.89	0.0844
470	3.241	400	477.59	3.30	0.1403

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The vapor and liquid phase composi-tions have been determined for the (1)-(2) system in the two-phase hydrocarbon-rich liquid region. Equilibrium points were obtained by incremental addition of water followed by stirring, settling, sampling and chromatographic analy-sis. This procedure was continued until addition of water resulted in no pressure increase, indicating three-phase conditions. Many de-tails are given in the paper.	(1) Phillips Petroleum Company; 99.5% purity. (2) laboratory distilled.

	ESTIMATED ERROR:
	soly. ± 0.004 weight fraction of the (2) present.

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3] 2. Water; H_2O; [7732-18-5]	Rebert, C. J.; Hayworth, K. E.; *Am. Inst. Chem. Engnrs. J.* 1967, *13*, 118-121.
VARIABLES: Pressure and temperature along one phase-two phase boundary.	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

Smoothed data

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{14}}$
603	330	12.90	1870	2.0	0.0042
613	340	14.67	2127		
623	350	16.65	2414		
633	360	18.83	2731		
643	370	21.46	3112		
644	371	21.77	3157		
645.0[a]	371.8	22.23	3223		
644	371	22.17	3214		
643	370	22.02	3193		
633	360	20.27	2939		
623	350	18.72	2715		
613	340	17.43	2527		
608	335	16.96	2459		
605	332	16.78	2433		
603	330	16.70	2422		
601	328	16.67	2417		
599	326	16.69	2420		
597	324	16.76	2430		
595	322	16.90	2450		
591	318	17.71	2568		
588	315	19.24	2790		
573	300	8.92	1294	15.4	0.0367
583	310	10.48	1520		
593	320	12.19	1768		

(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Samples of mixtures of known composition confined over mercury. Samples heated in a vapor bath and the pressure-temperature phase boundaries determined by direct observation of appearance or disappearance of a phase. Apparatus similar to that described in ref. (1).	1. No details given.
	ESTIMATED ERROR: $\delta T/K = \pm 0.05$; $\delta p/psi = \pm 1$.
	REFERENCES: 1. Rebert, C. J.; Kay, W. B. *Am. Inst. Chem. Engnrs. J.* 1959, *5*, 285.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3]	Rebert, C. J.; Hayworth, K. E.
2. Water; H_2O; [7732-18-5]	*Am. Inst. Chem. Engnrs. J.*
	<u>1967</u>, *13*, 118-121.

EXPERIMENTAL VALUES:

<u>Smoothed data</u>

T/K	T/°C	P/MPa	p/psi	g (1)/100 g (soln.)	$x_{C_6H_{14}}$
598	325	13.13	1904	15.4	0.0367
603	330	14.11	2046		
608	335	14.88	2158		
613	340	16.13	2339		
618	345	17.23	2498		
623	350	18.41	2670		
628	355	19.74	2862		
633	360	21.31	3090		
543	270	7.08	1026	50.57	0.1762
548	275	7.62	1105		
553	280	8.25	1196		
558	285	8.94	1297		
563	290	9.71	1408		
568	295	10.55	1530		
573	300	11.45	1660		
578	305	12.40	1798		
583	310	13.42	1946		
588	315	14.62	2120		
593	320	16.03	2324		
598	325	17.63	2556		
603	330	19.53	2832		
608	335	21.63	3136		
493	220	4.63	672	85.34	0.5489
498	225	5.06	734		
503	230	5.52	800		
508	235	6.01	871		
513	240	6.53	947		
518	245	6.97	1011		
523	250	7.74	1123		
528	255	8.49	1231		
533	260	9.31	1350		
538	265	10.23	1484		
543	270	11.34	1645		
548	275	12.92	1873		
553	280	14.88	2158		
558	285	17.39	2522		

[a] Critical point.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-8] (2) Water; H_2O; [7732-18-5]	Nelson, H.D.; De Ligny, C.L. *Rec. Trav. Chim. Pays-Bas* <u>1968</u>, *87*, 528-44.
VARIABLES:	PREPARED BY:
Temperature: 4-55°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of hexane in water

$t/°C$	$10^6 x_1$	mg(1)/kg sln (compiler)
4.0	3.42 ± 0.34	16.4
14.0	3.17 ± 0.52	15.2
25.0	3.83 ± 0.47	18.3
35.0	2.69 ± 0.26	12.9
45.0	4.64 ± 0.72	22.2
55.0	4.42 ± 0.26	21.2

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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 (90% probability interval)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Roddy, J.W.; Coleman, C.F. *Talanta* <u>1968</u>, *15*, 1281-6.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 25°C was reported to be 0.00362 mol(2) dm^{-3} sln corresponding to a mole fraction, x_2, of 4.76 x 10^{-4}. The corresponding mass percent value calculated by the compiler is 0.00995 g(2)/100 g sln.

The compiler's calculation assumes a solution density of 0.6629 g/mL (the density of hexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A method of gravimetric absorption monitored by tritium tracer was used. (1) was equilibrated with a slight excess of tritiated water by shaking over a period of at least 8 hr in a thermostat. The phases were allowed to separate for at least 16 hr and then were sampled for tritium analysis. Most of the (1) phase was weighed into a boiling flask of a closed distillation system and then distilled through a magnesium perchlorate weighing tube. The magnesium perchlorate was then dissolved for measurement of its tritium content by liquid scintillation counting with a Packard Tri-Carb Scintillation Spectrometer.	(1) Phillips Petroleum Co.; 99%; purified by shaking with concentrated sulphuric acid, washed with water and dried with sodium sulphate. (2) tritiated water at 5 Ci/mL; New England Nuclear Corp.; diluted to about 1 mCi/mL.

ESTIMATED ERROR:

soly. better than 1% (type of error not specified)

REFERENCES:

1. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) Hexane; C_6H_{14}; [110-54-3]
 	
(2) Water; H_2O; [7732-18-5]
	Benkovski, V.G.; Nauruzov, M.H.;
	  Bogoslovaskaya, T.M.
	
	Tr. Inst. Khim. Nefti Prir. Solei
	  Akad. Nauk Kaz. SSR <u>1970</u>, *2*,
	  25-32.

VARIABLES:	PREPARED BY:
One temperature: 303 K	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in hexane at 303 K was reported to be

0.0051 g(2)/100 g sln.

The corresponding mole fraction, x_2, value calculated by compiler

is 0.00024.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; purified; purity not specified. (2) distilled.
	ESTIMATED ERROR: Not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* <u>1973</u>, *13*, 885-7.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be $x_1 = 2.8 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 1.3×10^{-3} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; CP reagent; purity not specified. (2) distilled.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Leinonen, P.J.; Mackay, D. *Can. J. Chem. Eng.* <u>1973</u>, *51*, 230-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be
12.3 mg(1)dm^{-3} sln corresponding to a mole fraction, x_1, of
2.5 x 10^{-6}.

The corresponding mass percent calculated by the compiler is
0.00123 g(1)/100 g sln.

The compiler's calculation assumes a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was equi-librated for at least 12 hrs in a 200 mL Teflon stoppered vessel with gentle shaking. The solution was allowed to settle for 6 hrs and the aqueous phase was tested (Tyndall effect). Both phases were analysed by the gas chromatographic tech-nique of internal standardization. The (1) in the aqueous phase was extracted into 5 mL of heptane and the extract analysed by GLC. The instrument was a Hewlett-Packard model equipped with a flame ioniza-tion detector.	(1) Phillips Petroleum Co.; research grade; purity 99%+; used without further purification. (2) doubly distilled.

ESTIMATED ERROR:
temp. ± 0.1 K soly. ± 1 mg(1)dm^{-3} sln

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* __1973__, *51*, 4018-23.
VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of hexane in water

t/°C	mg(1)/kg sln	x_1 (compiler)
0[a]	16.5[c]	3.44×10^{-6}
25[b]	12.4[c]	2.59×10^{-6}

Solubility of water in hexane

t/°C	mg(2)/kg sln	x_2 (compiler)
0[a]	28[d]	1.34×10^{-4}
25[b]	90[e]	4.30×10^{-4}

[a-e] see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.
	ESTIMATED ERROR:
	temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%; e) ± 3.1% (mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	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 the value of 16.2 mg(1)dm^{-3} sln for the
solubility of hexane in water. With the assumption of a solution
density of 1.00 g cm^{-3}, the corresponding mass percent, calculated
by the compiler, is 0.00162 g(1)/100 g sln and the corresponding
mole fraction, x_1, is 3.4 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 10% (compiler)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemstov, M.S. *Zh. Fiz. Khim.* <u>1976</u>, *50*, 1344. *Deposited doc.* <u>1976</u>, VINITI 438-76.
VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of hexane in water at 20°C was reported to be $x_1 = 3 \times 10^{-6}$.

The corresponding mass percent calculated by the compiler is 0.0014 g(1)/100 g sln.

The solubility of water in hexane at 20°C was reported to be $x_2 = 3.7 \times 10^{-4}$.

The corresponding mass percent calculated by the compiler is 0.0077 g(2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by glc. The solubility of (2) in (1) was determined by Karl Fischer reagent method.	(1) source not specified; pure or analytical reagent grade; purity <99.9%. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Namiot, A.Yu.; Skripka, V.G.; Lotter, Yu.G. *Zh. Fiz. Khim.* 1976, *50*, 2718 Deposited doc. 1976, VINITI 1213-76.

VARIABLES:	PREPARED BY:
Temperature: 200 and 220°C Pressure: 2.0-5.2 MPa	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in hexane

$t/°C$	$p/kg\ cm^{-2}$	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
200	20	2.0	0.006	0.13
200	25	2.5	0.024	0.51
200	30	2.9	0.051	1.11
200	35	3.4	0.084	1.92
200	37	3.6	0.097	2.2
220	25	2.5	0.002	0.04
220	30	2.9	0.023	0.49
220	35	3.4	0.053	1.16
220	40	3.9	0.088	1.98
220	45	4.4	0.129	3.00
220	50	4.9	0.179	4.36
220	53.3	5.2	0.216	5.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The static method for vapor-liquid equilibrium described in ref 1 was used. No more details were reported in the paper.	(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:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	PREPARED BY:
Temperature: 25-151.8°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of hexane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	9.47 ± 0.20	0.000947	1.98
40.1	10.1 ± 0.3	0.00101	2.11
55.7	13.2 ± 0.5	0.00132	2.76
69.7	15.4 ± 1.9	0.00154	3.22
69.7	15.2 ± 0.5	0.00152	3.18
99.1	22.4 ± 1.0	0.00224	4.68
114.4	29.2 ± 1.0	0.00292	6.10
121.3	37.6 ± 1.2	0.00376	7.86
137.3	56.9 ± 2.3	0.00569	11.89
151.8	106.0 ± 4.0	0.0106	22.2

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1 K soly. range of values given above
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (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.E. *Zh. Fiz. Khim.* 1973, *47*, 1035. Deposited doc. 1976, VINITI 5347-72

VARIABLES:	PREPARED BY:
Temperature: 200 and 220°C Pressure: 3.6-78.5 MPa	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of water in hexane

$t/°C$	$p/\text{kg cm}^{-2}$	p/MPa (compiler)	x_2	g(2)/100 g sln (compiler)
200	37	3.6	0.097	2.20
	50	4.9	0.094	2.12
	100	9.8	0.084	1.88
	200	19.6	0.072	1.60
	300	29.4	0.065	1.43
	400	39.2	0.060	1.32
	500	49.0	0.055	1.20
	600	58.8	0.051	1.11
	700	68.6	0.047	1.02
	800	78.5	0.041	0.89
220	50.8	5.0	0.187	4.59
	80	8.3	0.145	3.42
	100	9.8	0.134	3.13
	200	19.6	0.113	2.59
	300	29.4	0.102	2.32
	400	39.2	0.092	2.07
	500	49.0	0.083	1.86
	600	58.8	0.074	1.64
	700	68.6	0.068	1.50
	800	78.5	0.065	1.43

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The experimental technique was described in ref 1. No details reported in the paper.	(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.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water, H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. *87*:87654

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of hexane in water at 20°C was reported to be
0.14 g(1)dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.014 g(1)/100 g sln and 2.9×10^{-5}.

The compiler's calculation assumes a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Sugi, H.; Katayama, T. *J. Chem. Eng. Jap.* <u>1977</u>, *10*, 400-2.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 25°C was reported to be in mole fraction, $x_2 = 5.1 \times 10^{-4}$. The corresponding mass percent calculated by the compiler is 0.01066 g (2)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The Karl Fischer method was used. The experimental apparatus and procedures are given in ref 1.	(1) Merck Uvasol spectrograde chemical; used without further purification. (2) deionized and fractionated twice in an all-glass distillation flask.
	ESTIMATED ERROR: not specified.
	REFERENCES: 1. Sugi, H.; Nitta, T.; Katayama, T. *J. Chem. Eng. Jap.* <u>1976</u>, *9*, 12.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Charykov, A.K.; Tikhomirov, V.I.; Potapova, T.M. *Zh. Obshch. Khim.* <u>1978</u>, *48*, 1916-21.
VARIABLES: One temperature: 20°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in hexane at 20°C was reported to be
0.0035 mol(2) dm^{-3} sln corresponding to a mole fraction, x_2, of
0.00046. The mass percent calculated by the compiler is
0.0084 g(2)/100 g sln. The compiler's calculation assumes a solution
density of 0.663 g/mL (the density of hexane reported in ref 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The saturation of (1) with (2) was obtained by shaking definite volumes of (1) and (2) in a mechanical shaker for 2-3 hrs. (2) was determined in an aliquot (0.2-5 mL) of (1) by the Karl Fischer method. No more details are given.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES: 1. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* <u>1978</u>, *51*, 957-8.

VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 0.16 g(1)dm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.016 g(1)/100 g sln and 3.3×10^{-5}.

The compiler's calculation assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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).	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. 0.01 g(1)dm^{-3} sln (standard deviation from 6 determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (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 hexane in water at 25°C was reported to be
9.47 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 9.47 x 10^{-4} g(1)/100 g sln and 1.98 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.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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. 0.3 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y. J. Chem. Eng. Data <u>1979</u>, 24, 30-4.
VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of hexane in water at 25°C was reported to be 0.0123 g(1) dm^{-3} sln.

With the assumption of a solution density of 1.00 g cm^{-3}, the corresponding mass percent is 0.00123 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.57 x 10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions were prepared by adding an excess of (1) in (2) for 24 h, followed by settling in the water-bath for at least 48 hrs. The dissolved (1) was extracted by helium and trapped in liquid nitrogen. (1) was then injected into the GC column. The gas chromatograph was a Hewlett-Packard Model equipped with a flame ionization detector. The technique is described in ref 1.	(1) Fisher Scientific; pure grade (99 mol%). (2) not specified.
	ESTIMATED ERROR: soly. ± 0.0004 g(1) dm^{-3} sln (type of error not specified).
	REFERENCES: 1. Mackay, D.; Shiu, W.Y. Bull. Environ. Contam. Toxicol. <u>1974</u>, 15, 101.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3] 2. Water; H_2O; [7732-18-5]	De Loos, Th. W.; Penders, W. G.; Lichtenthaler, R. N. *J. Chem. Thermodyn.* <u>1982</u>, *14*, 83-91.
VARIABLES: Temperature, pressure	PREPARED BY: C. L. Young

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	P/MPa	Mole fraction of hexane	q (1)/ 100 g soln.	T/K	P/MPa	Mole fraction of hexane	q (1)/ 100 g soln.
631.5	18.33	0.005	2.4	623.1	19.63	0.005	2.4
633.8	18.82			620.7	19.37		
635.9	19.31			618.3	19.23		
637.7	19.80			616.4	19.15		
639.7	20.27			614.8	19.10		
641.4	20.76			613.4	19.10		
643.5	21.25			610.9	19.20		
644.8	21.74			609.5	19.20		
645.5	22.08			608.4	19.25		
645.4	22.20			607.5	19.40		
645.3	22.22			606.3	19.45		
644.2	22.23			605.1	19.66		
643.3	22.18			604.2	19.80		
642.1	22.08			603.2	20.00		
641.2	21.99			601.8	20.30		
640.0	21.89			600.4	20.63		
640.0	21.78			597.6	21.92		
639.7	21.35			596.7	22.41		
634.6	21.13			596.3	24.69		
632.4	20.73			595.9	25.25		
628.4	20.34			595.9	26.23		
625.1	19.97						(cont.)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Static visual cell fitted with magnetic stirrer. Composition of homogeneous phase determined from weighing cell charge at ambient temperature. Details of cell and procedure given in ref.(1). Pressure measured with a pressure balance and temperature measured with Pt resistance thermometer.	1. Merck sample, purity at least 99.0 moles per cent. Degassed. 2. Doubly distilled. Conductivity less than 10^{-6} S cm^{-1}.

	ESTIMATED ERROR: $\delta T/K = \pm 0.1$ K; $\delta P/MPa = \pm 0.02$ up to 40 MPa, ± 0.05 above 40 MPa; $\delta x = \pm 0.002$.

	REFERENCES:
	1. De Loos, Th. W.; Wijen, A. J. M.;
	   Diepen, G. A. M.
	   J. Chem. Thermodyn.
	   <u>1980</u>, *12*, 193.

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3]	De Loos, Th. W.; Penders, W. G.;
2. Water; H_2O; [7732-18-5]	Lichtenthaler, R. N.
	J. Chem. Thermodyn.
	1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
629.9	18.33	0.015	6.8	635.8	23.22	0.025	10.9
632.0	18.82			635.0	23.35		
634.9	19.56			633.8	23.53		
637.7	20.29			633.2	23.62		
639.3	20.76			632.6	23.72		
641.1	21.25			631.6	23.92		
642.7	21.99			630.2	24.46		
643.0	22.23			628.1	25.00		
642.4	22.47			627.1	25.40		
641.8	22.52			626.4	25.79		
641.6	22.54			626.2	25.94		
641.3	22.57			626.1	26.18		
641.2	22.58			625.6	26.68		
640.8	22.60			625.1	27.17		
637.4	22.74			624.9	27.65		
635.4	22.79			624.8	28.15		
633.5	22.86			624.6	29.12		
629.5	22.94			624.4	30.10		
627.9	23.01			624.5	31.09		
626.3	23.05			624.5	32.56		
624.8	23.15			624.9	33.54		
620.8	24.48			625.2	35.50		
620.3	24.72			625.9	36.97		
619.5	24.97			627.2	40.21		
618.3	25.21			629.0	45.08		
617.2	26.10			633.2	54.89		
616.9	29.64			638.8	64.68		
616.5	31.89			643.9	74.46		
616.6	34.54			649.4	86.68		
617.9	40.23			657.6	101.40		
622.9	59.82			663.1	118.56		
633.5	74.49			669.5	135.70		
639.0	86.73			635.8	21.02	0.030	12.9
645.1	106.32			636.2	21.18		
650.7	118.56			636.9	21.56		
655.4	129.84			637.4	21.71		
629.6	18.84	0.025	10.9	637.9	22.01		
630.7	19.06			638.0	22.35		
631.6	19.31			638.0	22.74		
632.5	19.56			637.5	22.84		
634.3	20.04			637.0	22.99		
635.1	20.29			636.6	23.08		
636.7	20.78			636.3	23.13		
638.0	21.19			636.0	23.20		
639.5	21.74			635.7	23.23		
640.1	22.23			635.6	23.28		
639.4	22.58			635.2	23.33		
639.3	22.63			634.9	23.43		
638.9	22.72			634.3	23.53		
638.4	22.82			633.3	23.72		
637.8	22.94			632.9	23.82		
637.5	22.99			632.5	23.92		
637.1	23.03			632.2	24.01		
636.8	23.08			631.9	24.12		
636.5	23.13			631.5	24.22		
636.1	23.18						

(cont.)

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3]	De Loos, Th. W.; Penders, W. G.;
2. Water; H_2O; [7732-18-5]	Lichtenthaler, R. N.
	J. Chem. Thermodyn.
	1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	P/MPa	Mole fraction of hexane	q (1)/ 100 g soln.	T/K	P/MPa	Mole fraction of hexane	q (1)/ 100 g soln.
631.0	24.31	0.030	12.9	632.1	20.78	0.042	17.3
630.8	24.41			633.3	21.27		
630.5	24.51			634.2	21.76		
630.0	24.60			635.0	22.25		
629.8	24.70			635.3	22.74		
629.5	24.80			634.7	23.13		
628.1	25.43			633.9	23.48		
627.1	26.08			632.4	24.01		
626.5	26.68			631.9	24.22		
626.3	27.17			631.5	24.31		
626.1	27.65			631.3	24.41		
626.0	27.85			631.2	24.46		
625.8	28.24			631.1	24.51		
625.7	28.83			631.0	24.55		
625.4	30.10			630.8	24.62		
625.5	30.89			630.0	24.95		
625.6	31.38			628.6	25.82		
625.7	31.78			627.8	26.50		
625.9	32.17			627.5	26.92		
626.3	33.05			627.3	27.27		
627.4	35.99			627.1	27.65		
627.9	37.22			626.8	28.15		
629.0	40.18			626.7	28.63		
637.0	57.34			626.6	29.12		
620.0	17.14	0.038	15.9	626.6	30.10		
624.1	18.11			626.7	31.09		
626.9	18.84			626.9	32.07		
630.0	19.82			627.2	33.54		
631.7	20.29			628.8	36.94		
633.8	21.02			629.2	38.31		
635.3	21.76			631.4	42.63		
636.0	22.25			633.7	47.53		
635.8	22.74			639.1	57.23		
635.8	22.89			643.9	66.12		
635.6	22.99			648.7	74.44		
634.7	23.23			655.9	88.41		
632.9	23.72			659.8	96.49		
632.3	23.82			664.4	106.30		
632.0	23.96			671.2	122.95		
631.7	24.06			616.3	16.65	0.049	19.8
630.9	24.26			618.3	17.02		
630.1	24.72			622.3	18.06		
629.1	25.21			623.4	18.35		
627.9	26.18			626.6	19.23		
627.1	27.17			628.4	19.80		
626.5	28.15			629.9	20.29		
626.2	29.62			631.4	20.78		
626.3	31.57			632.0	21.02		
627.0	33.54			632.5	21.27		
628.0	37.46			633.0	21.51		
632.2	45.08			633.4	21.76		
641.1	622.22			633.8	22.01		
625.0	18.59	0.042	17.3	633.9	22.10		
626.7	19.08			634.1	22.99		
628.3	19.56			634.0	23.08		
630.8	20.29			634.0	23.18		(cont.)

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C₆H₁₄; [110-54-3]	De Loos, Th. W.; Penders, W. G.;
2. Water; H₂O; [7732-18-5]	Lichtenthaler, R. N.
	J. Chem. Thermodyn.
	<u>1982</u>, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
633.5	23.43	0.049	19.8	629.9	25.29	0.060	23.4
633.2	23.58			628.8	26.26		
632.6	23.82			628.3	26.90		
632.3	23.96			628.1	27.46		
632.0	24.12			627.9	27.85		
631.0	24.55			627.8	28.24		
630.5	24.79			627.7	28.83		
630.1	24.90			627.7	29.42		
629.8	25.05			627.6	30.20		
629.8	25.15			627.7	30.89		
629.4	25.38			627.8	31.57		
629.0	25.63			628.1	32.56		
628.9	25.77			628.3	33.52		
628.6	26.02			628.7	34.50		
628.2	26.41			629.7	36.94		
627.5	27.22			631.5	40.18		
627.3	28.32			635.0	47.05		
627.3	29.62			641.9	56.82		
627.4	30.60			647.7	68.33		
627.6	31.57			653.5	78.63		
627.8	32.07			660.1	91.45		
628.0	32.80			663.9	98.94		
628.6	34.50			618.9	18.25	0.070	26.5
629.1	35.47			619.3	18.35		
629.4	36.50			620.1	18.59		
629.6	36.84			621.0	18.84		
630.1	37.93			622.5	19.33		
631.4	40.18			626.1	20.70		
633.0	42.38			627.3	21.34		
634.0	45.08			628.6	22.15		
641.2	57.56			629.3	22.74		
643.2	60.75			629.4	23.53		
648.3	69.54			629.2	24.12		
653.0	78.36			628.9	24.54		
653.8	79.35			628.6	25.00		
657.7	86.68			628.4	25.52		
665.9	102.87			627.9	26.18		
618.5	17.61	0.060	23.4	627.5	27.17		
620.3	18.11			627.3	28.15		
621.2	18.35			627.2	29.12		
622.9	18.84			627.3	30.10		
625.9	19.82			627.5	31.09		
627.7	20.56			627.8	31.07		
628.4	20.78			628.0	33.05		
629.5	21.27			628.3	34.00		
630.0	21.51			628.7	34.99		
630.6	21.76			628.6	34.50		
631.2	22.25			631.6	40.18		
631.6	22.74			634.4	45.08		
631.8	22.94			643.7	59.79		
631.9	23.53			652.9	74.44		
631.7	23.92			660.7	86.68		
631.4	24.12			616.3	17.78	0.081	29.7
631.2	24.31			617.3	18.13		
630.9	24.55			619.0	18.40		
630.5	24.95			621.3	19.33		

(cont.)

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3]	De Loos, Th. W.; Penders, W. G.;
2. Water; H_2O; [7732-18-5]	Lichtenthaler, R. N.
	J. Chem. Thermodyn.
	1982, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
622.8	19.82	0.081	29.7	628.5	34.50	0.094	33.2
624.0	20.31			630.5	37.93		
625.2	20.80			633.3	42.63		
626.1	21.29			634.8	45.08		
627.0	21.78			637.8	49.98		
627.6	22.27			641.0	54.87		
628.3	23.23			644.4	59.72		
628.3	24.22			645.9	62.22		
628.2	25.19			647.1	64.68		
628.0	25.70			653.3	74.44		
627.5	26.68			660.1	86.68		
627.4	27.65			667.9	101.40		
627.3	28.63			673.9	111.20		
627.4	29.62			613.4	17.98	0.102	35.2
627.7	30.60			613.8	18.03		
627.9	31.57			614.5	18.37		
628.2	32.54			615.2	18.61		
628.5	33.52			616.1	18.86		
629.0	34.50			617.4	19.35		
629.7	35.47			618.7	19.82		
630.1	36.94			619.8	20.31		
631.0	38.41			621.1	20.80		
632.1	40.18			622.0	21.29		
632.3	40.67		.	623.4	22.27		
632.8	41.40			624.1	22.96		
633.1	41.90			624.9	23.74		
633.5	42.63			625.3	24.72		
633.8	43.12			625.6	25.94		
634.3	43.85			625.9	27.17		
645.0	60.26			626.4	28.63		
647.2	64.66			626.7	30.10		
650.1	69.54			627.1	31.09		
654.5	76.79			627.5	32.07		
657.9	83.02			627.9	33.05		
662.7	92.08			628.9	34.50		
665.4	98.94			630.0	36.94		
671.2	108.75			632.8	41.40		
671.7	109.98			643.9	59.77		
608.9	16.65	0.094	33.2	652.9	74.44		
612.1	17.47			653.1	74.44		
615.0	18.37			653.5	75.67		
618.3	19.33			654.2	76.90		
619.5	19.77			660.0	86.68		
621.1	20.31			666.6	98.94		
621.5	20.55			610.2	18.08	0.119	39.3
622.1	20.80			613.1	19.10		
622.8	21.29			614.2	19.84		
623.8	21.78			617.7	21.12		
624.6	22.27			618.7	21.78		
625.6	23.25			620.5	23.01		
626.0	24.72			621.4	23.74		
626.1	25.70			622.1	24.48		
626.3	27.17			622.6	25.21		
626.6	29.62			623.2	26.18		
627.0	31.09			623.6	27.17		
627.6	32.56			624.2	28.15		
628.1	33.54						

(cont.)

COMPONENTS:	ORIGINAL MEASUREMENTS:
1. Hexane; C_6H_{14}; [110-54-3] 2. Water; H_2O; [7732-18-5]	De Loos, Th. W.; Penders, W. G.; Lichtenthaler, R. N. *J. Chem. Thermodyn.* <u>1982</u>, *14*, 83-91.

EXPERIMENTAL VALUES:

Values of pressure and temperature on one phase-two phase boundary

T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.	T/K	P/MPa	Mole fraction of hexane	g (1)/ 100 g soln.
624.6	29.12	0.119	39.3	616.8	21.31	0.135	42.7
625.1	30.10			617.7	21.60		
625.7	31.09			618.4	22.27		
626.2	32.07			619.1	22.76		
627.0	33.54			620.3	23.74		
627.6	34.52			621.0	24.72		
628.3	35.47			622.2	26.18		
629.4	37.43			622.9	27.17		
631.3	40.18			623.4	28.15		
632.9	42.63			624.1	29.12		
635.4	46.55			624.9	30.60		
637.7	49.98			625.8	32.07		
642.5	57.32			627.3	34.52		
645.6	62.22			628.2	35.96		
648.6	67.09			629.4	37.93		
652.7	74.44			631.2	40.18		
656.8	81.79			632.7	42.63		
662.3	91.59		.	634.2	45.08		
667.2	101.40			635.9	47.53		
672.1	111.20			643.7	59.77		
608.3	17.87	0.135	42.7	647.0	64.68		
609.1	18.13			653.1	74.44		
609.8	18.37			659.9	86.68		
611.3	18.86			666.5	98.94		
615.0	20.33			672.6	111.20		
616.0	20.82						

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* 1982, 9, 279-86.
VARIABLES: Temperature: 15-35°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of hexane in water

$t/$°C	mg(1)/kg sln	10^3g(1)/100g sln (compiler)	$10^6 x_1$ (compiler)
15	10.72	1.07	2.24
20	10.32	1.03	2.15
25	10.09	1.01	2.11
30	10.02	1.00	2.09
35	10.10	1.01	2.11

[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:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Fluka, > 99.7%, 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:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Water; H_2O; [7732-18-5]	Tsonopoulos, C.; Wilson, G.M. *A. I. Ch. E. J.* <u>1983</u>, *29*, 990-9.

VARIABLES:	PREPARED BY:
Temperature: 311-473 K Pressure: 0.05-3.5 MPa	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of hexane in water

T/K	p^a/MPa	$10^4\ x_1$	10^2 g(1)/100 g sln (compiler)
310.93	$-^a$	0.238	0.114
366.48	$-^a$	0.573	0.274
367.55	$-^a$	0.535	0.256
373.15	0.3482	0.621	0.297
422.04	$-^a$	2.71	1.30
423.15	1.2548	3.39	1.62
473.15	3.516	18.5	8.85

a Not specified.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
All experimental details are given in an Appendix deposited in a Documentation Centre rather than in the original paper. The solubility of (1) in (2) was measured by gas chromatography, whilst that of (2) in (1) was measured by Karl Fischer titration.	(1) No details given (2) No details given

ESTIMATED ERROR:
soly. ± 5% relative; repeatability of replicate analyses. temp. not stated. press. ± 1%; type of error not stated.

REFERENCES:

(1) Hexane; C_6H_{14}; [110-54-3]
(2) Water; H_2O; [7732-18-5]

(continued)

The solubility of water in hexane

T/K	p^a/MPa	$10^2\ x_2$	g(2)/100 g sln (compiler)
313.15	0.04537	0.117,0.123	0.025^b
367.55	$-^a$	0.595	0.124
373.15	0.3482	0.709	0.148
423.15	1.2548	3.11	0.667
473.15	3.516	11.0	2.52

a Not specified.
b Average value.

The three phase critical point was reported to be 496.7 K, 5.295 MPa and $x_1 = 4.982 \times 10^{-4}$ (0.238 g(1)/100 g sln, compiler).

The authors also report equations fitted to their own and literature data over the range 273-497 K, *viz.*

$$\ln x_1 = -367.9847 + 16128.646/T + 52.820813 \ln T$$
$$\ln x_2 = -45.1714 - 1635.73/T + 7.53503 \ln T$$

COMPONENTS:	EVALUATOR:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of hexane (1) in seawater (2) at 298 K has been reported in two works:

Authors	Method	Salinity g salts/kg sln	g(1)/100 g sln
Krasnoshchekova and Gubergrits (ref 1)	GLC	6	7.55×10^{-3}
Aquan-Yuen *et al.* (ref 2)	Spectro-fluorometry	35.3	7.86×10^{-4}

These two determinations were made at somewhat different salinities and thus cannot be directly compared. Because the presence of sea salts is expected to depress the solubility value below the value for pure water (tentative value 1.3×10^{-3} g(1)/100 g sln) the tentative value of 7.86×10^{-4} g(1)/100 g sln is adopted for hexane in seawater at the indicated temperature and salinity. The value of Krasnoshchekova and Gubergrits is considered doubtful. Freegarde *et al.* (ref 3) also measured the solubility of hexane in seawater. However, since they did not report temperature or salinity, their work is rejected. Aquan-Yuen *et al.* have also measured solubility over a range of salinities.

SOLUBILITY OF HEXANE (1) IN SEAWATER (2)
TENTATIVE VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	35.3	7.86×10^{-4}

REFERENCES

1. Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.

2. Aquan-Yuen, M.; Mackay, D; Shiu, W.Y. *J. Chem. Eng. Data* 1979, *24*, 30-4.

3. Freegarde, M.; Hatchard, C.G.; Parker, C.A. *Lab. Pract.* 1971, *20*, 35-40.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Seawater	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* 1973, *13*, 885-8.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of hexane in seawater was reported to be

7.55×10^{-3} g(1)/100 g sln and the corresponding mole

fraction, $x_1 = 1.3 \times 10^{-5}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) "chemically pure" (2) distilled water plus salt mixture.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Hexane; C_6H_{14}; [110-54-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Aquan-Yuen, M.; Mackay, D.; Shiu, W.Y. *J. Chem. Eng. Data* <u>1979</u>, *24*, 30-4.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 18-130 g(2)/kg sln.	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of hexane in aqueous NaCl

mol(2)/L sln	g(2)/kg sln[a]	mg(1)/L sln	10^4mass%(1)[a]	$10^6 x_1$[a]
0.31	17.9	10.48	10.35	2.19
0.62	35.3	8.06	7.86	1.68
1.00	56.2	7.54	7.25	1.58
1.50	82.6	4.88	4.60	1.08
2.00	108.2	3.75	3.47	0.846
2.50	132.7	2.55	2.32	0.583

'a' calculated by compilers

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) 99% pure from Fisher Scientific. (2) reagent grade.
	ESTIMATED ERROR: soly ± 1 relative %.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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 system toluene (1) and water (2) have been reported in the references listed in Table 1.

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

Reference	T/K	Solubility	Method
Jaeger (ref 1)	353-573	(1) in (2)	synthetic
Fühner (ref 2)	289	(1) in (2)	titration
Uspenskii (ref 3)	283,295	mutual	titration, analytical
Rosenbaum and Walton (ref 4)	283-323	(2) in (1)	analytical
Gross and Saylor (ref 5)	303	(1) in (2)	interferometric
Tarassenkow and Poloshinzewa (ref 6,7)	264-366	(2) in (1)	synthetic
Booth and Everson (ref 8)	298	(1) in (2)	residue volume
Andrews and Keefer (ref 9) (ref 9)	298	(1) in (2)	spectrophotometric
Klevens (ref 10)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 11)	273-318	(1) in (2)	spectrophotometric
Morrison and Billet (ref 12)	298	(1) in (2)	analytical
Wing and Johnston (ref 13)	298	(2) in (1)	radiotracer
Caddock and Davis (ref 14)	293	(2) in (1)	radiotracer
Guseva and Parnov (ref 15,16)	363-497	(1) in (2)[a]	synthetic?
Jones and Monk (ref 17)	298	(2) in (1)	radiotracer
McAuliffe (ref 18)	298	(1) in (2)	GLC
Hoegfeldt and Bolander (ref 19)	298	(2) in (1)	Karl Fischer
Englin et al. (ref 20)	273-323	(2) in (1)	analytical
Connolly (ref 21)	553-583[b]	(1) in (2)	cloud point
Johnson et al. (ref 22)	298	(2) in (1)	Karl Fischer
McAuliffe (ref 23)	298	(1) in (2)	GLC
Gregory et al. (ref 24)	298	(2) in (1)	Karl Fischer
Benkovski et al. (ref 26)	303	(2) in (1)	Karl Fischer
Glasoe and Schultz (ref 28)	288-303	(2) in (1)[a]	Karl Fischer
Pierotti and Liabastre (ref 29)	278-318	(1) in (2)	GLC
Bradley et al. (ref 31)	298-328[b]	(1) in (2)	spectrophotometric
Polak and Lu (ref 32)	273-298	mutual	GLC, Karl Fischer

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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 1 continued)

Reference	T/K	Solubility	Method
Brown and Wasik (ref 33)	278-293	(1) in (2)	GLC
Krasnoshchekova and Gubergrits (ref 34)	298	(1) in (2)	GLC
Mackay and Shiu (ref 35)	298	(1) in (2)	GLC
Sada *et al.* (ref 36)	298	(1) in (2)	titration
Sutton and Calder (ref 37)	298	(1) in (2)	GLC
Price (ref 39)	298	(1) in (2)	GLC
Korenman and Aref'eva (ref 40,41)	293,298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 42)	298	(1) in (2)	GLC
Banerjee *et al.* (ref 43)	298	(1) in (2)	radiotracer
Schwarz (ref 44)	297	(1) in (2)	chromatographic
Rossi and Thomas (ref 45)	298	(1) in (2)	GLC
Sanemasa *et al.* (ref 46)	288-318	(1) in (2)	spectrophotometric
Sanemasa *et al.* (ref 47)	288-318	(1) in (2)	spectrophotometric
Sanemasa *et al.* (ref 48)	298	(1) in (2)	spectrophotometric

a Data also given for D_2O
b Pressure also varied, see Table 4

The original data in all of the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation.

As indicated in the footnotes to Table 1, quantitative solubility data for toluene in heavy water (ref 15) and D_2O in toluene (ref 28), have been reported. However, since no other comparable data are available, no critical evaluation of the reliability of these data can be made. The interested user is referred to the relevant Data Sheets for experimental solubilities. Solubility values reported by Price (ref 30) were not available for inspection. Solubility data may also be calculated from the calorimetric data of Gill *et al.* (ref 38).

Critical point data have been reported by Alwani and Schneider (ref 25) and Roof (ref 27) and are discussed in section 3 below.

In the toluene-water system the mutual solubilities are sufficiently low to enable data reported in w/v fractions (or equivalent) to be converted to mass percent solubilities with reasonable precision by assuming solution densities to be the same as the pure solvents. These conversions are given

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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)

in the Data Sheets and the data are included in this Evaluation. The data of Jaeger (ref 1), Booth and Everson (ref 8), Wing and Johnston (ref 13), Jones and Monk (ref 7) and Sada *et al*. (ref 36) given in v/v fractions have not been converted and so have been excluded from this Evaluation.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation or extrapolation of the original measurements given in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits. The letter (*R*) indicates "Recommended" data. Data are "Recommended" if two or more apparently reliable studies are in reasonable agreement (± 5% relative). All other data are regarded as "Tentative". For convenience, further discussion of this system will be divided into three parts.

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

The solubility of toluene in water has been investigated on numerous occasions (Table 1).

The large amount of data at 298K enables a particularly critical assessment of the reported values. Data have been rejected if they deviated significantly (> 3 σ_n) from the average value. Thus, at 298K, the value of Krasnoshchekova and Gubergrits (ref 34), which is markedly lower than all other values, and Bohon and Claussen (ref 11), Pierotti and Liabastre (ref 29), Korenman and Aref'eva (ref 41), Banerjee *et al*. (ref 43) and Schwarz (ref 44, 297K), which are higher, have all been rejected. The datum of Krzyzanowska and Szeliga (ref 42) has not been included in the Critical Evaluation because it does not appear to be independent of that of Price (ref 38).

At temperatures other than 298K, the data of Fühner (ref 2) and Uspenskii (ref 3) are markedly lower than all other values and are rejected. All other data are included in Table 2 except for the high temperature data which are discussed in section 3 below.

Agreement among the studies (ref 11,29,33,46,47) which report solubilities over a range of temperatures below 323K is disappointing (see Table 2 and Figure 1). For example, although the solubility data of Pierotti and Liabastre (ref 29) are usually markedly higher than Recommended values in well-characterised systems (e.g. benzene in water) their toluene results lie

COMPONENTS:	EVALUATOR:
(1) Toluene, C_7H_8; [108-88-3]	G.T. Hefter, School of Mathematical
(2) Water; H_2O; [7732-18-5]	and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	May 1986

CRITICAL EVALUATION: (continued)

within the range of values reported by other workers. Even the averaged "Best" solubilities, which usually show a smoother variation with temperature than individual data sets, show a good deal of scatter (e.g. compare Figure 1 with the analogous diagram for benzene and water).

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

T/K	Solubility values ($\pm \sigma_n$)		
	Reported values $10^2 g(1)/100g$ sln	"Best" values $10^2 (1)/100g$ sln	$10^4 x_1$
273	6.60* (ref 11), 7.24 (ref 32)	6.9 ± 0.3	1.35
278	6.42* (ref 11), 6.36 (ref 29), 6.08* (ref 33)	6.3 ± 0.1	1.23
283	6.28* (ref 11), 6.32 (ref 29), 5.82* (ref 33), 5.24 (ref 46)	5.9 ± 0.4	1.15
293	6.18* (ref 11), 6.06 (ref 29), 5.67 (ref 33), 5.7 (ref 40), 5.45 (ref 46), 5.18* (ref 47)	5.7 ± 0.3	1.11
298	5.3 (ref 9), 5.00 (ref 10), 5.36 (ref 12), 5.38 (ref 18), 5.15 (ref 23), 5.47 (ref 31), 5.73 (ref 32), 5.20 (ref 35), 5.35 (ref 37), 5.54 (ref 39), 5.07 (ref 45), 5.57 (ref 46), 5.25 (ref 47), 5.19 (ref 48)	5.3 ± 0.2 (R)	1.04 (R)
303	5.7 (ref 5), 6.40 (ref 11), 6.5* (ref 29), 5.7* (ref 31), 5.73* (ref 46), 5.32* (ref 47)	5.9 ± 0.4	1.15
313	6.82* (ref 11), 6.7* (ref 29), 6.6* (ref 31), 6.12* (ref 46), 5.57 (ref 47)	6.4 ± 0.5	1.25
318	7.15* (ref 11), 6.72 (ref 29), 7.22 (ref 31), 6.35 (ref 46), 5.78 (ref 47)	6.6 ± 0.5	1.29
328	8.6 (ref 31)	8.6	1.68

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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)
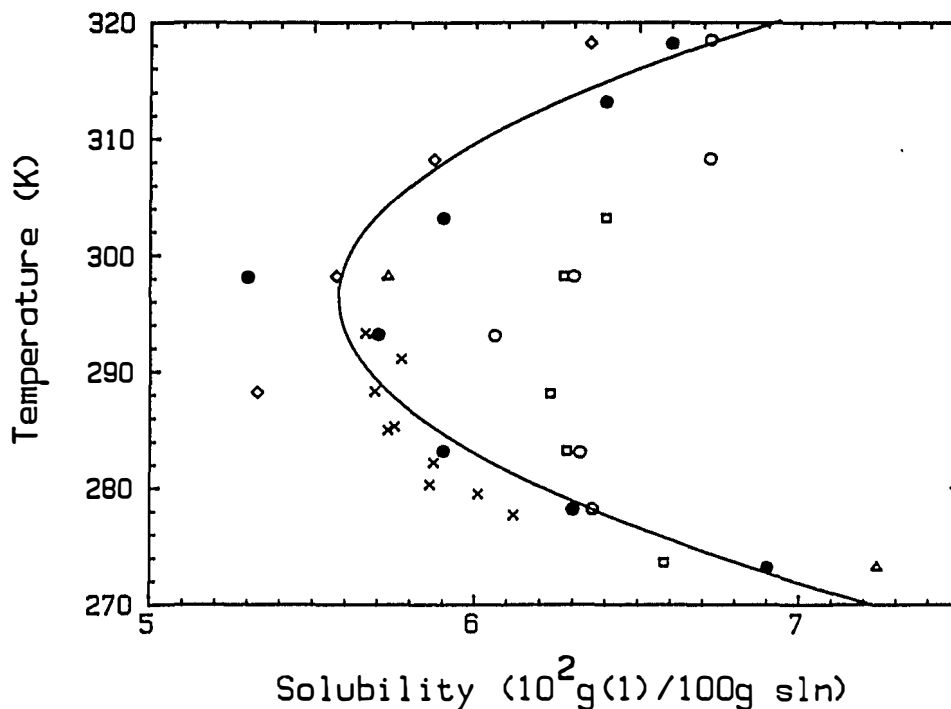
FIGURE 1. Solubility of toluene in water, selected data:ref 11(□); ref 29(o); ref 32 (Δ); ref 33 (x); ref 46 (◊); "Best" values (●, full line).

Thermodynamic data calculated by application of the van't Hoff equation to the variable temperature solubility studies are summarized in Table 3. As might be expected from the scatter in the reported solubilities none of the derived therodynamic functions agree closely with reliable calorimetric values (Table 3). Even the averaged "Best" solubilities which should show minimal systematic (temperature dependent) errors give a disappointing value for $\Delta C_{p,sln}$.

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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 3:   Thermodynamic Functions Calculated from Solubility Data

Reference	ΔH_{sln} kJ mol^{-1}	$\Delta C_{p,sln}$ J K^{-1} mol^{-1}
Bohon and Claussen (ref 11)	2.3	292
Guseva and Parnov (ref 15,16)	35.3	-62
Pierotti and Liabastre (ref 29)	1.5	168
Brown and Wasik (ref 33)	4.7	590
Sanemasa *et al.* (ref 46)	3.7	160
Sanemasa *et al.* (ref 47)	2.1	181
"Best" values (Table 2)	1.7	566
Gill *et al.* (ref 38)	1.73 ± 0.04[a]	263 ± 13[a]

a Calorimetric data

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

A reasonable amount of data is available for the solubility of water in toluene over the temperature range 273-323K.

In spite of the difficulties of accurate analysis at the relatively low concentrations involved, the results are generally in good agreement and a number of "Best" values have been "Recommended" (Table 4).

Except for the low temperature ($T < 313K$) values of Tarassenkow and Poloshinzewa (ref 6,7) and the datum of Benkovski *et al.* (ref 26), which are markedly lower than all other values and are therefore rejected, all the available data are listed in Table 4. Selected data are also plotted in Figure 2 (on the next page but one).

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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 4: Recommended (R) and Tentative Values of the Solubility of Water (2) in Toluene (1)

T/K	Reported values 10^2g(2)/100g sln	"Best" values (± σ_n) 10^2g(2)/100g sln	$10^3 x_2$
273	2.74 (ref 20), 2.28 (ref 32)	2.5 ± 0.2	1.3
283	4.26 (ref 3), 3.35 (ref 4), 3.16 (ref 10)	3.6 ± 0.5	1.8
293	5.1* (ref 3), 4.50 (ref 4), 4.6 (ref 14), 4.60 (ref 20), 4.7* (ref 28)	4.7 ± 0.2 (R)	2.4 (R)
298	5.6* (ref 3), 5.7 (ref 4), 5.4 (ref 19), 5.3* (ref 20), 5.72 (ref 22), 5.60 (ref 24), 5.45 (ref 28), 5.43 (ref 32)	5.5 ± 0.1 (R)	2.8 (R)
303	6.00 (ref 4), 6.15 (ref 20), 6.15 (ref 28)	6.1 ± 0.1 (R)	3.1 (R)
313	7.33 (ref 4), 7.3* (ref 6,7), 7.50 (ref 20)	7.4 ± 0.1 (R)	3.8 (R)
323	9.53 (ref 4), 10.2* (ref 6,7), 9.65 (ref 20)	9.8 ± 0.3 (R)	5.0 (R)
333	15.0* (ref 6,7)	15	7.7
343	21.0* (ref 6,7)	21	11
353	28.7* (ref 6,7)	29	15

Despite the relatively small differences between the data of Tarassenkow and Poloshinzewa (ref 6,7) and the "Best" values of Table 4 (see Figure 2 on next page), application of the van't Hoff equation yields quite different values for ΔH_{sln} (31 and 21 kJ mol^{-1}) and $\Delta C_{p,sln}$ (-24 and +239 J K^{-1} mol^{-1}, respectively). Comparison with similar reactions (e.g. water in benzene: ΔH_{sln}=24 kJ mol^{-1} and $\Delta C_{p,sln}$=99 J K^{-1} mol^{-1}) suggests the "Best" values may be more reliable.

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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. May 1986

CRITICAL EVALUATION: (continued)
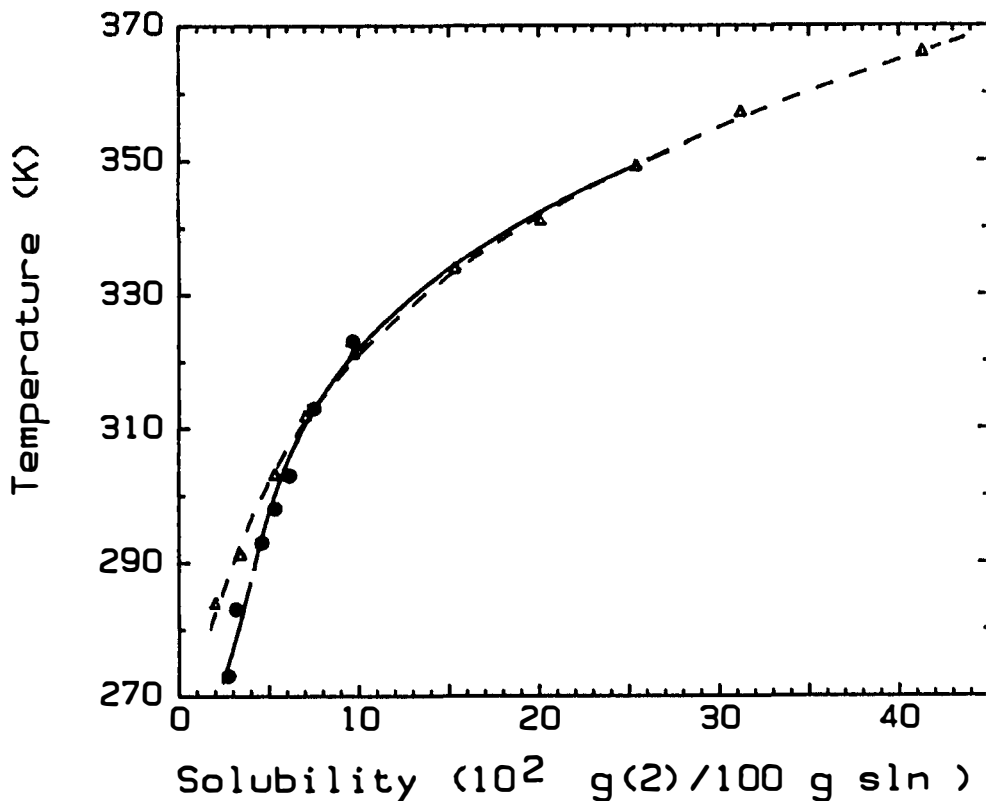
FIGURE 2. Solubility of water in toluene: ref 6,7 (△, broken line); Table 3 "Best" values (●, full line).

3.   MUTUAL SOLUBILITIES OF TOLUENE (1) AND WATER (2) AT ELEVATED PRESSURES

Solubilities in the toluene + water system have been studied at higher than atmospheric pressure in a few publications but the system lacks a comprehensive study. Table 5 gives the range of conditions under which the system has been studied.

As can be seen there is little overlap between the various workers and a meaningful comparison cannot be made. The interested user is referred to the relevant Data Sheets for experimental solubilities. However, it should be noted that thermodynamic functions calculated from the data of Guseva and Parnov (ref 15,16) disagree markedly with other values and are unlikely to be correct.

COMPONENTS:	EVALUATOR:
(1) Toluene, C_7H_8; [108-88-3] (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.
	May 1986

CRITICAL EVALUATION: (continued)

The phase behaviour of this system is similar to that of benzene + water. here are two critical loci, one starting at the critical point of water and eventually approaching high pressure. The second starts at the critical point of toluene and ends in a critical end point on a three phase line. The topology of the pressure -temperature projection is similar to that given for benzene + water except that the temperature at which the vapor pressures of the two pure components are equal is considerably lower than in the benzene + water system.

In the region above the three phase line on the pressure - temperature 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 toluene it is possible to have one or two phases present depending on the overall composition.

Roof (ref 27) has determined the temperature and pressure of the critical end point in this system to be T = 558.1K, P = 10.10MPa.

TABLE 5:   Solubility Studies of the Toluene + Water
System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Guseva and Parnov (ref 15,16)	$-^a$	363-497	(1) in (2)
Connolly (ref 21)	15-45	553-583	(1) in (2)
Alwani and Schneider (ref 25)	$-^b$	$-^b$	$-^b$
Roof (ref 27)	$-^b$	$-^b$	$-^b$
Bradley et al. (ref 31)	1,100	273-303	(1) in (2)

a Along three phase line
b Critical point data only

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COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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)

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COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (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)

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COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Jaeger, A. *Brennst. Chem.* <u>1923</u>, *4*, 259.
VARIABLES:	PREPARED BY:
Temperature: 100-300°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of toluene in water

$t/°C$	mL(1)/100 mL(2)
150	0.2
200	0.7
250	2.8
300	13.0

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Fuhner, H. *Ber. Dtsch. Chem. Ges.* <u>1924</u>, *57*, 510-5.

VARIABLES:	PREPARED BY:
One temperature: 16°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of toluene in water at 16°C was reported to be
0.047 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers
is 9.2×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm³ (2) until a completely clear solution was no longer obtained at the experimental temperature.	(1) source not specified; commercial grade; used as received, (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Uspenskii, S.P. *Neft. Khoz.* <u>1929</u>, *11-12*, 713-7.

VARIABLES:	PREPARED BY:
Temperature: 10 and 22°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of toluene in water

$t/°C$	$g(1)/100 \ g \ sln$	$10^5 x_1$ (compiler)
10	0.0368 ± 0.0002	7.20
22	0.0492 ± 0.0003	9.62

Solubility of water in toluene

$t/°C$	$g(2)/100 \ g \ sln$	$10^3 x_2$ (compiler)
10	0.0426 ± 0.0011	2.18
22	0.0526 ± 0.0016	2.68

AUXILIARY INFORMATION

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

The solubility of (1) in (2) was determined by titration. The solubility of (2) in (1) was determined by Clifford's (ref 1), method. Dried air was passed through the vessel with a saturated solution of (2) in (1) and U-tubes with $CaCl_2$ and next the adsorbed (2) was weighed.	(1) source not specified;
	    b.p. 109.8°C at 752 mm Hg,
	    d_4^{22} 0.8636, d_4^{10} 0.8743.
	
	(2) not specified.

	ESTIMATED ERROR: soly. see experimental values above.
	REFERENCES: 1. Clifford, C.W. *Ind. Eng. Chem.* <u>1921</u>, *13*, 628.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water, H_2O; [7732-18-5]	Rosenbaum, C.K.; Walton, J.H. *J. Am. Chem. Soc.* <u>1939</u>, *52*, 3568-73.

VARIABLES:	PREPARED BY:
Temperature: 10-50°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in toluene

t/°C	g(2)/100 g (1)	$10^3 x_2$ (compiler)
10	0.0335	1.71
20	0.0450	2.30
30	0.0600	3.06
40	0.0733	3.74
50	0.0953	4.85

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The organic phase was first saturated by shaking with water in a flask at a high temperature and then allowing the flask to cool in a thermostat to the desired temperature, with the resulting separation of excess water. After one day or more the solution was allowed to react with added calcium hydride in dry solvent. Hydrogen was evolved and the gas volume was read.	(1) source not specified; purified by keeping over mercury, refluxing with phosphorus pentoxide and fractionating; b.p. range 110.4-110.6°C (760 torr). (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Gross, P.M.; Saylor, J.H. *J. Am. Chem. Soc.* <u>1931</u>, *53*, 1744-51.
VARIABLES: One temperature: 30°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of toluene in water at 30°C was reported to be
0.57 g(1)/kg(2) and 0.0062 mol(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.057 g(1)/100 g solution and 1.12×10^{-4}.

AUXILIARY INFORMATION

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

Saturated solutions were prepared
by shaking in a thermostat and
were analyzed by means of an inter-
ferometer. The instrument used
was a combination liquid and gas
interferometer made by Zeiss.
	(1) Baker's CP analyzed grade;
	    distilled;
	    b.p. 110.74 ± 0.02°C
	
	(2) distilled.

	ESTIMATED ERROR: soly. 2.0% (from values of duplicate determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Tarassenkow, D.N.; Poloshinzewa, E.N. *Ber. Dtsch. Chem. Ges.* <u>1932</u>, *65B*, 184-6.

VARIABLES:	PREPARED BY:
Temperature: (-9)-93°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in toluene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
-9	0.002	0.1
-3.5	0.005	0.3
10.5	0.020	1.0
18	0.034	1.7
30	0.053	2.7
38.5	0.070	3.6
48	0.097	4.9
60.5	0.153	7.8
68	0.201	10.2
76	0.254	12.9
84	0.312	15.8
93	0.413	20.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Alexejew's method was used (ref 1). No additional details were reported in the paper.	(1) Kahlbaum, CP; dried over calcium chloride and distilled from sodium; purity not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 0.01% (not specified).
	REFERENCES: 1. Alexejew, W. *Wied. Ann. Physik* <u>1886</u>, *28*, 35.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Booth, H.S.; Everson, H.E. *Ind. Eng. Chem.* 1948, *40*, 1491-3.

VARIABLES:	PREPARED BY:
One temperature: 25.0°C (298.2 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25.0°C was reported to be 0.04 mL (1)/100 mL (2).

The solubility of (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate solution was also reported to be 1.20 mL (1)/100 mL sulfonate sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 0.02 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.	(1) "Highest grade commercial sample available"; no other details given. (2) Distilled.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Andrews, L.J.; Keefer, R.M. *J. Am. Chem. Soc.* <u>1949</u>, *71*, 3644-77.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be 0.053 g(1)/100 g sln.

The corresponding mole fraction, x_1, calculated by the compilers is 1.04×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Eastman Kodak Co. best grade; washed successively with concentrated sulfuric acid, water, and dilute sodium hydroxide; dried, and distilled; b.p. 110.4°C. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Klevens, H.B. *J. Phys. Chem.* <u>1950</u>, *54*, 283-98.

VARIABLES:	PREPARED BY:
Temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be 0.500 g(1) dm^{-3} sln and 0.00543 mol(1) dm^{-3} sln.
The corresponding mass percent and mole fraction, x_1, calculated by the compiler assuming a solution density of 1.00 g/mL are 0.05 g(1)/100 g sln and 9.80 x 10^{-5}.

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:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Bohon, R.L.; Claussen, W.F. *J. Am. Chem. Soc.* <u>1951</u>, *73*, 1571-8.

VARIABLES:	PREPARED BY:
Temperature: 0.4-45.3°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of Toluene in water

t/°C	g(1)/100g sln[a] (compiler)	$10^4 x_1$ (compiler)
0.4	0.0658	1.29
3.6	0.0646	1.26
10.0	0.0628	1.23
11.2	0.0624	1.22
14.9	0.0623	1.22
15.9	0.0621	1.21
25.0	0.0627[b]	1.23[b]
25.6	0.0625	1.22
30.0	0.0640	1.25
30.2	0.0642	1.25
35.2	0.0657	1.28
42.8	0.0701	1.37
45.3	0.0717	1.40

[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 0.627g(1)/L sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co., 99+%, used as received. (2) Air-free conductivity water, no further details given.

ESTIMATED ERROR:

Temp. ±0.02°C
Soly. ±0.5% relative

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Morrison, T.J.; Billett, F. *J. Chem. Soc.* <u>1952</u>, 3819-22.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be
0.00582 mol(1)/1000 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by compilers are 0.0536 g(1)/100 g sln and $x_1 = 1.05 \times 10^{-4}$.

The compiler's calculations assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
After an excess of (1) had been shaken with about 1 dm³ 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.	(1) source not specified; purest obtainable material; distilled; purity not specified. (2) not specified.

	ESTIMATED ERROR:
	temp. ± 0.1 K soly. ± 0.5% (mean of large numbers of determinations)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Wing, J.; Johnston, W.H. *J. Am. Chem. Soc.* <u>1957</u>, *79*, 864-5.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in toluene at 25°C was reported to be
0.0334 mL(2)/100 mL sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A small amount of (2) was equi- librated with 20 mL of (1) using a Teflon stirrer in a 100 mL flask in a Sargent constant temperature bath. At the end of two hours, the mixture was poured into a test tube immersed in the bath and the organic phase separated from water by gra- vitation. The determination of THO in the organic phase was done by isotopic dilution with a large excess of H_2O. The tritium activ- ities in the tritiated water samples were determined by the acetylene method described in ref 1.	(1) source not specified, chemical grade; redistilled in a column of 50 theoretical plates; purity not specified. (2) Tracerlab, Inc., tritiated water with an activity of approximately 1 µCi/mL.
	ESTIMATED ERROR: temp. ± 0.02 K soly. 0.8% (st. dev. from 5 deter- minations).
	REFERENCES: 1. Wing, J; Johnson, W.H. *Science* <u>1955</u>, *121*, 674.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Caddock, B.D.; Davies, P.L. *J. Inst. Petrol.* <u>1960</u>, *46*, 391-6.
VARIABLES: One temperature: 20°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in toluene at 20°C was reported to be
46 mg(2)/100 g(1).

The corresponding mass percent and mole fraction, x_2, calculated
by the compiler are 0.046 g(2)/100 g sln and 0.0023.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A sample of (1) was equilibrated at 20°C with an air stream containing a known amount of water vapor tagged with HTO. At equilibrium a sample of (1) was taken and its (2) content determined by liquid scintillation counting.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.01 K
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim* <u>1963</u>, *18*, 76-9. *Radiokhimiya* <u>1963</u>, *5*, 507-9.
VARIABLES: Temperature: 90-224°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of toluene in water

$t/°C$	g(1)/100 g sln	$10^3 x_1$ (compiler)
90	0.42	0.83
114	0.823	1.619
147	1.640	3.248
169	2.387	4.737
183	2.790	5.579
207	4.113	8.314
224	5.072	10.336

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The measurements were made in sealed glass tubes. No details were reported in the paper.	(1) source not specified; n_D^{20} 1.4970. (2) doubly distilled.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Jones, J.R.; Monk, C.B. *J. Chem. Soc.* <u>1963</u>, 2633-5.

VARIABLES:	PREPARED BY:
Temperature: 25-35°C	A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

Solubility of water in toluene

$t/°C$	10^4 mL(2)/mL(1)
25	4.0
30	4.8
35	5.9

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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) 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 quenching effects (due to solvent) on the scintillator.	(1) 'AnalaR' grade; repurified by conventional methods, ref 1. (2) not specified.

ESTIMATED ERROR:
soly. ± 5% to ± 1% (average deviation)

REFERENCES:
1. Vogel 'Practical Organic Chemistry', Longmans, Green and Co., London, 1956.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported
to be 0.0538 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compilers
is 1.05×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+%; used as received. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1.5 K soly. 0.0017 (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Hoegfeldt, E.; Bolander, B. *Ark. Kemi,* <u>1964</u>, *21*, 161-86.
VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in toluene was reported to be

0.026 mol(2) dm^{-3} sln.

The corresponding mass percent and mol fraction, x_2, calculated

by the compilers are 0.054 g(2)/100 g sln and 2.8 x 10^{-3}.

The assumption that 1 dm^3 sln = 862 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The water determination was carried out according to Johansson's modification of the Karl Fischer titration in ref 1, 2.	(1) Kebo; purity 99.0%; used as received. (2) not specified.

<table>
<tr><td></td><td>ESTIMATED ERROR:

temp. ± 0.3 K
soly. ± 0.001 mol(2) dm^{-3} sln
(type of error not specified)</td></tr>
<tr><td></td><td>REFERENCES:
1. Hardy, C.J.; Greenfield, B.F.; Scargill, D.
   J. Chem. Soc. <u>1961</u>, *90*.
2. Johansson, A.
   Sv. Papperstidn. <u>1947</u>, *11B*, 124.</td></tr>
</table>

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (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: Temperature: 0-50°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in toluene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
0	0.02704	1.382
10	0.0316	1.61
20	0.0460	2.35
30	0.0615	3.14
40	0.0750	3.82
50	0.0965	4.92

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Connolly, J.F. *J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

VARIABLES:	PREPARED BY:
Temperature: 280-310°C Pressure: 150-600 atm	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of toluene in water

t/°C	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
280	150	15	6.8	0.0141
	250	25.3	6.8	0.0141
	410	41.5	6.6	0.0136
	600	60.8	5.8	0.0119
300	170	17.2	14.2	0.0313
	250	25.3	14.1	0.0311
	300	30.4	14.0	0.0308
305	160	16.2	18.0	0.0411
	180	18.2	19.0	0.0438
	200	20.3	19.5	0.0452
	250	25.3	19.0	0.0438
	285	28.9	18.0	0.0411
310	145	14.7	18.0	0.0411
	150	15.2	19.6	0.0455
	155	15.7	21.7	0.0514
	165	16.7	23.9	0.0578
	170	17.2	26.7	0.0590
	175	17.7	29.6	0.0759
	180	18.2	33.1	0.0882
	180	18.2	36.3	0.1002
	270	27.3	50.5	0.1663
	265	26.9	48.6	0.1560

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected until either a cloud or a small droplet of a second phase appeared at the top of the cell. Then mercury was injected to change pressure, more (1) was injected and the measurement was repeated.	(1) Phillips reagent grade; better than 99.8 %; used as received. (2) distilled and deaerated.

ESTIMATED ERROR:
temp. ± 0.02 K pressure ± 2 atm.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3]	Connolly, J.F.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

Solubility of toluene in water

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
	260	26.3	46.5	0.1452
	260	26.3	44.3	0.1346
	260	26.3	41.9	0.1236
	260	26.3	39.2	0.1119
	260	26.3	36.3	0.1002
310	260	26.3	33.1	0.0882
	275	27.9	29.6	0.0759
	295	29.9	26.7	0.0665
	325	32.9	23.8	0.0575
	405	41.0	19.5	0.0452
	455	46.1	11.0	0.0411

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (3) Water; H_2O; [7732-18-5]	Johnson, J.R.; Christian, S.D.; Affsprung, H.E. *J. Chem. Soc. A.* <u>1966</u>, 77-8.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in toluene at 25°C was reported to be
0.0274 mol(2) dm^{-3} sln.
The corresponding mass percent and mole fraction, x_2, calculated
by the compilers are 0.0572 g(2)/100 g sln and 2.92 x 10^{-3}.
The assumption that 1 dm^3 sln = 862 g sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The apparatus described in ref 1 was used without modification. Samples were equilibrated in a constant-temperature water-bath maintained at 25 ± 0.1°C. Water solubilities were determined by using a Beckman Model KF-3 Aquameter.	(1) source not specified; certified or reagent grade; distilled through a 30-plate Oldershaw column. (2) not specified.

ESTIMATED ERROR:

temp. ± 0.1 K
soly. ± 0.0005 mol(2) dm^{-3} sln
(type of error not specified)

REFERENCES:

1. Christian, S.P.; Affsprung, H.E.;
   Johnson, J.R.; Worley, J.D.
   J. Chem. Educ. <u>1963</u>, *40*, 419.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported
to be 515 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0515 g(1)/100 g sln and 1.01×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 17 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Gregory, M.D.; Christian, S.D.; Affsprung, H.E. *J. Phys. Chem.* <u>1967</u>, *71*, 2283-9.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of water in toluene at 25°C was reported to be
0.0268 mol(2) dm^{-3} sln.

The corresponding mass percent and mole fraction, x_2, calculated
by the compilers are 0.0560 g(2)/100 g sln and 2.86 x 10^{-3}.

The assumption that 1 dm^3 sln = 863 g sln was used in the calculation.

AUXILIARY INFORMATION

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

A solution of (2) in (1) was ob-
tained using solute isopiestic
equilibrator described in ref 1.
Water concentration was determined
with a Beckman KF-3 aquameter by
the Karl Fischer analysis.
	(1) source not specified, reagent
	    grade; fractionally distilled
	    using a 30-plate Oldershaw,
	
	(2) not specified.

ESTIMATED ERROR:
temp. ± 0.05 K

REFERENCES:

1. Christian, S.D.; Affsprung,
    H.E.; Johnson, J.R.; Warley,
    J.D. *J. Chem. Educ.* <u>1963</u>,
    40, 419.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Benkovski, V.G.; Naruzov, M.H.; Bogoslovskaya, T.M. *Tr. Inst. Khim. Nefti Prir. Solei Akad. Nauk Kaz. SSR* <u>1970</u>, *2*, 25-32.
VARIABLES:	PREPARED BY:
One temperature: 303 K	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in toluene at 303 K was reported to be
0.0273 g(2)/100 g sln.

The corresponding mole fraction, x_2, value calculated by compiler
is 0.0739.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; purified; purity not specified. (2) distilled.
	ESTIMATED ERROR: Not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Glasoe, P.K.; Schultz, S.D. *J. Chem. Eng. Data*, <u>1972</u>, *17*, 66-8.

VARIABLES:	PREPARED BY:
Temperature: 15-30°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in toluene

$t/°C$	mol(2) dm^{-3} sln	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
15	0.0200 ± 0.0006	0.0413	2.11
25	0.0261 ± 0.0004	0.0545	2.78
30	0.0293 ± 0.0004	0.0615	3.14

The compilers calculations assume a solution density of 0.862 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Dried (1) was saturated with (2) by allowing it to stand in contact with (2) in a closed system, protected from atmospheric moisture. This two-phase system was kept in a pyrex storage bottle which was immersed in a constant temperature water bath. The concentration of (2) in (1) was determined by the Karl Fischer method.	(1) source not specified; reagent grade; purified by distillation and dried over molecular sieve, (2) distilled in a pyrex system.
	ESTIMATED ERROR:
	soly. as indicated above. (type of error not specified)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., <u>1972</u>, No. 21163, 113 p.
VARIABLES: Temperature: 278.16-318.46 K	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of toluene (2) in water (1)

$T/$ K	g(1)/100 g sln	$10^3 x_1$
278.16	0.06357 ± 0.0017	0.1243
283.06	0.06324 ± 0.0016	0.1236
293.06	0.06606 ± 0.0018	0.1292
298.16	0.06299 ± 0.0013	0.1232
308.26	0.06721 ± 0.0011	0.1314
318.46	0.06717 ± 0.0020	0.1313

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Fisher Scientific Co., Chromatoquality; 99+mole%; used as received. (2) laboratory distilled water.

ESTIMATED ERROR:
soly.: standard deviation from at least 15 measurements are given above.

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Bradley, R.S.; Dew, M.J.; Munro, D.C. *High Temp. High Press.* <u>1973</u>, *5*, 169-76.

VARIABLES:	PREPARED BY:
Temperature: 25-55°C Pressure: 1-1200 bar	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of toluene in water

t/°C	p/bar[b]	mol/L sln	g(1)/100g sln[a] (compiler)	$10^4 x_1$[a] (compiler)
25	1	0.00595	0.0547	1.07
45	1	0.00785	0.0722	1.41
55	1	0.0094	0.086	1.68
45	1000	0.0121	0.111	2.17
55	1000	0.0131	0.121	2.37

[a] Assuming a solution density of 1.00kg/L at all temperatures and pressures.

[b] 1 bar = 0.1 MPa exactly.

Data at other pressures are presented in graphical form. Data are also presented for the solubility of (1) in aqueous solutions of $AgNO_3$ and KNO_3 at various temperatures and pressures.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility of (1) in (2) at room temperature and pressure was determined in a stoppered 1mm silica cuvette placed in a Unicam SP500 spectrophotometer and stirred magnetically. Measurements were made until a constant concentration was reached. The value was cross-checked against a 2-L sample of saturated solution which had been equilibrated for some months.

Solubilities at higher temperatures and pressures were similarly determined in a special cell fitted into the spectrophotometer. Many details of the apparatus are given in the paper.

SOURCE AND PURITY OF MATERIALS:

(1) Not specified

(2) Distilled, air-free

ESTIMATED ERROR:
 Not specified

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C.-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of toluene in water

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
0(a)	724(c)	0.0724	1.42
25(b)	573(c)	0.0573	1.12

Solubility of water in toluene

$t/°C$	mg(2)/kg(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
0(a)	228(d)	0.0228	1.17
25(b)	543(e)	0.0543	2.77

[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) Matheson, Coleman and Bell, spectroquality grade reagent; shaken three times with distilled water.

(2) distilled.

ESTIMATED ERROR:

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

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Brown, R.L.; Wasik, S.P. *J. Res. Natl. Bur. Stds.* <u>1974</u>, *78*, 453-60.

VARIABLES:	PREPARED BY:
Temperature: 4.5-20.1°C (277.7-293.3 K)	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of toluene in water:

$t/°C$	$g(1)/100 \ g \ sln^a$	$10^4 \ x_1$ (compiler)
4.5	0.0612 ± 0.0010	1.20
6.3	0.0601 ± 0.0011	1.18
7.1	0.0586 ± 0.0018	1.15
9.0	0.0587 ± 0.0011	1.15
11.8	0.0573 ± 0.0014	1.12
12.1	0.0575 ± 0.0012	1.13
15.1	0.0569 ± 0.0013	1.11
17.9	0.0577 ± 0.0013	1.13
20.1	0.0566 ± 0.0011	1.11

[a] Errors given as standard deviations.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 cm³ 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.	(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:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Vodnye. Resursy.* <u>1975</u>, *2*, 170-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be
0.220 mg (1) cm^{-3} sln.

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.022 g(1)/100 g sln and 4.3×10^{-5}.

The compiler's calculations assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) described in ref (1). (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1 K

	REFERENCES:
	1. Krasnoshchekova, P.Ya.; Gubergritz, M.Ya. *Neftekhimiya* <u>1973</u>, *13*, 885.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* <u>1975</u>, *53*, 239-41.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be 0.5195 g(1) dm^{-3}.

The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 0.05195 g(1)/100 g sln and 1.015 x 10^{-4}.

The compiler's calculations assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined by gas chromatography. The gas chromatograph was Hewlett-Packard Model 5750 equipped with a hydrogen flame ionization detector. Many details are given in the paper.	(1) Phillips Petroleum Co.; research grade; 99.9+%; used as received. (2) not specified.
	ESTIMATED ERROR: temp. ± 0.1 K soly. ± 0.0096 g(1) dm^{-3}
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Sada, E.; Kito, S.; Ito, Y. *J. Chem. Eng. Data* 1975, *20*, 373-5.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be 0.5633 mL(1)/1000 mL(2).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Sudan IV was used to dye (1). The experimental apparatus and procedure used in this work were similar to those of Sobotka and Khan (ref 1). To make the measurements more accurate, the apparatus used consisted of a 1-liter dissolution flask and a 2-mL microburet. The scale was calibrated in advance by use of mercury. The dissolution flask was immersed in a water bath controlled thermostatically at 25°C. To avoid condensation of (1) from the gas phase, the temperature of gas phase in the dissolution flask was kept 1°C higher than that of the liquid phase. The dissolution flask and the microburet were connected tightly.

SOURCE AND PURITY OF MATERIALS:

(1) source not specified; reagent grade; used as received; purity not specified.

(2) pure.

ESTIMATED ERROR:

temp. ± 0.01 K
soly. less than 0.008 mL(1)/1000 mL sln (type of error not specified)

REFERENCES:

1. Sobotka, H.; Kahn, J. *J. Am. Chem. Soc.* 1948, *53*, 2935.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	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 toluene in water at 25°C was reported to be

534.8 mg(1)/kg(2). The corresponding mass percent and mole fraction,

x_1, calculated by the compilers are 0.05348 g(1)/100 g sln and

1.046×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chroma- tography.	(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 0.1 K soly. 4.9 mg(1)/kg(2) (the standard deviation of the mean for six replicates)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C and at system pressure
was reported to be 554.0 mg(1)/kg(2). The corresponding mass percent
and mole fraction, x_1, calculated by the compiler are 0.0554 g(1)/
100 g sln and 1.08×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.

ESTIMATED ERROR:
temp. ± 1 K soly. ± 15 mg(1)/kg(2)

REFERENCES:

HWW 2-BB

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. *87*:87654

VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of toluene in water at 20°C was reported to be
0.57 g(1)dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.057 g(1)/100 g sln and 1.11 x 10^{-4}.

The compiler's calculations assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. *Zh. Prikl. Khim.* <u>1978</u>, *51*, 957-8.

VARIABLES:	PREPARED BY:
Temperature: 25°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be
0.65 $g(1)dm^{-3}$ sln.

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.065 g(1)/100 g sln and 1.27×10^{-4}.

The compilers' calculations assume a solution density of 1.00 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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).	(1) not specified. (2) not specified.

ESTIMATED ERROR:
soly. ± 0.01 $g(1)dm^{-3}$ sln (standard deviation from 6 determinations).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported

to be 554.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated

by compiler are 0.0554 g(1)/100 g sln and 1.08×10^{-4}.

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:	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. 11.0 mg(1)/kg(2) (standard deviation from 7-9 determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Banerjee, S.; Yalkowsky, S.H.; Valvani, S.C. *Environ. Sci. Technol.* <u>1980</u>, *14*, 1227-9.
VARIABLES: One temperature: 25°C	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of toluene in water was reported to be 1.68×10^{-2} 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 0.155 g(1)/100 g sln and 3.04×10^{-4} respectively.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experiments were performed in sealed stainless steel centrifuge tubes. An excess of ^{14}C labelled toluene 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, and each analysis was also conducted in duplicate.

SOURCE AND PURITY OF MATERIALS:

(1) ^{14}C-labelled toluene: New England Nuclear, used without further purification.

(2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.2 K

Solubility: ±2.3% rel. (representing one std. dev.)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *Anal. Chem.* <u>1980</u>, *52*, 10-15.

VARIABLES:	PREPARED BY:
One temperature: 23.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of toluene in water at 23.5°C

g(1)/100 g sln	$10^4 x_1$ (compiler)
0.0670 ± 0.0015	1.31
0.0660 ± 0.0006	1.29

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa).	(1) 99.9% purity used without further purification (2) distilled
As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.	ESTIMATED ERROR: temp. ± 1.5°C soly. 1.5% (average std. dev.)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Rossi, S.S.; Thomas, W.H. *Env. Sci. Technol.* <u>1981</u>, *15*, 715-6.

VARIABLES:	PREPARED BY:
One temperature: 25°C (298 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of toluene in distilled water at 25°C was reported to be 506.7 µg/g, corresponding to a mole fraction, x_1, of 5.5 x 10^{-6}. The corresponding mass per cent calculated by the compiler is 0.0507 g(1)/ 100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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. Toluene was extracted (>99%) by passing known volumes through 0.6 x 6 cm columns of a superficially porous bonded C_{18} stationary-phase adsorbent and eluted with trichlorofluoromethane. Toluene levels in eluates were determined on a Hewlett-Packard Model 5840A gas chromatograph equipped with a flame ionisation detector and an electronic integrator using a $\frac{1}{8}$ in x 8 ft stainless-steel column of 10% TCEP on 10/120 Chromsorb or a WCOTSP-2100 glass column (0.25 mm x 30 m). Hydrocarbon concentrations in eluates were additionally determined by UC spectrophotometry.	(1) Burdick & Jackson; purified by triple distillation in glass. (2) Doubly distilled in all-glass apparatus; free of trace organics.
	ESTIMATED ERROR: Temperature: ±0.1°C Solubility: ±6.1 µg/g (std. dev. for 6 determinations).
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H. *Chem. Lett.* <u>1981</u>, 225-8.

VARIABLES:	PREPARED BY:
Temperature: 15-45°C	M.C. Haulait-Pirson and G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of toluene in water

$t/°C$	$g(1)/L$	$g(1)/100$ g sln[a]	$10^4 x_1$[a]
15	0.533 ± 0.017	0.0533	1.04
25	0.557 ± 0.007	0.0559	1.09
35	0.587 ± 0.015	0.0590	1.16
45	0.635 ± 0.019	0.0641	1.25

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	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 toluene in water

t /°C	10^3 mol(1)/dm^3 sln	g(1)/100 g sln (compiler)[a]	10^4 x_1 (compiler)[a]
15	5.58 ± 0.11	0.0514	1.01
25	5.71 ± 0.14	0.0526	1 03
35	5.88 ± 0.16	0.0545	1.07
45	6.28 ± 0.10	0.0584	1.14

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

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 99.0%, used without further purification. (2) Redistilled; no further details given.

Below the SOURCE AND PURITY section:

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) Toluene; C_7H_8; [108-88-3] (2) Water; H_2O; [7732-18-5]	Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. *Bull. Chem. Soc. Jpn.* <u>1984</u>, *57*, 1539-44.

VARIABLES:	PREPARED BY:
One Temperature: 25°C	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of toluene in water at 25°C was reported to be 5.65×10^{-3} mol(1)/dm^3 sln. Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of 0.0521 g(1)/100 g sln, $x_1 = 1.02 \times 10^{-4}$, calculated by the compiler.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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.* <u>1982</u>, *55*, 1054-62.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Deuterium oxide, (Heavy water); D_2O; [7789-20-0]	Guseva, A.N.; Parnov, E.I. *Radiokhimiya* <u>1963</u>, *5*, 507-9.

VARIABLES:	PREPARED BY:
Temperature: 87-203°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of toluene in Deuterium oxide

t/°C	$10^3 \, x_1$	g(1)/100 g sln (compiler)
87	0.682	0.313
123	1.81	0.828
164.5	4.22	1.91
203	7.51	3.37

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in ref 1.	(1) not specified. (2) distilled.

ESTIMATED ERROR:

Not specified.

REFERENCES:

1. Khazanova, P.E. *Tr. Gos. inst. azotn. promyshl.* <u>1954</u>, *4*, 5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Deuterium oxide, (heavy water); D_2O; [7789-20-0]	Glasoe, P.K.; Schultz, S.D. *J. Chem. Eng. Data,* <u>1972</u>, *17*, 66-8.

VARIABLES:	PREPARED BY:
Temperature: 15-30°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of deuterium oxide in toluene

$t/°C$	mol(2) dm^{-3} sln	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
15	0.0162	0.0372	1.71
25	0.0213	0.0504	2.31
30	0.0240	0.0560	2.57

The compilers calculations assume a solution density of 0.862 g/mL.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Dried (1) was saturated with (2) by allowing it to stand in contact with (2) in a closed system, protected from atmospheric moisture. This two-phase system was kept in a pyrex storage bottle which was immersed in a constant temperature water bath. The concentration of (2) in (1) was determined by the Karl Fischer method.	(1) source not specified; reagent grade; purified by distillation and dried over molecular sieve, (2) distilled in a pyrex system.
	ESTIMATED ERROR: soly ± 0.0004 mol(2) dm^{-3} sln (type of error not specified)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Toluene; C_7H_8; [108-88-3] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA December 1982

CRITICAL EVALUATION:

The solubility of toluene (1) in seawater (2) at 298 K has been reported
as follows:

Authors	Method	Salinity g salts/kg sln	10^2 g(1)/100 g sln
Mackay and Shiu (ref 2)	GLC	35.0	3.79
Sada et al. (ref 3)	Cloud Point	28.72	3.48
Sutton and Calder (ref 4)	GLC	34.5	3.793
Price (ref 5)	GLC	34.47	4.02
Rossi and Thomas (ref 6)	GLC	35	4.2

At 298 K and a salinity of 35 g salts/kg sln, the values of Mackay and Shiu,
Sutton and Calder, and Price are in very good agreement. Each group of
workers has also determined the solubility of toluene in pure water and
obtained results within experimental error of the value recommended in
this volume. Therefore, the mean of the reported values, 3.87 x 10^{-2} g(1)/
100 g sln, is accepted as the recommended value at the indicated temperature
and salinity. Mackay and Shiu measured solubility over a range of sali-
nities and reported their data in terms of the Setschenow equation. Their
values may be used to interpolate solubilities at other salinities up to
200 g salts/kg sln.

Brown et al. (ref 1) determined the solubility of toluene in seawater at
a salinity of 34.42 g salts/kg sln over the temperature range 273 to 293 K.
Linear extrapolation by the evaluator of these results to 298 K gives a
value of 3.80 x 10^{-2} g(1)/100 g sln. This suggests that the results of
Brown et al. may be consistent with the recommended value. The values
reported by Sada et al. and by Rossi and Thomas are in poorer agreement
with the remaining data.

<div align="center">

SOLUBILITY OF TOLUENE (1) IN SEAWATER (2)
RECOMMENDED VALUE

</div>

T/K	g salts/kg sln	g(1)/100 g sln
298	35	3.87 x 10^{-2}

REFERENCES
1. Brown, R.L.; Wasik, S.P. J. Res. Natl. Bur. Stds. A 1974, 78, 453-60.
2. Mackay, D.; Shiu, W.Y. Can. J. Chem. Eng. 1975, 53, 239-42.
3. Sada, E.; Kito, S.; Ito, Y. J. Chem. Eng. Data 1975, 20, 373-5.
4. Sutton, C.; Calder, J.A. J. Chem. Eng. Data 1975, 20, 320-2.
5. Price, L.C. Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.
6. Rossi, S.S.; Thomas. W.H. Environ. Sci. Technol. 1981, 15, 715-6.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Artificial seawater	Brown, R.L.; Wasik, S.P. *J. Res. Natl. Bur. Stds. A.* <u>1974</u>, *78*, 453-60.
VARIABLES:	PREPARED BY:
Temperature: 0-20°C Salinity: 34.42 g salts/kg sln	G.T. Hefter and D.G. Shaw

EXPERIMENTAL VALUES:

Solubility of toluene in artificial seawater

$t/°C$	g(1)/100 g sln[a]	$10^5 x_1$ (compiler)
0.19	0.0449 (0.0006)	9.0
5.32	0.0429 (0.0007)	8.60
10.05	0.0416 (0.0008)	8.34
14.96	0.0405 (0.0008)	8.12
20.04	0.0397 (0.0008)	7.96

[a] numbers in parentheses are standard deviations from 4 observations

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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 cm³ 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.	(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) Toluene; C_7H_8; [108-88-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Mackay, D.; Shiu, W.Y. *Can. J. Chem. Eng.* 1975, *53*, 239-42.
VARIABLES: One temperature: 25°C Salinity: 0-200 g(2)/kg sln	PREPARED BY: M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

The solubility of toluene in solutions of sodium chloride is reported in terms of the Setschenow equation:

$$\log(S_0/S) = K_s C_s$$

where, S_0 is the solubility of toluene in water (mg/L)

S is the solubility of toluene in solution (mg/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_2 0-4 mol/L, K_s = 0.2052 ± 0.0056 (standard error) with S_0 = 519.5 ± 9.6.

The corresponding mass percent and mole fraction, x_1, at salinity = 35 g(2)/kg sln calculated by the compilers are 3.79 x 10^{-2} g(10)/100 g sln and 7.743 x 10^{-5} assuming a density of 1.025 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Solubility was determined by vapor phase extraction and gas chromatographic analysis. This method does not require the preparation of saturated solutions and thus avoids one of the major sources of error of other methods.	(1) research grade, 99.9+%, from Phillips Petroleum Co. (2) and (3) not specified.
	ESTIMATED ERROR: Temp. ±0.1 K Soly. 95% confidence limit is about 8%
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:

(1) Toluene; C_7H_8; [108-88-3]
 	
(2) Sodium chloride; NaCl;
    [7647-14-5]
 	
(3) Water; H_2O; [7732-18-5]
	Sada, E.; Kito, S.; Ito, Y.
	
	J. Chem. Eng. Data <u>1975</u>, *20*
	    373-5.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 29 - 108 g(3)/kg sln	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of toluene in aqueous sodium chloride solutions

mol(2)/L	g(2)/kg sln[a]	L (1)/10^3 L sln	Mass%(1)[a]	$10^5 x_1$[a]
0.5011	28.72	0.410	0.0348	6.95
0.9991	56.14	0.298	0.0248	5.06
1.4933	82.66	0.223	0.0182	3.76
1.9933	107.9	0.169	0.0136	2.87

[a] calculated by compilers using density and other physical data for NaCl solutions from ref 1 and the assumption that the density of (1) is 0.8669 kg/L.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Experimental apparatus and procedure used similar to those in ref 2. Toluene stained with 0.1% by weight Sudan IV was added dropwise from a microburet into aqueous salt solution retained in a 1-L dissolution flask which was kept at 25.00° ± 0.01°C in a thermostatically controlled water bath. The aqueous salt solution was violently stirred by a magnetic stirring device.	(1),(2): reagent grade, source not specified. (3): not specified.

Before saturation was reached, the Sudan IV was precipitated and floated on the surface as a solid. At saturation, the excess toluene appeared as immiscible red liquid droplets suspended in the aqueous solution. To ensure complete saturation, 24 hr was allowed for equilibration.	ESTIMATED ERROR: Soly 0.008 x 10^{-3} L (1)/L sln.
	REFERENCES: 1. Weast, R.C. CRC Handbook of Chemistry and Physics, 59th Ed. <u>1978</u>, CRC Press, pp D299 - D300. 2. Sobotka, H.; Kahn, J. *J. Am. Chem. Soc.* <u>1948</u>, *53*, 2935.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (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 toluene in artificial seawater is reported to be

379.3 mg(1)/kg sln. The corresponding mass percent and mole fraction,

x_1 calculated by the compiler are 0.03793 g(1)/100 g sln and 7.61×10^{-5}

assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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 K soly. 2.8 (std. dev.)

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Sodium chloride; NaCl; [7647-14-5] (3) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 1-360 g(2)/kg sln	M. Kleinschmidt and D. Shaw

EXPERIMENTAL VALUES:

Solubility of Toluene in Aqueous NaCl

Salinity g(2)/kg sln	Mass Percent g(1)/100 g sln	Mole fraction, $10^5 x_1$ (compilers)
1.002	0.0526	10.3
10.000	0.0490	9.65
34.472[a]	0.0402	8.04
50.030	0.0359	7.26
125.100	0.0182	3.85
199.900	0.0106	2.34
279.800	0.00538	1.24
358.700	0.00372	0.890

[a]Artificial seawater, composition not specified but probably
similar to ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Details given in source. (1) was equilibrated with NaCl solution for one month. An aliquot was analyzed directly by gas chromatography.	(1) commercial, 99 + % pure
	ESTIMATED ERROR: Temperature ± 1 K Solubility ± 10 relative %
	REFERENCES: 1. Lyman, J.; Fleming, R.H.; *J. Mar. Res.* <u>1940</u>, *3*, 135.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Toluene; C_7H_8; [108-88-3] (2) Seawater; natural; H_2O	Rossi, S.S.; Thomas, W.H. *Environ. Sci. Technol.* <u>1981</u>, *15*, 715-6.

VARIABLES:	PREPARED BY:
Temperature: 15 - 25°C Salinity: 35 g/kg sln	W.Y. Shiu, D. Mackay

EXPERIMENTAL VALUES:

Solubility of toluene in seawater

t/°C	μg(1)/g sln	Mass percent g(1)/100 g sln	Mole fraction $10^5 x_1$
15	410	0.041	8.2
20	410	0.041	8.2
25	418.5	0.042	8.4

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solution was prepared by equilibrating seawater with an excess of hydrocarbon for 24 hrs. in a constant temperature gyrotary shaker followed by 12 hrs. 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.	toluene: from Burdick and Jackson, triple distilled in glass. 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°/₀₀.

ESTIMATED ERROR:

  temp. ± 0.1 K

  soly. ± 2%

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,5-Norbornadiene; C_7H_8; [121-46-0] (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: 20-50°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in 2,5-norbornadiene

$t/°C$	g(2)/100g sln	$10^3 x_2$ (compiler)
20	0.0295	1.51
30	0.0383	1.96
50	0.0675	3.44

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia November 1984.

CRITICAL EVALUATION:

Quantitative solubility data for the system 1,3,5-cycloheptatriene (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of
1,3,5-Cycloheptatriene (1) in Water (2)

Reference	T/K	Solubility	Method
Englin *et al.* (ref 1)	293-323	(2) in (1)	analytical
McAuliffe (ref 2)	298	(1) in (2)	GLC
Pierotti and Liabastre (ref 3)	278-318	(1) in (2)	GLC

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.   THE SOLUBILITY OF 1,3,5-CYCLOHEPTATRIENE (1) IN WATER (2)

Solubility values of (1) in (2) are listed in Table 2 and plotted in Figure 1. The data at 298 K are in reasonable agreement. However, it should be noted that the results of Pierotti and Liabastre (ref 2) are generally higher than "Recommended" values in well characterised systems (e.g. benzene in water). Their results at temperatures other than 298 K should be regarded with some caution.

TABLE 2: Tentative Values for the Solubility
of 1,3,5-Cycloheptatriene (1) in Water (2)

T/K	Reported values[a] 10^2 g(1)/100 g sln	"Best" values ($\pm \sigma_n$)[b] 10^2 g(1)/100 g sln	$10^3 x_1$
278	5.80* (ref 3)	5.8	1.1
288	6.64* (ref 3)	6.6	1.3
298	6.20 (ref 2), 6.69* (ref 3)	6.4 ± 0.2	1.25
308	7.40* (ref 3)	7.4	1.4
318	7.63* (ref 3)	7.6	1.5

a Values marked with an asterisk (*) obtained by the Evaluator by graphical intrapolation of original data.

b "Best" values obtained by averaging where appropriate; σ_n has no statistical significance.

(continued next page)

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COMPONENTS:	EVALUATOR:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (2) Water; H_2O; [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. November 1984.

CRITICAL EVALUATION: (continued)

FIGURE 1. Solubility of 1,3,5-cycloheptatriene (1) in water:
ref 2 (x); ref 3 (o).

2.   THE SOLUBILITY OF WATER (2) IN 1,3,5-CYCLOHEPTATRIENE (1)

The solubility of water in 1,3,5-cycloheptatriene has been reported only by
Englin *et al*. (ref 1) and so no Critical Evaluation can be made. The
interested user is referred to the appropriate Data Sheet for solubility
values. However, it should be noted that the data of Englin *et al*. are
generally reliable at lower temperatures but are high when $T > 300$ K.

REFERENCES

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

2.   McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

3.   Pierotti, R.A.; Liabastre, A.A. *Structure and properties of water
      solutions*, U.S. Nat. Tech. Inform. Serv., PB Rep. <u>1972</u>, No.21163,
      113 pp.

ACKNOWLEDGEMENT

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (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: Temperature: 30-50°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in 1,3,5-cycloheptatriene

$t/°C$	g(2)/100 g sln	$10^3 \, x_2$ (compiler)
30	0.0630	3.21
40	0.0773	3.94
50	0.0993	5.06

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (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 1,3,5-cycloheptatriene in water at 25°C was reported to be 620 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0620 g(1)/100 g sln and 1.21×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 20 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3,5-Cycloheptatriene; C_7H_8; [544-25-2] (2) Water; H_2O; [7732-18-5]	Pierotti, R.A.; Liabastre, A.A. "Structure and properties of water solutions." U.S. Nat. Tech. Inform. Serv., PB Rep., 1972, No. 21163, 113 p.
VARIABLES: Temperature: 278.26-318.36 K	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 1,3,5-cycloheptatriene in water

$T/$ K	g(1)/100 g sln	$10^3 x_1$
278.26	0.05809 ± 0.0014	0.1136
288.36	0.06645 ± 0.0017	0.1299
298.26	0.06694 ± 0.0019	0.1309
308.36	0.07418 ± 0.0019	0.1450
318.36	0.07648 ± 0.0022	0.1495

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
10 mL of (2) were placed along with 4-10 drops of (1) in 10 mL serum bottles, which were then tightly capped, and placed in the rotating basket and rotated for 24 hours. The bottles were then hand shaken to remove (1) droplets from the stoppers and then replaced in the bath with the tops down for an additional 24 hours. The solute concentrations were determined by use of a flame-ionization gas chromatograph. Many details about equipment, operating conditions and calculation are given in the paper.	(1) Columbia Organic Chemicals Co., Inc.; Tech 83%; used as received. (2) laboratory distilled water.
	ESTIMATED ERROR: soly.: standard deviation from at least 15 measurements are given above.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,6-Heptadiyne; C_7H_8; [2396-63-6] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,6-heptadiyne in water at 25°C was reported
to be 1650 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.1650 g(1)/100 g sln and 3.23×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 25 g(1)/10^6 g(2)
           (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Methylcyclohexene; C_7H_{12}; [591-49-1] (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-methylcyclohexene in water at 25°C was reported to be 52 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0052 g(1)/100 g sln and 9.7 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.

ESTIMATED ERROR:
temp. ± 1.5 K soly. 52 g(1)/10^6 g(2) (standard deviation of mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cycloheptene; C_7H_{12}; [628-92-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
VARIABLES: One temperature: 25°C	PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of cycloheptene in water at 25°C was reported
to be 66 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0066 g(1)/100 g sln and 1.2×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 4 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,6-Heptadiene; C_7H_{12}; [3070-53-9] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1,6-heptadiene in water at 25°C was reported to be 44 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated by the compilers are 0.0044 g(1)/100 g sln and 8.2×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 3 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptyne; C_7H_{12}; [628-71-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 1-heptyne in water at 25°C was reported
to be 94 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0094 g(1)/100 g sln and 1.76×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 3 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylcyclopentane; C_7H_{14}; [1640-89-7] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1964</u>, *19*, 77-8.
VARIABLES: Temperature: 70.5-203°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of ethylcyclopentane in water

$t/°C$	g(1)/100 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
70.5	0.0219	0.0219	0.40
113	0.0525	0.0525	0.96
168.5	0.224	0.224	4.10
203	0.759	0.759	13.89

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylcyclopentane; C_7H_{14}; [1640-89-7] (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 ethylcyclopentane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.0071	3.87
20	0.0119	6.49
30	0.0186	10.14

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.

ESTIMATED ERROR:
not specified.

REFERENCES:

COMPONENTS:	EVALUATOR:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (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. November 1984

CRITICAL EVALUATION:

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

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

Reference	T/K	Solubility	Method
Guseva and Parnov (ref 1)	341-488	(1) in (2)	synthetic?
Englin et al. (ref 2)	283-303	(2) in (1)	analytical
McAuliffe (ref 3)	298	(1) in (2)	GLC
Price (ref 4)	298-423	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 5)	298	(1) in (2)	GLC
Rudakov and Lutsyk (ref 6)	298	(1) in (2)	partition coefficient

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

At 298K the various solubility values (ref 3, 4, 6) are in good agreement (Table 2). The datum of Krzyzanowska and Szeliga (ref 5) has been excluded from consideration because it does not appear to be independent of that of Price (ref 4).

At other temperatures the values of Guseva and Parnov (ref 1), probably obtained in sealed tubes at unspecified pressures, are almost an order of magnitude larger than those of Price (ref 4) and are thus rejected. All other data are listed in Table 2 and plotted in Figure 1.

Roof (ref 7) has reported a critical end point at 572.2K and 3.47 MPa.

COMPONENTS:	EVALUATOR:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (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. November 1984

CRITICAL EVALUATION: (continued)

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

T/K	Solubility values		
	Reported values[a] 10^3 g(1)/100g sln	"Best" values (± σ_n) 10^3 g(1)/100g sln	$10^6 x_1$
298	1.4 (ref 3), 1.60 (ref 4), 1.53 (ref 6)	1.51 ± 0.08 (R)	2.94 (R)
303	1.7* (ref 4)	1.7	3.1
313	1.8* (ref 4)	1.8	3.3
323	1.9* (ref 4)	1.9	3.5
343	2.2* (ref 4)	2.2	4.0
363	2.9* (ref 4)	2.9	5.3
383	5.2* (ref 4)	5.2	9.6
403	18.8* (ref 4)	11	20
423	24.5* (ref 4)	25	46

a Values marked with an asterisk (*) have been obtained by the Evaluators by graphical interpolation of the original data.
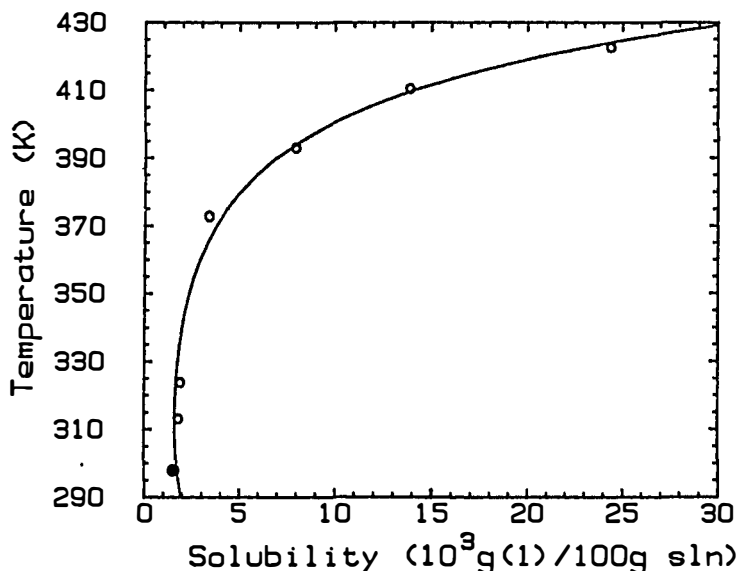
FIGURE 1. Solubility of methylcyclohexane in water : ref 4 (o); average of ref 3, 4 & 6 (●).

COMPONENTS:	EVALUATOR:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (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. November 1984

CRITICAL EVALUATION: (continued)

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

The solubility of water in methylcyclohexane has been reported only by Englin *et al.* (ref 2) and so no critical evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it should be noted that the data of Englin *et al.* are generally reliable at lower temperatures but are high when $T > 300K$.

REFERENCES

1.   Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* __1964__, *19*, 77-8.

2.   Englin, B.A.; Plate, A.F.; Tugolikov, V.M.; Pryanishnikova, M.A. *Khim. Tekhnol. Topl. Masel* __1965__, *10*, 42-6.

3.   McAuliffe, C. *J. Phys. Chem.* __1966__, *70*, 1267-75.

4.   Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* __1976__, *60*, 213-44.

5.   Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* __1978__, *34*, 413-7.

6.   Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* __1979__, *53*, 1298-1300.

7.   Roof, J.G.; *J. Chem. Eng. Data* __1970__, *15*, 301-3.

ACKNOWLEDGEMENT

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Vestn. Mosk. Univ. Khim.* <u>1964</u>, *19*, 77-8.

VARIABLES:	PREPARED BY:
Temperature: 68-215°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of methylcyclohexane in water

$t/°C$	g(1)/100 g(2)	g(1)/100 g sln (compiler)	$10^4 x_1$ (compiler)
68	0.011	0.011	0.20
120.5	0.0363	0.0363	0.67
157.5	0.0933	0.0933	1.71
215	0.759	0.759	13.90

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Presumably the measurements were made in sealed glass tubes, as reported in ref 1. No more details were reported in the paper.	(1) not specified. (2) not specified.

ESTIMATED ERROR:

not specified.

REFERENCES:
1. Guseva, A.N.; Parnov, E.I.
    Vestn. Mosk. Univ. Khim. <u>1963</u>,
    18, 76.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (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 methylcyclohexane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.0061	3.33
20	0.0116	6.32
30	0.0179	9.75

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.

	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of methylcyclohexane in water at 25°C was reported to be 14 mg (1)/kg sln (0.0014 g(1)/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 2.6×10^{-6}.

The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1.5 K soly. 1.2 mg (1)/kg sln (standard deviation from mean)

	REFERENCES:
	1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
Temperature: 25-149.5°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of methylcyclohexane in water at system pressure

$t/°C$	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	16.0 ± 0.2	0.00160	2.9
40.1	18.0 ± 0.6	0.00180	3.3
55.7	18.9 ± 0.5	0.00189	3.5
99.1	33.8 ± 1.0	0.00338	6.2
120.0	79.5 ± 2.2	0.00795	14.6
137.3	139.0 ± 8.0	0.01390	25.5
149.5	244.0 ± 10.0	0.02440	44.8

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

ESTIMATED ERROR:

temp. ± 1 K
soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of methylcyclohexane in water at 25°C was reported
to be 16.0 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 0.0016 g(1)/100 g sln and 2.93 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:	SOURCE AND PURITY OF MATERIALS:
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 mea-sured 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 solu-tions of heptane in (2) were used as standard solutions.	(1) not specified. (2) not specified.
	ESTIMATED ERROR:
	soly. 0.5 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Methylcyclohexane; C_7H_{14}; [108-87-2] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of methylcyclohexane between the gas and aqueous phase. α = 16 ± 1. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 46.33$ mm of Hg and $\log C_g = \log p - 4.269$ = -2.60 expressed in moles per liter. Therefore $C_s = 1.56 \times 10^{-4}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.0015 g(1)/100 g sln and the corresponding mole fraction, x_1, is 2.7×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.	(1) not specified. (2) not specified. **ESTIMATED ERROR:** soly. ± 10% (estimated by the compiler) **REFERENCES:** 1. Hine, J.; Mooker, P.K. *J. Org.* *Chem.* <u>1975</u>, *4*, 292.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Cycloheptane; C_7H_{14}; [291-64-5]	McAuliffe, C.
(2) Water; H_2O; [7732-18-5]	*J. Phys. Chem.* 1966, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of cycloheptane in water at 25°C was reported to be 30 mg (1)/kg sln (0.0030 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 5.5 x 10^{-6}.
The same value is also reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.

ESTIMATED ERROR:

temp. ± 1.5 K
soly. 1.0 mg (1)/kg sln (standard
         deviation from mean)

REFERENCES:

1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	EVALUATOR:
(1) 1-Heptene; C_7H_{14}; [592-76-7] (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 data for the solubility of water (2) in 1-heptene (1) have been reported in the publications listed in Table 1.

TABLE 1:   Quantative Solubility Studies of Water (2) in 1-Heptene (1)

Reference	T/K	Method
Black *et al.* (ref 1)	283-294	radiotracer
Englin *et al.* (ref 2)	283-303	analytical

The solubility of 1-heptene in dilute aqueous HNO_3 solutions have also been reported (ref 3). However, as no other data are available for comparison these values will not be considered in this Evaluation. The interested user is referred to the relevant Data Sheet immediately following this Critical Evaluation.

The reported values (ref 1 and 2) for the solubility of water in 1-heptene are listed in Table 2.

The data are in very poor agreement. In the absence of confirmatory studies selection of best values is difficult. However, it may be noted that in well characterized systems (e.g., water in benzene) the results of Englin *et al.* at $T < 300K$ are generally reliable whilst those of Black *et al.* generally differ markedly from Recommended values. Thus, values of Englin *et al.* (ref 2) have been selected as the "Best" values available although, in the absence of confirmatory studies, it is not possible at this stage to reject outright the data of Black *et al.* (ref 1).

COMPONENTS:	EVALUATOR:
(1) 1-Heptene; C_7H_{14}; [592-76-7] (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 Water (2) in 1-Heptene (1)

T/K	Solubility Values		
	Reported values $10^2 g(2)/100g$ sln	"Best" values[a] $10^2 g(2)/100g$ sln	$10^3 x_2$
283	6.92 (ref 1), 1.86 (ref 2)	1.9	1.0
293	11.2 (ref 1), 2.49 (ref 2)	2.5	1.4
298	3.2^b (ref 2)	3.2	1.7
303	3.75 (ref 2)	3.8	2.0

[a]Rounded values of Englin *et al.* (ref 2); see text.

[b]Obtained by the Evaluator by graphical interpolation.

REFERENCES

1. Black, C.; Joris, G.G.; Taylor, H.S.   *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.

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

3. Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data.* <u>1972</u>, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptene; C_7H_{14}; [592-76-7] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.

VARIABLES:	PREPARED BY:
Temperature: 10 - 21.2°C	A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in 1-heptene

$t/°C$	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^3 x_2$ (compiler)
10.0	0.0692	0.0692	3.76
20.1	0.1126	0.1126	6.11
20.5	0.1047	0.1047	5.68
21.2	0.1158	0.1158	6.28

(at total saturation pressure of 1 atm)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Air saturated with radioactive water vapor was bubbled through (1) until saturation was attained. Dissolved water was separated from (1) by absorption on calcium oxide. The tritium was transferred into the counter by equilibration with ethanol vapor. The method is described in ref (1).	(1) Havard University; purity not specified; used as received. (2) not specified.

ESTIMATED ERROR:
soly. ± 1% (type or error not specified)

REFERENCES:
1. Joris, G.G.; Taylor, H.S.   *J. Chem. Phys.* <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptene; C_7H_{14}; [592-76-7] (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: Temperature: 10-30°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in 1-heptene

$t/°C$	g(2)/100 g sln	$10^3 x_2$ (compiler)
10	0.0186	1.01
20	0.0249	1.36
30	0.0375	2.04

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1-Heptene; C_7H_{14}; [592-76-7] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9

VARIABLES:	PREPARED BY:
Temperature: 20-30°C	M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of 1-heptene in 0.001 mol L^{-1} HNO_3 solution

$t/°C$	10^4 mol L^{-1} sln^a	10^3 g(1)/100 g sln^b (compiler)	10^6 x_1 (compiler)
20	3.16 ± 0.13	3.1	5.7
25	2.81 ± 0.12	2.8	5.1
30	2.45 ± 0.15	2.4	4.4

a Uncertainties stated to be "standard deviations from means".
b Assuming a solution density of 1.00 g mL^{-1} at all temperatures.

<u>Compiler's note</u>: 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^{-1} HCℓ .

AUXILIARY INFORMATION	

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Matheson, Coleman and Bell; 99%. (2) Not specified.

	ESTIMATED ERROR: Temp. ± 0.05 K Soly. see table above.
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2-Heptene; C_7H_{14}; [592-77-8]	G.T. Hefter
	School of Mathematical and Physical
(2) Water; H_2O; [7732-18-5]	Sciences, Murdoch University,
	Perth, Australia.
	July 1985

CRITICAL EVALUATION:

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

TABLE 1:   Quantitative Solubility Studies of
2-Heptene (1) in Water (2)

| Reference | T/K | Method | Solubility values[a] | |
			10^3g(1)/100g sln	$10^6 x_1$
McAuliffe (ref 1)	298	GLC	15 (R)	2.7 (R)
Schwarz (ref 2)	297	chromatographic	15 (R)	2.7 (R)

[a] (R) - Recommended value

The agreement between the two studies is excellent and although the measurement temperatures differ slightly this effect should be minor. The values in Table 1 are therefore Recommended.

Solubility values of 2-heptene in various salt solutions have also been reported (ref 3) but, although in broad agreement with the values given in Table 1 will not be considered in this Evaluation. No data are available for the solubility of water in 2-heptene.

REFERENCES

1. McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.
2. Schwarz, F.P. *Anal. Chem.* <u>1980</u>, *52*, 10-15.
3. Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Heptene; C_7H_{14}; [592-77-8] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of 2-heptene in water at 25°C was reported
to be 15 g(1)/10^6 g(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compilers are 0.0015 g(1)/100 g sln and 2.7 x 10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum or Columbia Chemical; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 1.4 g(1)/10^6 g(2) (standard deviation of mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Heptene; C_7H_{14}; [592-77-8] (2) Water; H_2O; [7732-18-5]	Schwarz, F.P. *Anal. Chem.* __1980__, *52*, 10-15.
VARIABLES: One temperature: 23.5°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2-heptene in water at 23.5°C was reported to be
0.00150 ± 0.00003 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler
is 2.75×10^{-6}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
An elution chromatography method was used where (1) was the stationary phase and (2) the mobile phase. A transparent column was packed with an inert support (chromosorb P) coated with a known amount of the liquid solute (1). This solute column was connected to a water reservoir (connected to a compressed gas regulator). Water was forced through the column by the pressure of the compressed gas (ca. 14 kPa). As the total volume of water flowing through the column increased, a solute depleted zone, different in color from the stationary phase, developed and increased in length. The solubility is calculated from the amount of solute removed from the column, i.e. length of the solute depleted zone, and the volume of water passed through the column. Many details about preparation of the solute column and calculation are given in the paper.	(1) 99% purity used without further purification (2) distilled
	ESTIMATED ERROR: temp. ± 1.5°C soly. 2% (average std. dev.)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Heptene; C_7H_{14}; [592-77-8] (2) Water; H_2O; [7732-18-5]	Natarajan, G.S.; Venkatachalam, K.A. *J. Chem. Eng. Data* <u>1972</u>, *17*, 328-9
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson, G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of 2-heptene in water was reported to be 2.716×10^{-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, 0.00266 g(1)/100 g sln and 4.89×10^{-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:	SOURCE AND PURITY OF MATERIALS:
15 mL of the aqueous medium was equilibrated with 1 mL of (1) by mechanical shaking in a thermostated 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.	(1) Prepared by dehydration of 2-heptanol and then washed, dried and fractionated. Purity (no specification) was determined by chromatography. (2) Not specified
	ESTIMATED ERROR: Temp. ± 0.05 K Soly. not specified
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2,3-Trimethylbutane; C_7H_{16}; [464-06-2] (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: 0-50°C	A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in 2,2,3-trimethylbutane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0027	1.50
10	0.0057	3.17
20	0.0106	8.90
30	0.0184	10.23
40	0.0315	17.51
50	0.0507	28.15

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylpentane; C_7H_{16}; [590-35-2] (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 2,2-dimethylpentane in water at 25°C and at system pressure was reported to be 4.40 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.4×10^{-4} g(1)/100 g sln and 7.9×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 cHewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.11 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,2-Dimethylpentane; C_7H_{16}; [590-35-2] (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 2,2-dimethylpentane in water at 25°C was reported
to be 4.40 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 4.4×10^{-4} g(1)/100 g sln and 7.9×10^{-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:
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. 0.13 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylpentane; C_7H_{16}; [565-59-3] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3-dimethylpentane in water at 25°C and at system pressure was reported to be 5.25 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 5.25 x 10^{-4} g(1)/100 g sln and 9.43 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.02 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,3-Dimethylpentane; C_7H_{16}; [565-59-3] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,3-dimethylpentane in water at 25°C was reported to be 5.25 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 5.25 x 10^{-4} g(1)/100 g sln and 9.43 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:
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. 0.16 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (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 November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 2,4-dimethylpentane (1) and water (2) are reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies for
the 2,4-Dimethylpentane (1) - Water (2) System

Reference	T/K	Solubility	Method
McAuliffe (ref 1)	298	(1) in (2)	GLC
McAuliffe (ref 2)	298	(1) in (2)	GLC
Polak and Lu (ref 3)	273,298	mutual	GLC, Karl Fischer
Price (ref 4)	298	(1) in (2)	GLC
Krzyzanowska and Szeliga (ref 5)	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 2,4-DIMETHYLPENTANE (1) IN WATER (2)

Solubility data for 2,4-dimethylpentane in water (ref 2,4) are listed in Table 2 with the following exceptions. The datum of Krzyzanowska and Szeliga (ref 5) has been excluded because it does not appear to be independent of that of Price (ref 4). The earlier datum of McAuliffe (ref 1) is presumably superceded by his later determination (ref 2) and has also been excluded.

The 298K datum of Polak and Lu (ref 3) is considerably higher (ca. 25% relative) than other reported values (ref 2,4). Furthermore, the increase in solubility between 298 and 273K, as for other hydrocarbons investigated by these authors, is unusually large. The data of Polak and Lu (ref 3) are therefore rejected.

COMPONENTS:	EVALUATOR:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (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 November 1984

CRITICAL EVALUATION: (continued)

TABLE 2: Recommended (R) Value of the Solubility of 2,4-Dimethylpentane (1) in Water (2)

T/K	Solubility values		
	Reported values 10^4g(1)/100g sln	"Best" values ($\pm \sigma_n$)^a 10^4g(1)/100g sln	$10^7 x_1$
298	4.06 (ref 2), 4.4 (ref 4)	4.2 ± 0.2 (R)	7.6 (R)

"Best" values obtained by averaging; σ_n has no statistical significance.

2.   THE SOLUBILITY OF WATER (2) IN 2,4-DIMETHYLPENTANE (1)

The solubility of water in 2,4-dimethylpentane has been reported only by Polak and Lu (ref 3) and thus no critical evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it can be noted that the data of Polak and Lu are generally close to "Recommended" values in well characterized systems.

REFERENCES

1.   McAuliffe, C. *Nature*   *1963*, *200*, 1092-3.

2.   McAuliffe, C. *J. Phys. Chem.* *1966*, *70*, 1267-75.

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

4.   Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* *1976*, *60*, 213-44.

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1093-3.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,4-dimethylpentane in water at 25°C was reported
to be 3.62 mg (1)/kg sln (0.00362 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is
6.5×10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
20-50 mL of (1) was added to (2) and vigorously shaken or stirred several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbon-saturated water was directly injected into the gas chromatograph fitted with a suitable fractionator to absorb water. A hydrogen-flame ionization detector was used.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.

ESTIMATED ERROR:
temp. ± 1.5 K   soly. 0.10 mg (1)/kg sln (standard deviation from mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* 1966, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,4-dimethylpentane in water at 25°C was reported to be 4.06 mg (1)/kg sln (0.00406 g(1)/100 g sln).

The corresponding mole fraction, x_1, calculated by the compiler, is 7.3×10^{-7}.

The same value is also reported in ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 0.29 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* 1964, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 2,4-dimethylpentane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	6.50^c	1.17×10^{-6}
25^b	5.50^c	9.88×10^{-7}

Solubility of water in 2,4-dimethylpentane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	31^d	1.73×10^{-4}
25^b	81^e	4.51×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

ESTIMATED ERROR:
temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 1.7%; d) ± 4.7%;   e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane; C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,4-dimethylpentane in water at 25°C and at system pressure was reported to be 4.41 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 4.41 x 10^{-4} g(1)/100 g sln and 7.92 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.05 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2,4-Dimethylpentane, C_7H_{16}; [108-08-7] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2,4-dimethylpentane in water at 25°C was reported to be 4.41 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 4.41×10^{-4} g(1)/100 g sln and 7.92×10^{-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:	SOURCE AND PURITY OF MATERIALS:
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. 0.14 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3,3-Dimethylpentane; C_7H_{16}; [562-49-2] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.

VARIABLES:	PREPARED BY:
Temperature: 25-150.4°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of 3,3-dimethylpentane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^6 x_1$ (compiler)
25.0	5.92 ± 0.06	0.000592	1.06
40.1	6.78 ± 0.20	0.000678	1.22
55.7	8.17 ± 0.46	0.000817	1.47
69.7	10.3 ± 0.7	0.00103	1.85
99.1	15.8 ± 0.7	0.00158	2.84
118.0	27.3 ± 0.4	0.00273	4.91
140.4	67.3 ± 1.7	0.00673	12.10
150.4	86.1 ± 1.8	0.00861	15.48

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

	ESTIMATED ERROR:
	temp. ± 1 K soly. range of values given above

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3,3-Dimethylpentane; C_7H_{16}; [562-49-2] (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 3,3-dimethylpentane in water at 25°C was reported to be 5.94 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 5.94×10^{-4} g(1)/100 g sln and 1.07×10^{-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). Consequently, this system has not been evaluated.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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. 0.18 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylhexane; C_7H_{16}; [591-76-4] (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-methylhexane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
10	0.0056	3.12
20	0.0103	5.73
30	0.0182	10.12

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylhexane; C_7H_{16}; [591-76-4] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 2-methylhexane in water at 25°C and at system pressure was reported to be 2.54 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.54 x 10^{-4} g(1)/100 g sln and 4.57 x 10^{-7}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.02 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 2-Methylhexane; C_7H_{16}; [591-76-4] (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 2-methylhexane in water at 25°C was reported
to be 2.54 mg(1)/kg(2).
The corresponding mass percent and mole fraction, x_1, calculated
by compiler are 2.54 x 10^{-4} g(1)/100 g sln and 4.57 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:
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. 0.09 mg(1)/kg(2) (standard deviation from 7-9 determinations)
	REFERENCES:

COMPONENTS:	EVALUATOR:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (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. November 1984

CRITICAL EVALUATION:

Quantitative solubility data for the system 3-methylhexane (1) and water (2) have been reported in the publications listed in Table 1.

TABLE 1:   Quantitative Solubility Studies of   ·

the System 3-Methylhexane (1) - Water (2)

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 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 3-METHYLHEXANE (1) IN WATER (2)

Although the solubility of 3-methylhexane in water has been reported in three publications (ref 1,2,3) the datum of Krzyzanowska and Szeliga (ref 3) does not appear to be independent of that of Price (ref 2) and is thus excluded from consideration. The remaining 298K data, of Price (ref 2) and Polak and Lu (ref 1), are in poor agreement. In the absence of confirmatory studies the average of these two studies: $(3.8\pm0.9)\times10^{-4}$g(1)/100g sln, $x_1=6.8\times10^{-7}$, is regarded as the "Tentative" solubility of 3-methylhexane in water. However, it may be noted that Polak and Lu's values for other hydrocarbon water systems are often higher and Price's values often lower than "Recommended" values.

2.   THE SOLUBILITY OF WATER (2) IN 3-METHYLHEXANE (1)

The solubility of water in 3-methylhexane has been reported only by Polak and Lu (ref 1) ans so no critical evaluation can be made. The interested user is referred to the relevant Data Sheet for solubility values. However, it can be noted that the data of Polak and Lu are generally close to "Recommended" values in well characterized systems.

REFERENCES

1.   Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

2.   Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

3.   Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)* <u>1978</u>, *34*, 413-7.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of 3-methylhexane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	5.24^c	9.41×10^{-7}
25^b	4.95^c	8.89×10^{-7}

Solubility of water in 3-methylhexane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	25^d	1.39×10^{-4}
25^b	74^e	4.12×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

ESTIMATED ERROR:
temp. a) ± 0.02 K; b) ± 0.01 K
soly. c) ± 1.7%; d) ± 4.7%;
      e) ± 3.1% (mean)

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* <u>1976</u>, *60*, 213-44.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylhexane in water at 25°C and at system pressure was reported to be 2.64 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1, calculated by the compiler are 2.64 x 10^{-4} g(1)/100 g sln and 4.75 x 10^{-7}.

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

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+%. (2) distilled.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 0.08 mg(1)/kg(2)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 3-Methylhexane; C_7H_{16}; [589-34-4] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, <u>1978</u>, *12*, 413-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of 3-methylhexane in water at 25°C was reported to be 2.64 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated by compiler are 2.64×10^{-4} g(1)/100 g sln and 4.75×10^{-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:	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:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (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 heptane (1) - water (2) system have been reported in the references listed in Table 1.

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

Reference	T/K	Solubility	Method
Fuhner (ref 1)	289	(1) in (2)	cloud point
Milligan (ref 2)	298	(1) in (2)	partition coefficient
Black *et al.* (ref 3)	283-298	(2) in (1)	radiotracer
Booth and Everson (ref 4)	298	(1) in (2)	residue volume
Durand (ref 5)	289	(1) in (2)	cloud point
McCants *et al.* (ref 6)	311	(1) in (2)	cloud point
Guseva and Parnov (ref 7)	345-460	(1) in (2)[a]	not specified
Schatzberg (ref 8)	298	(2) in (1)	Karl Fischer
Englin *et al.* (ref 9)	273-323	(2) in (1)	analytical
Zel'venskii *et al.* (ref 10)	296	(2) in (1)	radiotracer
Connolly (ref 11)	568-628[b]	(1) in (2)	cloud point
McAuliffe (ref 12)	298	(1) in (2)	GLC
Nelson and DeLigny (ref 13)	277-318	(1) in (2)	GLC
Ghanem *et al.* (ref 14)	296	(2) in (1)	radiotracer
Krasnoshchekova and Gubergrits (ref 15)	298	(1) in (2)	GLC
Polak and Lu (ref 16)	273,298	mutual	GLC, analytical
Budantseva *et al.* (ref 17)	293-313	mutual	not specified
Price (ref 18)	298-424	(1) in (2)	GLC
Korenman and Aref'eva (ref 19)	293	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 20)	298	(1) in (2)	GLC
Bittrich *et al.* (ref 21)	298-313[c]	mutual	GLC
Rudakov and Lutsyk (ref 22)	298	(1) in (2)	partition coefficient
Jonsson *et al.* (ref 23)	288-308	(1) in (2)	partition coefficient

a Solubility in D_2O also reported.
b Pressure also varied.
c Temperature not specified for solubility of (1) in (2).

The original data in all the publications listed in Table 1 are compiled in the Data Sheets immediately following this Critical Evaluation with the exception of that of Milligan (ref 2) who employed a petroleum fraction of unspecified composition. Phase studies and critical phenomena have also been reported at elevated pressures (ref 25,26) but contain insufficient data to justify compilation.

COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (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)

As indicated in the footnotes to Table 1, quantitative solubility data for heptane in D_2O (ref 7) are available. However, as no comparable data have been reported no critical evaluation of the reliability of these data can be made. The interested user is referred to the relevant data sheets.

In the heptane-water system the mutual solubilities are sufficiently low to enable data reported in w/v fractions (or equivalent) to be converted to mass percent solubilities with reasonable precision by assuming solution densities to be the same as the pure solvents. These conversions are made on the Data Sheets and the data so obtained are included in this Evaluation. For convenience, further discussion of this system will be divided into three parts.

In the Tables which follow, values obtained by the Evaluator by graphical interpolation or extrapolation of the original measurements in the Data Sheets are indicated by an asterisk (*). "Best" values have been obtained by simple averaging. The uncertainty limits (σ_n) attached to these values do not have statistical significance and should be regarded only as a convenient representation of the spread of values rather than as error limits.

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

The extremely low solubility of heptane in water presents a daunting analytical problem. Nevertheless, all the modern investigations (ref 12, 13, 15, 16, 18), employing GLC, are in good agreement. The older studies, by Fuhner (ref 1), Durand (ref 5) and Guseva and Parnov (ref 7), and the more recent measurements of Budantseva *et al.* (ref 17) and Korenman and Aref'eva (ref 19), are an order of magnitude higher than the GLC results and are therefore rejected. The value of Bittrich *et al.* (ref 21) at an unspecified temperature and the order of magnitude data of Booth and Everson (ref 4) and McCants *et al.* (ref 6) are also rejected. All other data are included in Table 2 except for the value of Krzyzanowska and Szeliga (ref 20) which does not appear to be independent of that of Price (ref 18) and has therefore been excluded from consideration.

Selected data from Table 2 are also plotted in Figure 1 which emphasises the general agreement between the various independent studies. Application of the van't Hoff equation to the data in Table 2 gives $\Delta H_{sln}^{\infty} = -2.43$ kJ mol^{-1} and $\Delta C_{p,sln}^{\infty} = 472$ JK^{-1} mol^{-1} which are similar to calorimetric values reported for closely related hydrocarbons (ref 24).

COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (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: Tentative Values of the Solubility of Heptane (1) in Water (2)

T/K	Solubility Values		
	Reported values 10^4 g(1)/100g sln	"Best" values ($\pm \sigma_n$) 10^4 g(1)/100g sln	$10^7 x_1$
273	1.9* (ref 13), 4.39 (ref 16)	3 ± 1	5
283	2.0* (ref 13)	2.0	3.6
293	2.3* (ref 13), 2.57 (ref 23)	2.4 ± 0.2	4.3
298	2.93 (ref 12), 2.66 (ref 13), 2.8 (ref 15), 3.37 (ref 16), 2.24 (ref 18), 2.9 (ref 22), 2.51 (ref 23)	2.4 ± 0.2	4.3
303	2.2* (ref 13), 2.36* (ref 18), 2.49 (ref 23)	2.4 ± 0.1	4.1
313	2.3* (ref 13), 2.62 (ref 18)	2.5 ± 0.2	4.5
323	2.93* (ref 18)	2.9	5.2
333	3.3* (ref 18)	3.3	5.9
363	3.9* (ref 18)	3.9	7.0
373	5.8* (ref 18)	5.8	10
393	13* (ref 18)	13	23
413	31* (ref 18)	31	56
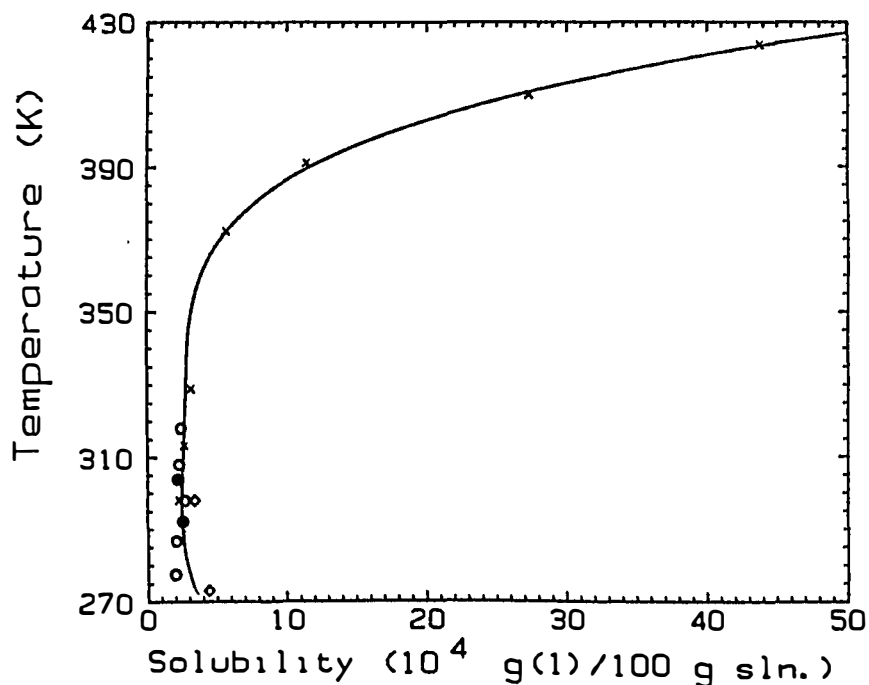
FIGURE 1. Solubility of heptane in water; selected data: ref 13 (O); ref 16 (◇); ref 18 (x), ref 23 (●).

COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (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)

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

In spite of the analytical difficulty of accurate determination of the low concentrations involved, the various reported values of the solubility of water in heptane are in reasonable agreement. However, the amount of data available is much smaller than for heptane in H_2O.

The values of Black *et al.* (ref 3), the higher temperature ($T > 293K$) data of Englin *et al.* (ref 9) and the value of Zelvenskii *et al.* (ref 10) are higher than other studies (ref 8,14,16,17,21) and are therefore rejected. All other values are listed in Table 3.

TABLE 3: Tentative Values of the Solubility of Water (2) in Heptane (1)

T/K	Solubility Values		
	Reported values 10^3 g(2)/100 g sln	"Best" values (± σ_n)[a] 10^3 g(2)/100 g sln	$10^4 x_2$
273	2.7 (ref 9), 2.6 (ref 16)	2.7	1.5
283	5.4 (ref 9)	5.4	3.0
293[b]	9.6 (ref 9), 9 (ref 17)	9	5.0
298	9.1 (ref 8), 8.2 (ref 16), 12.1 (ref 21)	10 ± 2	5.6
313	13 (ref 17), 15.6 (ref 21)	14	7.8

a Because of the limited amount of data at temperatures other than 298K, σ_n values would be misleading and have therefore not been calculated.
b A value of 5.73 x 10^{-3} g(2)/100 g sln reported at 295.7K in ref 14.

The data in Table 3 are also plotted in Figure 2. Application of the van't Hoff equation to the "Best" values of Table 3 gives ΔH^∞_{sln} = 23 kJ mol^{-1} and $\Delta C^\infty_{p,sln}$ = -1050 $JK^{-1}mol^{-1}$. Whilst the ΔH^∞_{sln} is reasonable by comparison with related systems (e.g. water in hexane), $\Delta C^\infty_{p,sln}$ values for the dissolution of water in hydrocarbons are normally *ca.* +100 $JK^{-1} mol^{-1}$. This is evidenced by a general flattening off for the solubility-temperature curve at higher temperatures (*e.g.* water in hexane or benzene) rather than the apparent increasing gradient seen in Figure 2. That is, the reported solubilities at higher temperatures are probably too low.

COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (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)
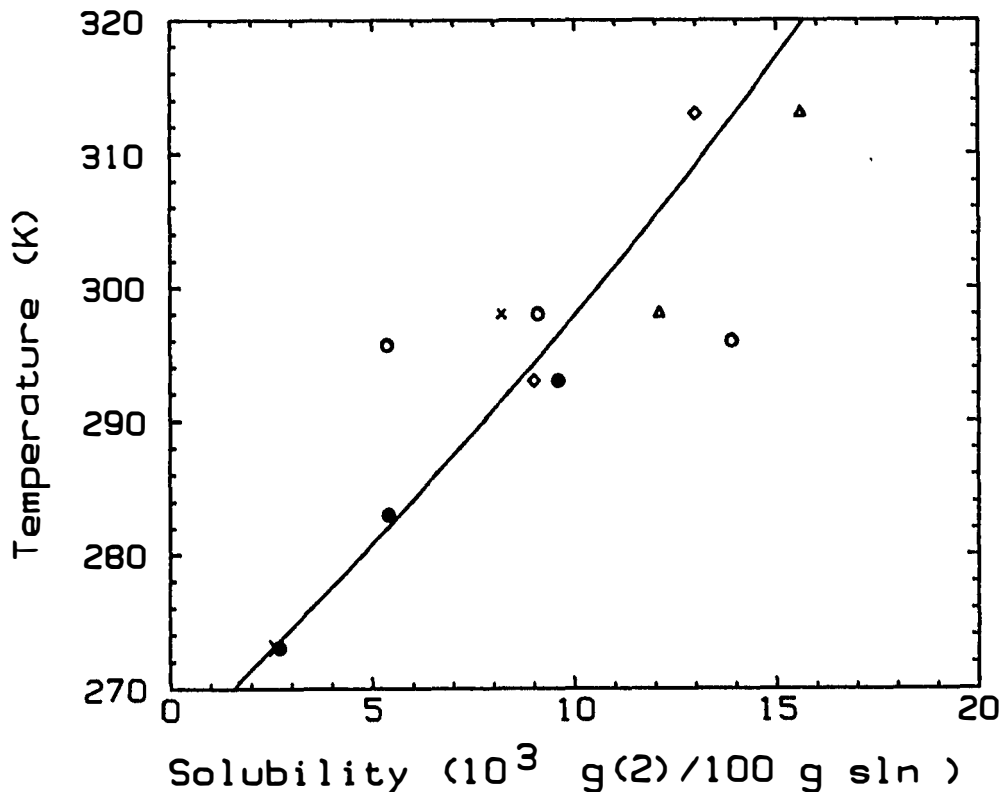
FIGURE 2.   Solubility of water in heptane: ref 9 (●); ref 16 (x); ref 17 (◇); ref 21 (Δ); other data (O). Full line represents curve of best fit.

3.   SOLUBILITY STUDIES OF THE HEPTANE (1) - WATER (2) SYSTEM AT ELEVATED PRESSURES

The phase behaviour type of this system is topographically similar to that of benzene + water.

Solubility studies on the heptane + water system at pressures higher than atmospheric are listed in Table 4. The solubility data obtained by Guseva and Parnov (ref 7) are considerably greater than that obtained by Price (ref 18) under comparable conditions. In the absence of further independent studies it is not possible to prefer either data set and the interested user is referred to the relevant Data Sheets for experimental values. Meaningful comparisons with the data of other workers is also precluded because of the differences in conditions.

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COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-83-5] (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)

TABLE 4. Solubility Studies of the Heptane + Water System at Elevated Pressures

Reference	p/MPa	T/K	Solubility
Guseva and Parnov (ref 7)	along 3-phase line	345-460	(1) in (2)
Connolly (ref 11)	17-55	568-628	(1) in (2)
Price (ref 18)	along 3-phase line	295-424	(1) in (2)
Bröllos et al. (ref 25)	_a	_a	_a
Roof (ref 26)	6.3[b]	519.0[b]	_b

a Qualitative statements and graph of phase behaviour only.
b Critical point of unknown composition.

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COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (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 (continued)

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26. Roof, J.G. *J. Chem. Eng. Data* 1970, *15*, 301-3.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Fühner, H. *Ber. Dtsch. Chem. Ges.* <u>1924</u>, *57*, 510-5.

VARIABLES:	PREPARED BY:
One temperature: 15.5°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of heptane in water at 15.5°C was reported to be
0.007 mL(1)/100 mL sln or 0.005 g(1)/100 g sln.
The corresponding mole fraction, x_1, calculated by the compiler
is 0.9×10^{-5}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
In a stoppered measuring cylinder pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100 or 1000 cm³ of (2) until a completely clear solution was obtained at the experimental temperature.	(1) source not specified; commercial grade; used as received. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Black, C.; Joris, G.G.; Taylor, H.S. *J. Chem. Phys.* <u>1948</u>, *16*, 537-43.
VARIABLES: Temperature: 10-25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in heptane
at a total saturation pressure of 1 atm

t/°C	g(2)/100 g(1)	g(2)/100 g sln (compiler)	$10^4 x_2$ (compiler)
10	0.0077	0.0077	4.28
20	0.0136	0.0136	7.56
20	0.0126	0.0126	7.00
25	0.0151	0.0151	8.39

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(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. <u>1948</u>, *16*, 45.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (1) Water; H_2O; [7732-18-5]	Booth, H.S.· Everson, H.E. *Ind. Eng. Chem.* <u>1948</u>, *40*, 1941-3.
VARIABLES: One temperature: 25.0°C (298.2 K)	PREPARED BY: G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *n*-heptane in water at 25.0°C was reported to be <0.04 mL (1)/100 mL (2). A similar request was reported for (1) in 40.0% (w/w?) aqueous sodium xylenesulfonate.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 0.02 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.	(1) "Highest grade commercial sample available"; no other details given. (2) Distilled.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Durand, R. *C.R. Hebd. Seances Acad. Sci.* 1948, *226*, 409-10.
VARIABLES: One temperature: 16°C	**PREPARED BY:** M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of heptane in water at 16°C was reported to be ·
0.015 cm^3(1)/dm^3(2).
With the assumption of a solution density of 1.00 g cm^{-3} and a
density value of 0.6868 g cm^{-3} for heptane at 16°C (ref 2), the
corresponding mass percent is 0.0010 g sln and the corresponding
mole fraction, x_1, is 1.8×10^{-6} (compiler).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The thermostatic method described in ref 1 was used. Addition of pipetted volumes of (1) to (2) followed by shaking is repeated till appearance of turbidity.	(1) not specified. (2) distilled.

	ESTIMATED ERROR: soly. ± 0.005 cm^3(1)/dm^3(2).

REFERENCES:

1. Durand, R. *C.R. Hebd. Seances Acad. Sci.* 1946, *223*, 898-900.

2. Timmermans, J. *Physico-chemical constants of pure organic compounds*, Elsevier, 1950.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5]	McCants, J.F.; Jones, J.H.; Hopson, W.H.
(2) Water; H_2O; [7732-18-5]	*Ind. Eng. Chem.* <u>1953</u>, *45*, 454-6.

VARIABLES:	PREPARED BY:
One temperature: 100°F (311 K)	G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of *n*-heptane in water at 100°F (311 K) was reported to be <0.1 g(1)/100 g sln. The corresponding mole fraction, x_1, calculated by the compiler, is <2 x 10^{-4}.

The solubility of water in *n*-heptane at 100°F (311 K) was reported to be 0.12 g(2)/100 g sln. The corresponding mole fraction, x_2, calculated by the compiler, is 6.6 x 10^{-3}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The method was essentially that of ref. 1 and involved titration of the second component to the cloud point, in a constant temperature bath.	(1) Phillips; pure grade; used without further purification; n_D^{20} 1.3974.
	(2) Distilled.

ESTIMATED ERROR:
Not specified.

REFERENCES:
1. Washburn, E.R.; Hnizda, V.; Vold, R.D., *J. Am. Chem. Soc.* <u>1931</u>, *53*, 3232.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Guseva, A.N.; Parnov, E.I. *Radiokhimiya* <u>1963</u>, *5*, 507-9.

VARIABLES:	PREPARED BY:
Temperature: 71.5-187°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of heptane in water

$t/°C$	$10^5 x_1$	g(1)/100 g sln (compiler)
71.5	1.8	0.010
108	2.9	0.016
181	11.4	0.0633
187	12.07	0.0671

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in ref 1.	(1) not specified. (2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Khazanova, P.E. *Tr. Gos. inst. azotn. promyshl.* <u>1954</u>, *4*, 5.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Schatzberg, P. *J. Phys. Chem.* <u>1963</u>, *67*, 776-9.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in heptane at 25°C was reported to be
91 mg(2)/kg sln corresponding to a mole fraction, x_2, of 5.06×10^{-4}
and to a mass percent of 0.0091 g(1)/100 g sln.

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AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
(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.	(1) Eastman Organic Chemicals; doubly distilled; 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 K soly. 0-6% (deviations from the mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (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: Temperature: 0-50°C	PREPARED BY: A. Maczynski and M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of water in heptane

$t/°C$	g(2)/100 g sln	$10^4 x_2$ (compiler)
0	0.0027	1.50
10	0.0054	3.00
20	0.0096	5.34
30	0.0172	9.57
40	0.0308	17.1
50	0.0480	26.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water, H_2O; [7732-18-5]	Zel'venskii, Ya.D; Efremov, A.A.; Larin, G.M. *Khim. Tekhnol. Topl. Masel* <u>1965</u>, *10*, 3-7.

VARIABLES:	PREPARED BY:
One temperature: 23°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of water in heptane at 23°C was reported to be 0.0139 g(2)/100 g sln.

The corresponding mole fraction, x_2, calculated by the compiler is 7.73 x 10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Saturated solutions of tritium labeled (2) in (1) were prepared in two ways. In the first, nitrogen was passed through the vessel with (2) and next through the vessel with (1) and frozen. In the second, about 500 mL of (1) and 1 mL (2) were stirred. The concentration of (2) in (1) was calculated from scintillation measurements.	(1) source not specified; pure grade; shaken with conc. H_2SO_4; washed with water, dried over sodium, and distilled; purity not specified. b.p. 98.43°C, m.p. -90.8°C. (2) source not specified; commercial; 1 Ci/mL HTO used as received.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Connolly, J.F. *J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6
VARIABLES:	**PREPARED BY:**
Temperature: 295-355°C Pressure: 170-700 atm	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of heptane in water

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
295	170	17.22	1.1	0.0020
	250	25.32	1.1	0.0020
	500	50.65	1.1	0.0020
	700	70.91	1.1	0.0020
330	200	20.26	3.3	0.0061
	300	30.39	3.3	0.0061
	500	50.65	3.3	0.0061
350	195	19.75	3.7	0.0069
	210	21.27	5.7	0.0107
	260	26.34	9.6	0.0187
	280	28.36	10.0	0.0196
	310	31.40	9.6	0.0187
	370	37.48	8.1	0.0156
	550	55.72	5.7	0.0107

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The cloud point method was used. Measurements were carried out in a 100 mL stainless-steel cell. The cell was loaded with 15 g (2) and brought to temperature. Mixing was started and (1) was injected, until either a cloud or a small portion of a second phase appeared at the top of the cell. Then mercury was injected to change the pressure, more (1) was injected and the procedure was repeated.	(1) Phillips reagent grade; better than 99.8%; used as received. (2) distilled and deaerated.
	ESTIMATED ERROR: temp. ± 0.02 K press. ± 2 atm (accuracy)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5]	Connolly, J.F.
(2) Water; H_2O; [7732-18-5]	*J. Chem. Eng. Data* <u>1966</u>, *11*, 13-6.

$t/°C$	p/atm	p/MPa (compiler)	g(1)/100 g sln	x_1 (compiler)
355	230	23.30	10.3	0.0202
	240	24.31	13.5	0.0273
	250	25.32	19.5	0.0417
	245	24.82	24.7	0.0557
	320	32.42	41.7	0.1139
	310	31.40	35.7	0.0885
	300	30.39	29.3	0.0693
	300	30.39	24.8	0.0559
	305	30.90	19.5	0.0417
	345	34.95	13.5	0.0273
	390	39.51	10.3	0.0202

COMMENTS AND ADDITIONAL DATA:

Upper critical solution temperature: 353°C at p = 290 atm (29.83 MPa).

The uncertainty in the CST is about 2°C and that of the corresponding pressure about 10 atm.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	McAuliffe, C. *J. Phys. Chem.* <u>1966</u>, *70*, 1267-75.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of heptane in water at 25°C was reported to be 2.93 mg (1)/kg sln (0.000293 g(1)/100 g sln).
The corresponding mole fraction, x_1, calculated by the compiler, is 5.3×10^{-7}.
The same value is also reported in refs 1 and 2.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; 99+% purity; used as received. (2) distilled.
	ESTIMATED ERROR: temp. ± 1.5 K soly. 0.20 mg (1)/kg sln (standard deviation from mean)
	REFERENCES: 1. McAuliffe, C. *Nature (London)* <u>1963</u>, *200*, 1092. 2. McAuliffe, C. *Am. Chem. Soc. Div. Petrol. Chem.* <u>1964</u>, *9*, 275.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Nelson, H.D.; De Ligny, C.L. *Rec. Trav. Chim. Pays-Bas* <u>1968</u>, *87*, 528-44.

VARIABLES:	PREPARED BY:
Temperature: 4.3-45°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of heptane in water

t/°C	$10^7 x_1$	mg(1)/kg sln (compiler)
4.3	3.51 ± 0.26	1.95
13.5	3.63 ± 0.51	2.02
25.0	4.78 ± 0.74	2.66
35.0	4.07 ± 0.95	2.27
45.0	4.32 ± 1.06	2.41

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips pure grade. (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 (90% probability interval)

	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Ghanem, N.A.; Marek, M.; Exner, J. *Int. J. Appl. Radiat. Isotop.* <u>1970</u>, 21, 239-40.

VARIABLES:	PREPARED BY:
One temperature: 22.5°	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of water in heptane at 22.5°C was reported to be 3.93×10^{-3} g(2)/100 mL (1) or 5.73×10^{-3} g(2)/100 g (1).
The corresponding mass percent and mole fraction, x_2, calculated by the compiler are 5.73×10^{-3} g(2)/100 g sln and 3.19×10^{-4}.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A volume of standardized radio-active water was injected in a vessel containing dry (1). The vessel was then closed and the contents were shaken and stirred. The vessel was then left for the excess water to settle to the bottom and sides and to ensure equilibrium. Portions of (1) saturated with (2) were added to a scintillation mixture and counted.	(1) source not specified; purified by shaking with a mixture of H_2SO_4 and P_2O_5, kept over KOH, then distilled and the distillate refluxed over NaH; residual water content $< 5 \times 10^{-6}$ mol·dm^{-3} (2) not specified.
	ESTIMATED ERROR: temp. ± 1 K soly. ± 10% (type of error not specified)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Krasnoshchekova, P.Ya.; Gubergrits, M.Ya. *Neftekhimiya* <u>1973</u>, *13*, 885-7.

VARIABLES:	PREPARED BY:
One temperature: 25°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of heptane in water at 25°C was reported to be
$x_1 = 5.0 \times 10^{-7}$.
The corresponding mass percent calculated by the compiler is
2.8×10^{-4} g(1)/100 g sln.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) source not specified; CP reagent; purity not specified. (2) distilled.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Polak, J.; Lu, B.C-Y. *Can. J. Chem.* <u>1973</u>, *51*, 4018-23.

VARIABLES:	PREPARED BY:
Temperature: 0-25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of heptane in water

$t/°C$	mg(1)/kg sln	x_1 (compiler)
0^a	4.39^c	7.9×10^{-7}
25^b	3.37^c	6.1×10^{-7}

Solubility of water in heptane

$t/°C$	mg(2)/kg sln	x_2 (compiler)
0^a	26^d	1.45×10^{-4}
25^b	82^e	4.56×10^{-4}

$^{a-e}$see "ESTIMATED ERROR"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Phillips Petroleum Co.; pure grade reagent (99%+); shaken three times with distilled water. (2) distilled.

	ESTIMATED ERROR: temp. a) ± 0.02 K; b) ± 0.01 K soly. c) ± 4%; d) ± 4.7%; e) ± 3.1% (mean)
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Budantseva, L.S.; Lesteva, T.M.; Nemtsov, M.S. *Zh. Fiz. Khim.* <u>1976</u>, *50*, 1344. *Deposited doc.* <u>1976</u>, VINITI 437-76.
VARIABLES: Temperature: 20 and 40°C	PREPARED BY: A. Maczynski

EXPERIMENTAL VALUES:

Solubility of heptane in water

$t/°C$	$10^5 \, x_1$	10^3 g(1)/100 g sln (compiler)
20	0.3	2
40	1	6

Solubility of water in heptane

$t/°C$	$10^4 \, x_2$	10^3 g(2)/100 g sln (compiler)
20	5	9
40	7	13

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
Nothing specified in the paper. .	(1) not specified. (2) not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Price, L.C. *Am. Assoc. Petrol. Geol. Bull.* 1976, *60*, 213-44.
VARIABLES:	PREPARED BY:
Temperature: 25-150.4°C	F. Kapuku

EXPERIMENTAL VALUES:

Solubility of heptane in water at system pressure

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	$10^7 x_1$ (compiler)
25.0	2.24 ± 0.04	0.000224	4.0
40.1	2.63 ± 0.05	0.000263	4.7
55.7	3.11 ± 0.11	0.000311	5.6
99.1	5.60 ± 0.17	0.000560	10.1
118.0	11.4 ± 0.4	0.00114	20.5
136.6	27.3 ± 0.9	0.00273	49.1
150.4	43.7 ± 1.0	0.00437	78.6

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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 al-lowed 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.	(1) Phillips Petroleum Company; 99+%. (2) distilled.

ESTIMATED ERROR:
temp. ± 1 K soly. range of values given above

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Korenman, I.M.; Aref'eva, R.P. Patent USSR, 553 524, 1977.04.05 C.A. *87*:87654.
VARIABLES:	PREPARED BY:
One temperature: 20°C	A. Maczynski

EXPERIMENTAL VALUES:

The solubility of heptane in water at 20°C was reported to be
0.06 g(1)dm^{-3}(2).

The corresponding mass percent and mole fraction, x_1, calculated
by the compiler are 0.006 g(1)/100 g sln and 1.1×10^{-5}. The
assumption that 1 dm^3 sln = 1 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: not specified.
	REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Krzyzanowska, T.; Szeliga, J. *Nafta (Katowice)*, <u>1978</u>, *12*, 413-7.
VARIABLES: One temperature: 25°C	PREPARED BY: M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of heptane in water at 25°C was reported

to be 2.24 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1, calculated

by compiler are 2.24×10^{-4} g(1)/100 g sln and 4.03×10^{-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.

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

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Bittrich, H.-J.; Gedan, H.; Feix, G. *Z. Phys. Chem., Leipzig* <u>1979</u>, *260*, 1009-13.

VARIABLES:	PREPARED BY:
Temperature: 25-40°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of heptane in water

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	x_1 (compiler)
unspecified	3.7	0.00037	6.6×10^{-7}

Solubility of water in heptane

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	x_2 (compiler)
25	121	0.0121	6.73×10^{-4}
40	156	0.0156	8.68×10^{-4}

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
A mixture of (1) and (2) was shaken with no access of air at a specified temperature and then thermostatted for 48 hr. The equilibrated phases were sampled and analysed by gas chromatography using a flame-ionization detector. A 3-m-steel column of 15% nitril silicone on Porolith, 110°C and a 3-m-steel column of 1.5 g CaC_2 and 10% SE 30 on chromaton N, 120°C were used for (1) and (2) respectively.	(1) source not specified; distilled or crystallized; purity tested by gas chromatography. (2) not specified.

ESTIMATED ERROR:
soly. ± 9% (type of error not specified).

REFERENCES:

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Rudakov, E.S.; Lutsyk, A.I. *Zh. Fiz. Khim.* <u>1979</u>, *53*, 1298-1300.

VARIABLES:	PREPARED BY:
One temperature: 25°C	M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The authors reported the partition coefficient α of heptane between the gas and aqueous phase. $\alpha = 84 \pm 4$. $\alpha = C_g/C_s$ with C_s being the concentration of the compound in dilute aqueous solution at 25°C and C_g the concentration in the gas phase in equilibrium with the aqueous solution (both in moles per liter).

The compiler has assumed that when (1) and (2) are not very soluble in each other, C_s may be taken as the water solubility and C_g as the vapor pressure of (1). The value of p (where p is the vapor pressure in mm of Hg) is taken from ref 1. $p = 45.81$ mm of Hg and $\log C_g = \log p - 4.269 = -2.61$ expressed in moles per liter. Therefore $C_s = 2.9 \times 10^{-5}$ moles per liter. With the assumption of a solution density of 1.00 g mL^{-1}, the corresponding mass percent is 0.00029 g(1)/100 g sln and the corresponding mole fraction, x_1, is 5.2×10^{-7}.

AUXILIARY INFORMATION	
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The equilibrium distribution was attained after shaking for 10 min the thermostatted reactor containing (2) and the (1) vapor. After being allowed to stand for 10 min, equal calibrated volumes of samples of the gas and solution were introduced by a syringe into a special cell for the removal of (1) by blowing, built into the gas line of the chromatograph and the partition coefficient α was determined as the ratio of the areas of the peaks of the substrate arising from the two phases.	(1) not specified. (2) not specified.
	ESTIMATED ERROR: soly. ± 10% (estimated by the compiler)
	REFERENCES: 1. Hine, J.; Mooker, P.K. *J. Org. Chem.* <u>1975</u>, *4*, 292.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Water; H_2O; [7732-18-5]	Jonsson, J.A.; Vejrosta, J.; Novak, J. *Fluid Phase Equil.* <u>1982</u>, *9*, 279-86.

VARIABLES:	PREPARED BY:
Temperature: 15-35°C	G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of heptane in water

$t/°C$	mg(1)/kg sln	10^4g(1)/100g sln (compiler)	$10^7 x_1$ (compiler)
15	2.67	2.67	4.80
20	2.57	2.57	4.62
25	2.51	2.51	4.51
30	2.49	2.49	4.47
35	2.52	2.52	4.53

^{a}Solubility values were calculated by the authors from their smoothed air-water partition çoefficient (K_{AW}) by assuming K_{AW} values obtained at infinite dilution were valid at the saturation pressure of (1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) Fluka, > 99.7%, used as received. (2) Not specified.
	ESTIMATED ERROR: Not specified.
	REFERENCES: 1. Vejrosta, J.; Novak, J.; Jonsson, J.A. *Fluid Phase Equil.* <u>1982</u>, *8*, 25-35.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Deuterium oxide (heavy water); D_2O; [7789-20-0]	Guseva, A.N.; Parnov, E.I. *Radiokhimiya* **1963**, *5*, 507-9.

VARIABLES:	PREPARED BY:
Temperature: 68-193°C	A. Maczynski

EXPERIMENTAL VALUES:

Solubility of heptane in deuterium oxide

$t/°C$	$10^5 x_1$	g(1)/100 g sln (compiler)
68	1.51	0.0076
109	2.8	0.0140
158	6.24	0.0312
193	14.9	0.0745

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The solubility of (1) in (2) was determined in sealed glass tubes. Details were reported in ref 1.	(1) not specified. (2) distilled.

ESTIMATED ERROR:

not specified.

REFERENCES:

1. Khazanova, P.E. *Tr. Gos. inst.*
   azotn. promyshl. **1954**, *4*, 5.

COMPONENTS:	EVALUATOR:
(1) Heptane; C_7H_{16}; [142-82-5] (2) Seawater	D.G. Shaw Institute of Marine Science University of Alaska Fairbanks, Alaska USA
	December 1982

CRITICAL EVALUATION:

The solubility of heptane (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	1.03×10^{-3}
Freegarde *et al.* (ref 2)	GLC	?	?	4×10^{-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 heptane in pure water at 298 K.

SOLUBILITY OF HEPTANE (1) IN SEAWATER (2)
DOUBTFUL VALUE

T/K	g salts/kg sln	g(1)/100 g sln
298	6	1.03×10^{-3}

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) Heptane; C_7H_{16}; [142-82-5] (2) Seawater	Krasnoshchekova, R.Ya.; Gubergrits, M.Ya. *Neftekhimiya* <u>1973</u>, *13*, 885-8.

VARIABLES:	PREPARED BY:
One temperature: 25°C Salinity: 6 g/kg sln	M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of heptane in seawater was reported to be

1.03×10^{-3} g(1)/100 g sln. and the corresponding mole fraction,

$x_1 = 1.9 \times 10^{-6}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
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.	(1) "chemically pure" (2) distilled water plus salt mixture.

	ESTIMATED ERROR: not specified.
	REFERENCES:

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