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SOLUBILITY DATA SERIES

Volume 58

POLYCYCLIC AROMATIC HYDROCARBONS: BINARY NON-AQUEOUS SYSTEMS
PART I: SOLUTES A–E

SOLUBILITY DATA SERIES

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SOLUBILITY DATA SERIES

Volume 58

POLYCYCLIC AROMATIC HYDROCARBONS: BINARY NON-AQUEOUS SYSTEMS PART I: SOLUTES A–E

Volume Editor

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CONTENTS

INTRODUCTION TO THE SOLUBILITY DATA SERIES

SOLUBILITY OF SOLIDS IN LIQUIDS

NATURE OF THE PROJECT

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

COMPILATIONS AND EVALUATIONS

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

Compilations

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

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

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

(a) saturating components:
(b) non-saturating components;
(c) solvents.

In each of (a), (b) or (c), the components are arranged in order according to the IUPAC 18-column periodic table with two additional rows:

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

The same order is followed in arranging the compilation sheets within a given volume.

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

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

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

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

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

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

The precision of the original data is preserved when derived quantities are calculated, if necessary by the inclusion of one additional significant figure. In some cases, compilers note that numerical data have been obtained from published graphs using digitizing techniques. In these cases, the precision of the data can be determined by the quality of the original graph and the limitations of the digitizing technique. In some cases graphs have been included, either to illustrate data more clearly, or if this is the only information in the original. Full grids are not usually inserted as it is not intended that users should read data from the graphs.

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

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

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

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

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

Evaluations

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

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

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

Critical Evaluation:

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

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

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

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

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

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

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

(f) Units. While the original data may be reported in the units used by the investigators, the final recommended values are reported in SI units (3) when the data can be accurately converted.

QUANTITIES AND UNITS USED IN COMPILATION AND EVALUATION OF SOLUBILITY DATA

Mixtures, Solutions and Solubilities

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

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

The *solubility* of a solute 1 (solid, liquid or gas) is the analytical composition of a saturated solution, expressed in terms of the proportion of the designated solute in a designated solvent (6).

"Saturated" implies equilibrium with respect to the processes of dissolution and precipitation; the equilibrium may be stable or metastable. The solubility of a substance in metastable equilibrium is usually greater than that of the same substance in stable equilibrium. (Strictly speaking, it is the activity of the substance in metastable equilibrium that is greater.) Care must be taken to distinguish true metastability from supersaturation, where equilibrium does not exist.

Either point of view, mixture or solution, may be taken in describing solubility. The two points of view find their expression in the reference states used for definition of activities, activity coefficients and osmotic coefficients.

Note that the composition of a saturated mixture (or solution) can be described in terms of any suitable set of thermodynamic components. Thus, the solubility of a salt hydrate in water is usually given as the relative proportions of anhydrous salt in solution, rather then the relative proportions of hydrated salt and water.

Physicochemical Quantities and Units

Solubilities of solids have been the subject of research for a long time, and have been expressed in a great many ways, as described below. In each case, specification of the temperature and either partial or total pressure of the saturating gaseous component is necessary. The nomenclature and units follow, where possible, ref. (3)

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

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

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

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

2. *Ionic mole fractions* of salt i, x_{i+}, x_{i-}:
For a mixture of s binary salts i, each of which ionizes completely into ν_{i+} cations and ν_{i-} anions, with $\nu_i = \nu_{i+} + \nu_{i-}$ and a mixture of p non-electrolytes k, of which some may be considered as solvent components, a generalization of the definition in (7) gives:

$$x_{+i} = \frac{\nu_{+i}x_i}{1+\sum_{j=1}^{s}(\nu_j-1)x_j}, \quad x_{-i} = \frac{\nu_{-i}x_{+i}}{\nu_{+i}} \quad i = 1...s \tag{2}$$

$$x_{ok} = \frac{x_k}{1+\sum_{j=1}^{s}(\nu_j-1)x_j}, \quad k = (s+1)...c \tag{3}$$

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

$$\sum_{i=1}^{s}(x_{+i}+x_{-i}) + \sum_{i=s+1}^{c} x_{oi} = 1 \tag{4}$$

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

$$x_1 = \frac{\nu_{+2}x_{o1}}{\nu_{+2}-(\nu_2-1)x_{+2}} \quad x_2 = \frac{x_{+2}}{\nu_{+2}-(\nu_2-1)x_{+2}} \tag{5}$$

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

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

$$w_1 = g_1/\sum_{s=1}^{c} g_s \tag{6}$$

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

4. *Solute mole fraction* of substance 1, $x_{s,1}$:

$$x_{s,1} = m_1/\sum_{s=1}^{c'} m_s = x_1/\sum_{s=1}^{c'} x_s \tag{7}$$

where c' is the number of solutes in the mixture. These quantities are sometimes called Jänecke mole (mass) fractions (8, 9). *Solute mass fraction* of substance 1, $w_{s,1}$, is defined analogously.

5. *Solvent mole fraction* of substance 1, $x_{v,1}$:

$$x_{v,1} = x_1/\sum_{s=1}^{p} x_s \tag{8}$$

Here, p is the number of solvent components in the mixture. *Solvent mass fraction* of substance 1, $w_{v,1}$, is defined analogously.

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

$$m_1 = n_1/n_2 M_2 \qquad [9]$$

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

7. *Aquamolality, Solvomolality* of substance 1 in a mixed solvent with components 2, 3 (10), $m_1^{(3)}$:

$$m_1^{(3)} = m_1\overline{M}/M_3 \qquad [10]$$

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

$$\overline{M} = x_{v,2}M_2+(1-x_{v,2})M_3 \qquad [11]$$

and $x_{v,2}$ is the solvent mole fraction of component 2. This term is used most frequently in discussing comparative solubilities in water (component 2) and heavy water (component 3) and in their mixtures.

8. *Amount concentration* of solute 1 in a solution of volume V, c_1:

$$c_1 = [\text{formula of solute}] = n_1/V \qquad [12]$$

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

9. *Mass concentration* of solute 1 in a solution of volume V, ρ_1:

$$\rho_1 = g_1/V = c_1M_1/V \qquad [13]$$

SI base units: kg m^{-3}.

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

$$r_{n,12} = n_1/n_2 \qquad [14]$$

Mass ratio, symbol $r_{m,12}$, may be defined analogously.

11. *Ionic strength*, I_m (molality basis), or I_c (concentration basis):

$$I_m = \frac{1}{2}\sum_i m_i z_i^2, \quad I_c = \frac{1}{2}\sum_i c_i z_i^2 \qquad [15]$$

where z_i is the charge number of ion i. While these quantities are not used generally to express solubilities, they are used to express the compositions of non-saturating components. For a single salt i with ions of charge numbers z_+, z_-,

$$I_m = |z_+z_-|\nu m_i, \quad I_c = |z_+z_-|\nu c_i \qquad [16]$$

Mole and mass fractions and mole ratios are appropriate to either the mixture or the solution point of view. The other quantities are appropriate to the solution point of view only. Conversions between pairs of these quantities can be carried out using the equations given in Table 1 at the end of this Introduction. Other useful quantities will be defined in the prefaces to individual volumes or on specific data sheets.

Salt hydrates are generally not considered to be saturating components since most solubilities are expressed in terms of the anhydrous salt. The existence of hydrates or solvates is noted carefully the critical evaluation.

Mineralogical names are also quoted, along with their CA Registry Numbers, again usually in in the text, and CA Registry Numbers (where available) are given usually in the critical evaluation.

In addition to the quantities defined above, the following are useful in conversions between concentrations and other quantities.

12. *Density*, ρ:

$$\rho = g/V = \sum_{s=1}^{c} \rho_s \qquad [17]$$

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

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

Thermodynamics of Solubility

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

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

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

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

PREFACE

The chemical literature contains solubility data for a large number of solutes dissolved in a single solvent. Solubility data for crystalline solutes in binary solvent systems are relatively scarce, and data for ternary (and higher-order) solvent systems are virtually nonexistent as experimental measurements become progressively more difficult, time-consuming and expensive with each additional solvent component. Despite continued efforts by experimentalists and scientific organizations, both in terms of new experimental measurements and critically evaluated data compilations, there still exist numerous systems for which actual solubility data are not readily available. To address this problem, researchers have to determine precise experimental data in binary solvents, and then use the measured results to check the predictive ability of modern semi-empirical relationships derived from basic thermodynamic principles.

With the afore mentioned ideas in mind, I compiled published solubility data for anthracene, naphthalene, phenanthrene, pyrene, fluorene, fluoranthene, carbazole, thianthrene, and other two- and three-ring polycyclic aromatic heteroatom compounds in pure and binary organic solvent mixtures so that experimental values will be readily available in a single reference source. Volume 54 in the IUPAC *Solubility Data Series* initiated this effort. The chemical literature contained far too many systems, however, to be accommodated within established page limits for a single volume. Volume 54 was limited in scope to polycyclic aromatic compounds dissolved in binary organic solvent systems. Pure, single component solvents were included in Volume 54 only if the solubility measurements were performed as part of the binary solvent study. A large number of solute-solvent systems were excluded under this criterion. The present two volume set is devoted to solubility of polycyclic aromatic compounds in pure, single component organic nonelectrolyte solvents. Experimental data for a very select number of binary solvent mixtures is also included in the set. For the most part, binary solvent data was published after Volume 54 was completed, and involves either anthracene or pyrene dissolved in alkane + alcohol and alcohol + alcohol mixtures. Solubility data for well over 250 different systems were retrieved from the chemical literature and are compiled in this volume. Literature sources searched include a complete coverage of *Chemical Abstracts* from 1907 to June 1994; Beilstein, *Handbuch der Organischen Chemie*; and the *International Critical Tables*.

Critical evaluation of published solubility data was performed only if four or more independent sources of experimental data could be found for the particular solute-solvent system under consideration. In the case of isothermal solubility data, where only a single temperature was studied, the published mole fraction solubilities were arithmetically averaged, and the mean and corresponding standard deviation are reported. If experimental solubilities were given at several temperatures, then the critical evaluation involved a linear least squares regression of the natural logarithm of mole fraction solubility versus the reciprocal of absolute temperature, in accordance with accepted thermodynamic practices. The mathematical equation for the least squares line and Ln x_1 versus $1/T$ graph are included in the volume. For a few systems, there was sufficient experimental data to permit construction of the binary phase diagram.

Polycyclic aromatic compounds are an important chemical class. They have been used as model compounds in coal liquefaction process design calculations, serve as the "parent" compound or base found in a number of drug molecules, and several are mutagens, carcinogens, or common organic pollutants resulting from oil spills. Moreover, many of the polycyclic aromatic compounds have very limited mole fraction solubilities, and from a thermodynamic modeling standpoint, saturated solutions are treated as infinitely dilute solutions. The solute is considered to be surrounded by solvent molecules. Solute-solute molecular interactions are ignored.

Compilations of published solubility data for crystalline polycyclic aromatic compounds dissolved in pure, single component solvents and in binary organic solvent systems alone, however, do not address entirely the needs of the scientific community. There are a number of systems that one encounters for which actual experimental data may consist solely of solute solubilities in the two pure solvents, and for which additional experimental measurements are not feasible. Solubility determinations are both time-consuming and expensive, and presume that the necessary chemicals and instrumentation have been procured. Research laboratories are not routinely equipped to measure solubility data, and one cannot always wait days for additional supplies to be delivered. In such instances, predictive expressions provide the sole means to generate desired values in timely fashion. Predictive methods facilitate interpolation between measured data points and help to screen data sets for possible outliers (incorrect entries) in need of redetermination.

Recognizing the increasing role that predictive expressions have enjoyed in modern science, I have decided to include in this volume a very brief survey of select methods currently being used to estimate solute solubilities in mixed solvents, particular binary alkane + alcohol and alcohol + alcohol systems. Admittedly, not every predictive expression can be presented. Several hundred pages of text would be required to adequately examine the various quantitative structure-activity relationships (QSARs), semi-empirical, stoichiometric complexation and group contribution models developed during the past fifty years. Discussion in the present volume is limited to basic thermodynamic principles governing the solubility of crystalline nonelectrolyte solutes, and predictive expressions actually used by the editor to screen the compiled solubility data sets for possible outliers. Agreement between theory and experimental solubilities indicates that the measured values are internally consistent. Such comparisons afford a convenient means to critically evaluate single measurement systems, as is the case with the majority of published solubility data for polycyclic aromatic compounds in binary solvent mixtures. Conventional methods of evaluation used in the *Solubility Data Series* are not applicable since data available from the different laboratories were not measured under the same conditions of temperature and solvent composition. For a more detailed treatment of solubility behavior, readers are referred to monographs by Acree (1), Grant and Higuchi (2), Hildebrand and Scott (3), James (4), Prausnitz *et al.* (5), and Shinoda (6).

BASIC THERMODYNAMIC PRINCIPLES

Composition of a liquid solution can be expressed in a variety of ways, as (1) the ratio of the amount of one component to the amount of a second component, n_1/n_2, etc., (2) amount concentration

$c_i = [i] = n_i/V$ SI base units: mol dm^{-3} [1]

(3) mole fraction

$x_1 = n_1/(n_1 + n_2 + n_3 + \ldots\ldots)$ [2]

or (4) volume fraction

$\phi_1 = n_1V_1/(n_1V_1 + n_2V_2 + n_3V_3 + \ldots\ldots)$ [3]

Strictly speaking, the true volume of a real solution is not equal to the sum of the volumes of the individual components but is the fractional sum of partial molar volumes, which for a ternary solution is $V = x_1V_1 + x_2V_2 + x_3V_3$. For purposes of this monograph, volume fractions are defined in terms of the molar volumes of the pure unmixed components $V_{m,i}$ (molar mass divided by density)

$\phi_1 = n_1V_{m,1}/(n_1V_{m,1} + n_2V_{m,2} + n_3V_{m,3} + \ldots\ldots)$ [4]

as this quantity serves as an input parameter in expressions for estimating solubilities in mixed solvents since it requires no *a priori* knowledge concerning volumetric behavior. Solute solubilities can be found in the chemical literature in terms of any of the aforementioned concentration variables, or as molality, m_i, which is the amount of solute i divided by the mass of the solvent

$m_i = n_i/n_s\ M_s$ SI base unit: mol kg^{-1} [5]

where M_s is the molar mass of the solvent.

Solubility is a strong function of the intermolecular forces between the solute and solvent molecules. The well-known adage *similis similibus solvuntur* (like is dissolved by like) serves merely as an empirical statement of the fact that, in the absence of specific interactions, the molecular forces between chemically similar species lead to a smaller endothermic enthalpy of solution than those between dissimilar species. Because dissolution must be accompanied by a decrease in the Gibbs energy, a low endothermic enthalpy is preferable to a large one. Factors other than the intermolecular forces between the solute and solvent, however, play an important role in determining the solubility of a crystalline material.

The solubility of a solid substance may be considered to arise from three, and in some cases four, contributions:

(a) The breaking of solute-solute interactions in the crystalline lattice;

(b) the breaking of solvent-solvent interactions, often referred to as cavity formation;

(c) the formation of solute-solvent interactions; and

(d) the perturbation of solvent-solvent interactions in the immediate vicinity of the solute, as in solvent structuring.

Each of these four contributions may be further divided into specific chemical (complexation) and nonspecific physical (simple dispersion) interactions. To illustrate, consider the solubilities of the two isomers phenanthrene and anthracene. The mole fraction solubility of phenanthrene in benzene at 298 K (x_1 = 0.2068) is approximately 25 times greater than that of anthracene (x_1 = 0.0074), even though both solutes are chemically similar to each other. The reason for this difference in solubility results from something that is all too often overlooked, that is, the solubility depends not only upon the activity coefficient of the solute (which reflects the intermolecular forces between the solute and solvent and between solute molecules), but also depends upon the chemical potential of the standard state to which the activity coefficient refers and on the chemical potential of the pure solid.

The thermodynamic criterion governing solute solubility (component 1) and solid-liquid equilibrium is

$$a_1 = a_1^* \qquad [6]$$

or

$$a_1^* = \gamma_1 \, x_1 \, a_1^{\circ} \qquad [7]$$

where * is the pure solid, x_1 is the mole fraction solubility of the solute in the solvent, γ_1 is the liquid-phase activity coefficient and a_1° is the standard state activity to which γ_1 refers. Selection of the standard state a_1° is arbitrary, the only thermodynamic requirement being that it must be at the same temperature as the saturated solution. For thermodynamic modeling of nonelectrolyte solutions, it is advantageous to define the standard state activity as the activity of the pure supercooled liquid, $a_1^*(l)$, at the solution's temperature and some specified pressure. Although this is a hypothetical standard state, it is one whose properties can be calculated with reasonable accuracy provided that the solution's temperature is not too far removed from the melting point temperature of the solute, T_{MP}.

The standard state activity is computed from the following three-step thermodynamic cycle:

Step I: Solute 1 (solid, T) $\longrightarrow$ Solute 1 (solid, T_{MP})

Step II: Solute 1 (solid, T_{MP}) $\longrightarrow$ Solute 1 (liquid, T_{MP})

Step III: Solute 1 (liquid, T_{MP}) $\longrightarrow$ Solute 1 (liquid, T)

with the overall process being

Solute 1 (solid, T) $\longrightarrow$ Solute 1 (supercooled liquid, T)

and

$$\Delta G = RT \ln a_1(s) = \Delta G_I + \Delta G_{II} + \Delta G_{III} \qquad [8]$$

Assuming that the difference in heat capacities between the solid and supercooled liquid remains constant over the temperature range from T to T_{MP}, the following expression is obtained

$$\ln a_1(s) = \ln (\gamma_1 x_1) = - \Delta H^{fus} (T_{MP} - T)/R \, T \, T_{MP} + \Delta C_p \, (T_{MP} - T)/RT - (\Delta C_p/R) \ln (T_{MP}/T) \qquad [9]$$

for the solubility of a crystalline solute in a liquid solvent. The expression for $a_1(s)$ must include additional term(s) if the solid undergoes a phase transition (7,8).

Melting point temperatures and enthalpy of fusion data are tabulated in Table I for 29 polycyclic aromatic hydrocarbons and hetero-atom derivatives. Excepted where noted, numerical values were taken from published compilations (9,10). For molecules

TABLE I. Enthalpies and Entropies of Fusion of Select Polycyclic Aromatic Hydrocarbons and Hetero-atom Derivatives[a]

Polycyclic Aromatic Compound	T_{MP}/K	ΔH^{fus}/(J mol^{-1})	ΔS^{fus}/(J mol^{-1} K^{-1})
Naphthalene	351.3	19,120	54.4
Acenaphthylene	362.1	10,960	30.3
Dibenzofuran	355.7	18,600	52.3
Dibenzothiophene	371.0	15,300	41.2
Thianthrene	428.5	25,440	59.4
Carbazole	516.2	29,420	57.0
Acenaphthene	366.6	21,540	58.8
Acridine	452.4	19,700	43.5
Fluorene	388.0	19,580	50.5
Xanthene	373.7	19,200	51.4
Anthracene	492.7	28,830	58.5
Phenanthrene	372.4	16,470	44.2
Pyrene	424.4	17,110	40.3
Fluoranthene	381.0	18,870	49.5
Chrysene	531.4	26,150	49.2
Triphenylene	473.5	25,100	53.0
Benz[a]anthracene	434.3	21,380	49.2
Benzo[c]phenanthrene	334.7	16,310	48.7
Perylene	553.9	31,750	57.3
Benzo[a]pyrene	454.2	17,320	38.1
Benzo[ghi]perylene	554.2	17,370	31.3
Dibenz[a,c]anthracene	553.5	25,820	46.6
Dibenzo[a,h]anthracene	544.2	31,160	57.3
Benzo[rst]pentaphene	556.8	27,870	50.1
Dibenzo[def,p]chrysene	501.2	24,680	49.2
Dibenzo[a,e]pyrene	520.2	30,500	58.6
Phthalazine	364.5	13,320	36.5
Quinazoline	320.9	16,950	52.8
Quinoxaline	305.7	11,800	38.6

[a] Melting point temperatures and enthalpy of fusion data for all polycylic aromatic compounds, except for phthalazine, quinazoline and quinoxaline, were taken from published compilations by Acree (9,10). Experimental data for the three diazanaphthalenes was from a calorimetric study by Sabbah and Pemenzi (62).

not listed in the table it is possible to estimate ΔH^{fus} from simple geometric considerations and/or group contribution parameters. Enthalpy and entropy are both state functions, and only the initial and final states, *i.e.*, the crystal and the melt, need to be defined. At the molecular level, the two states differ in their relative degree of geometric order. Intermolecular distance, spacial orientation and packing arrangement in the crystalline state are defined within a much narrower range than in the liquid melt.

For conceptualization, Yalkowsky and Valvani (11) divided the total melting process for rigid, nonspherical polycyclic aromatic compounds into the following subprocesses:

(a) Translational melting representing the change from the highly ordered arrangement of the molecular gravitational centers in the crystal to the more randomized, expanded arrangement in the liquid; and

(b) Rotational melting resulting from the change in ordered arrangement of the crystalline molecule's major axis to a randomly oriented arrangement in the liquid.

As noted by the authors, the molar entropy of fusion, ΔS^{fus}, is equal to the entropy of the liquid state minus the entropy of the crystal

$$\Delta S^{fus} = - R \ln P^{fus} \qquad [10]$$

where P^{fus} is the ratio of the number of ways of achieving the crystal to the number of ways of achieving the liquid. The ratio is equal to the probability (above the melting point temperature) of a collection of one mole of liquid molecules spontaneously arranging themselves in such a manner so as to fulfill the geometric requirements of the crystal. Since entropies of the translational melting and rotational melting subprocesses are related to their probability of occurrence by equations analogous to eqn. [10], and since the probabilities are assumed to be independent (*i.e.*, $P^{fus} = P^{trans} P^{rot}$), then entropies must be additive

$$\Delta S^{fus} = \Delta S^{trans} + \Delta S^{rot} \qquad [11]$$

The translational entropy was visualized by a two-dimensional analogy involving a field of checkers or disks that had been trapped into a nearly closest-packed two-dimensional crystalline arrangement. When the crystal melts, a slight expansion and randomization of the disk positions occur. The probability of two-dimensional fusion is equal to the total number of arrangements of the disks that are possible within the area allotted for the solid divided by the corresponding number of arrangements that are possible within the area allotted to the liquid melt. This, in turn, is related to the ratio of the free areas available within each phase for the disks to occupy. Free areas are replaced by free volumes in the case of a three-dimensional arrangement of molecules. Entropies of fusion for spherical molecules such as inert gases and for pseudospherical molecules such as tetrachloromethane typically range between 12.5 - 16.7 J mol^{-1} K^{-1}. Yalkowsky and Valvani (11) assumed the intermediate value of $\Delta S^{trans} = 14.6$ J mol^{-1} K^{-1} for the translational melting contribution to the entropy of fusion, though the authors did state that nonspherical molecules generally have a somewhat larger volume change associated with melting.

The rotational entropy of fusion results from differences in rotational degrees of freedom. In the crystal, molecules (with their centers of mass fixed) can wobble or vibrate approximately 10° in the spherical coordinates ϕ and θ from their most stable position after averaging over all axes. Molecules in the liquid phase have much greater orientational freedom and can rotate over a much wider range of ϕ and θ. If it is assumed for simplicity that liquid molecules can rotate freely, then any reference point will trace out a sphere about the center of gravity of the molecule. The reference point traces out only a spherical segment if the molecule's motion is restricted, as would be the case for the crystalline lattice. A ± 10° variation in ϕ and θ corresponds to a spherical segment that is roughly 0.00754 times that of a sphere of the same radius, or roughly a rotational entropy of fusion of $\Delta S^{fus} = 41.8$ J mol^{-1} K^{-1}. On the basis of the above discussion, the total entropy of fusion for a rigid polycyclic aromatic compound would be $\Delta S^{fus} = \Delta S^{trans} + \Delta S^{rot} \approx 56.4$ J mol^{-1} K^{-1}, which is in reasonable (though by no means perfect) agreement with experimental values listed in Table I.

Chickos and coworkers (12,13) derived a group additivity approach for estimating entropies of fusion based upon the mathematical relationships:

For acyclic and aromatic hydrocarbons

$$\Delta S^{fus} = \Sigma\, n_i\, C_i\, G_i + \Sigma\, n_j\, C_j\, G_j + \Sigma\, n_k\, C_K\, G_k \qquad [12]$$

For cyclic hydrocarbons

$$\Delta S^{fus} = [8.41 + 1.025\,(n - 3)] + \Sigma\, n_i\, C_i\, G_i + \Sigma\, n_j\, C_j\, G_j + \Sigma\, n_k\, C_K\, G_k \qquad [13]$$

For polycyclic molecules

$$\Delta S^{fus} = [8.41\,N + 1.025\,(R - 3N)] + \Sigma\, n_i\, C_i\, G_i + \Sigma\, n_j\, C_j\, G_j + \Sigma\, n_k\, C_K\, G_k \qquad [14]$$

where $K = \Sigma\, n_k$, n refers to the number of equivalent methylene groups necessary to simulate the size of the ring, R is the total number of ring atoms and N indicates the total number of rings in the polycyclic molecule. Hydrocarbon components are identified by the subscript *i*, the *j* subscript identifies the carbon(s) bearing the functional group(s) and the *k* subscript denotes the different functional groups in the molecule. Each group contribution to the entropy of fusion represents the product of the number of identical groups in the molecule (n) times the group value (G) times an empirical coefficient (C) which modifies each group contribution according to the structural environment around the carbon atom bearing substituent functional groups.

Inherent in the above group additivity estimational scheme is the underlying assumption that the contribution of any particular atom or group of atoms to the entropy change associated in going from a rigid anisotropic solid state to the highly isotropic liquid state is fundamentally constant. Entropies for mesomorphic liquid crystalline transitions are thus included in the overall melting process, if possible. The corresponding enthalpies of fusion, needed in the calculation of $a_1(s)$, are obtained by melting ΔS^{fus} by the observed melting point temperature, T_{MP}. Unpublished computations (14) for over 150 organic compounds not included in the original group parameter evaluation show that eqns. [12] - [14] provide very reasonable estimates of ΔS^{fus} and ΔH^{fus}. Average difference between predicted and observed values was approximately 7 %.

Enthalpies of fusion were discussed at length so that interested readers can calculate solute activity coefficients from the experimental solubility data tabulated in this volume. Enthalpy of fusion, activity coefficient and solute solubility are interrelated through eqn. [9]. Equation [9] immediately provides two useful conclusions regarding the solubility of solids in liquids. Although these conclusions rigorously apply to ideal solutions ($\gamma_1 = 1$), they serve as useful guidelines for other solutions that do not deviate excessively from ideal behavior.

(a) For a given solid-solvent system, the solubility increases with increasing temperature. The rate of increase is approximately proportional to the enthalpy of fusion and, to a first approximation, does not depend upon the melting point temperature.

(b) For a given solvent and at a fixed temperature, if two solids have a similar entropy of fusion then the solid with the lower melting temperature has the higher solubility. Similarly, if two solids have about the same melting temperature then the one with the lower enthalpy of fusion has the higher solubility.

In the preceding discussion Raoult's law is used to define the thermodynamic properties of an ideal solution. For very high molecular weight solvent systems, eqn. [9] (with $\gamma_1 = 1$) grossly underestimates solute solubilities. This is not too surprising because the Flory-Huggins model

$$G = RT\,[\,x_1 \ln \phi_1 + x_2 \ln \phi_2\,] \qquad [15]$$

$$\ln a_1 = \ln \phi_1 + \phi_2\,(1 - V_{m,1}/V_{m,2}) \qquad [16]$$

provides a more realistic description of solution ideality in polymer solutions. The corresponding expression for solubility is given by

$$\ln \phi_1 + (1 - \phi_1)(1 - V_{m,1}/V_{m,2}) = -\,\Delta H^{fus}\,(T_{MP} - T)/RT\,T_{MP} + \Delta C_p\,(T_{MP} - T)/RT - (\Delta C_p/R)\,\ln\,(T_{MP}/T) \qquad [17]$$

Chiou and Manes (15) compared experimental solubilities of 11 crystalline nonpolar polycyclic aromatic compounds and their derivatives in glycerol trioleate ($V_{m,s}$ = 966 $cm^3\ mol^{-1}$) to predictions based upon eqns. [9] and [17]. The authors' calculations revealed that the observed mole fraction solubilities are considerably higher than the predictions of eqn. [9] (with $\Delta C_p = 0$); the predictions in some instances being low by as much as 100 percent. In comparison, the observed volume fraction solubilities, ϕ_1, were comparable to or only slightly lower than the predictions of eqn. [17] (again with $\Delta C_p = 0$). The magnitude of the deviations from Raoult's law is well beyond the uncertainty of the observed solubilities. Since the solubility data can be explained by the Flory-Huggins model and since there is no convincing evidence to indicate strong specific solute-solvent interactions, the observed negative deviations from Raoult's law appears to be an artifact of the model caused by large molecular size disparity. The solubility measurements of Chiou and Manes, combined with an earlier study on glycerol trioleate/water partition coefficients (16), suggest that the Flory-Huggins model should be considered in systems having molar volume ratios of 4 or more.

SCATCHARD-HILDEBRAND SOLUBILITY PARAMETER THEORY

Elementary ideas from statistical thermodynamics lead to some general conclusions at the molecular level concerning nonideality of mixtures. Nonelectrolyte mixtures are classified according to their molecular properties by considering the kind of internal forces acting between like and unlike molecules. Such a division of intermolecular forces leads to classification of mixtures into simple and complex liquids. The interactions in simple liquids result exclusively from dispersion forces, or nonspecific interactions as they are often called. On the other hand, in complex liquids the molecules have a permanent nonuniform distribution of charge (polar liquids) so that they interact through electrostatic forces in addition to dispersion forces. The electrostatic interactions (primarily dipole-dipole interactions) lead to some degree of specific interactions resulting in a specific geometric orientation of one molecule with respect to an adjacent molecule. For this reason this interaction is sometimes called the orientation effect. If these interactions are strong enough, stable dimers or larger complexes may be formed and the liquid is said to be associated. The boundary between weakly polar liquids and associated liquids is nebulous, and there have been numerous disagreements in the published literature regarding the separation of specific and nonspecific interactions.

The Scatchard-Hildebrand solubility parameter model (6,17) provides reasonable estimates of solute solubility in systems containing only nonspecific interactions

$$RT \ln (a_1(s)/x_1) = V_{m,1} (1 - \phi_1)^2 (\delta_1 - \delta_{solvent})^2 \qquad [18]$$

where $\delta_{solvent}$ and δ_1 refer to the solubility parameters of the solvent and supercooled liquid solute, respectively, $V_{m,1}$ is the molar volume of the supercooled liquid solute, x_1 is the saturation mole fraction solubility, and ϕ_1 is the solute's volume fraction solubility calculated using the ideal molar volume approximation (eqn. [4]). For solvent components, the liquid molar volumes and solubility parameters are often tabulated in the literature (for example, see both Hoy (18) and Barton (17)), and when not available, they can be calculated directly from density and vapor pressure measurements on the pure liquid. Molar volumes of supercooled liquid solutes, $V_{m,1}$, on the other hand, are estimated either by group contribution methods or by the experimentally determined apparent partial molar volumes in the solvent of interest. Solubility parameters of the supercooled liquid can be obtained indirectly from solubility measurements or can be estimated by group contribution methods.

Tables II and III compare the predictions of eqn. [18] to experimental solubilities of naphthalene and biphenyl in a wide range of organic solvents. Properties used in the computations include the activities of the supercooled liquid solutes, a(s,biphenyl) = 0.384 and a(s,naphthalene) = 0.312, the molar volumes, $V_{m,biphenyl}$ = 149.4 cm^3 mol^{-1} and $V_{m,naphthalene}$ = 123.0 cm^3 mol^{-1}, and best estimates for the solubility parameters, $\delta_{biphenyl}$ = 20.05 $J^{1/2}$ $cm^{-3/2}$ and $\delta_{naphthalene}$ = 19.84 $J^{1/2}$ $cm^{-3/2}$. Inspection of Tables II and III reveals that the predicted values are, for the most part, within 10 % of the experimental solubilities.

The solubility parameter approach is extended to binary solvent mixtures by defining $\delta_{solvent}$

TABLE II. Comparison Between Experimental and Predicted Naphthalene Solubilities

Solvent	δ_2[a]	$V_{m,2}$[a]	x_1(exp)[b]	x_1(calc)
Dichloromethane	20.21	64.50	0.330	0.311
Chlorobenzene	19.78	102.26	0.311	0.312
Benzene	18.74	89.41	0.292	0.305
Trichloromethane	18.74	80.64	0.339	0.305
Methylbenzene	18.27	106.84	0.292	0.295
Ethylbenzene	18.08	123.08	0.289	0.289
Tetrachloromethane	17.49	97.08	0.255	0.275
Cyclohexane	16.75	108.76	0.147	0.242
Methylcyclohexane	15.95	128.32	0.147	0.189
n-Octane	15.42	163.48	0.142	0.146
n-Heptane	15.34	147.48	0.130	0.144
n-Hexane	14.87	131.51	0.122	0.119
Carbon disulfide	20.29	60.62	0.283	0.311

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[a] $\delta_2/(10^3\ \text{g/kg}^{1/2}\ \text{m}^{-1/2}\ \text{s}^{-1})$; $V_{m,2}/(\text{cm}^3\ \text{mol}^{-1})$.

[b] Experimental solubilites were determined by Chang (63).

TABLE III. Comparison Between Experimental and Predicted Biphenyl Solubilities

Solvent	δ_2[a]	$V_{m,2}$[a]	x_1(exp)[b]	x_1(calc)
Dichloromethane	20.21	64.50	0.412	0.384
Chlorobenzene	19.78	102.26	0.397	0.384
Benzene	18.74	89.41	0.381	0.374
Trichloromethane	18.74	80.64	0.422	0.375
Methylbenzene	18.27	106.84	0.377	0.362
Ethylbenzene	18.08	123.08	0.363	0.353
Tetrachloromethane	17.49	97.08	0.342	0.340
Cyclohexane	16.75	108.76	0.190	0.295
Methylcyclohexane	15.95	128.32	0.183	0.215
n-Octane	15.42	163.48	0.147	0.147
n-Heptane	15.34	147.48	0.138	0.145
n-Hexane	14.87	131.51	0.124	0.112
Carbon disulfide	20.29	60.62	0.369	0.384

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[a] $\delta_2/(10^3\ \text{g/kg}^{1/2}\ \text{m}^{-1/2}\ \text{s}^{-1})$; $V_{m,2}/(\text{cm}^3\ \text{mol}^{-1})$.

[b] Experimental solubilities were determined by Chang (63).

$$\delta_{\mathrm{solvent}} = (\phi_2\,\delta_2 + \phi_3\,\delta_3)/(\phi_2 + \phi_3) = \phi_2^{(s)}\,\delta_2 + \phi_3^{(s)}\,\delta_3 \qquad [19]$$

as a volume fraction average of the solubility parameters of the two pure solvents, δ_2 and δ_3. The superscript (s) indicates that the solvent composition is calculated as if the solute were not present.

The popularity of the solubility parameter approach arises because it relates the solubility of a solute in a given solvent, either pure or mixed, to the bulk properties of the pure components. Whereas this particular application of the solubility parameter theory has certain practical advantages in that it requires only a minimal number of experimental observations, a more flexible expression for binary solvent systems can be derived by replacing the individual δ_i values with the measured solubilities in the pure solvents and the measured thermodynamic excess properties of the solvent mixture.

To incorporate direct experimental observations into the basic solubility parameter model, first substitute eqn. [19] into eqn. [18]

$$(1 - \phi_1)^{-2}\,RT \ln\,(a_1(s)/x_1) = V_{m,1}\,(\phi_2^{(s)}\,\delta_2 + \phi_3^{(s)}\,\delta_3 - \delta_1)^2 \qquad [20]$$

and multiply out the squared term

$$(1 - \phi_1)^{-2}\,RT \ln\,(a_1(s)/x_1) = V_{m,1}\,[\,\phi_2^{(s)}\,(\delta_2 - \delta_1)^2 + \phi_3^{(s)}\,(\delta_3 - \delta_1)^2 - \phi_2^{(s)}\,\phi_3^{(s)}\,(\delta_2 - \delta_3)^2] \qquad [21]$$

Inspection of eqn. [21] reveals that, for model systems obeying this expression, the saturation solubility of the solute in a pure solvent (components 2 and 3) is described by

$$(G_1^{\mathrm{E}})_i^{\infty} = (1 - \phi_1)^{-2}\,RT \ln\,(a_1(s)/x_1) = V_{m,1}\,(\delta_i - \delta_1)^2 \qquad i = 2,3 \qquad [22]$$

The small subscripts i = 2 and i = 3 are used to distinguish the properties of the solute in a pure solvent from those in the binary solvent system. Similarly, the excess Gibbs energy of the binary solvent mixture can be expressed

$$G_{23}^{\mathrm{E}} = (x_2^{(s)}\,V_{m,2} + x_3^{(s)}\,V_{m,3})\,\phi_2^{(s)}\,\phi_3^{(s)}\,(\delta_2 - \delta_3)^2 \qquad [23]$$

in terms of solubility parameters.

Combining eqns. [21]-[23] one finds that the solubility of a solute in binary solvent mixtures containing only nonspecific interactions is

$$RT \ln\,(a_1(s)/x_1) = (1 - \phi_1)^2\,[\phi_2^{(s)}\,(G_1^{\mathrm{E}})_2^{\infty} + \phi_3^{(s)}\,(G_1^{\mathrm{E}})_3^{\infty} - V_{m,1}\,(x_2^{(s)}\,V_{m,2} + x_3^{(s)}\,V_{m,3})^{-1}\,G_{23}^{\mathrm{E}}\,] \qquad [24]$$

a volume fraction average of the solute's properties in the two pure solvents, $(G_1^{\mathrm{E}})_2^{\infty}$ and $(G_1^{\mathrm{E}})_3^{\infty}$, and a contribution due to the non-mixing of the solvent pair by the presence of the solute. Enhancement of the non-mixing term by a large solute molecule can lead to predictions of maximum ($G_{23}^{\mathrm{E}} > 0$) or minimum ($G_{23}^{\mathrm{E}} < 0$) mole fraction solubilities.

Thus far, attention has focussed primarily on the predictive aspects of the solubility parameter approach. It should be noted that the basic solution model can also serve as the point of departure for the mathematical representation of solubility data. The extended Hildebrand solubility equation

$$-\log x_1 = -\log a_1(s) + (V_{m,1}\,\phi^2_{\mathrm{solvent}}/2.303\,RT)\,[\delta^2_{\mathrm{solvent}} + \delta_1^2 - 2\,\Sigma\,A_i\,\delta^i_{\mathrm{solvent}}\,] \qquad [25]$$

derived by Martin and co-workers (19-21) reproduces very accurately the solubility behavior of many crystalline nonelectrolytes in very nonideal binary solvent mixtures. Numerical values of the various A_i-coefficients are computed from the solubility data using a least squares analysis. Mathematical representations, such as eqn. [25], do enable the calculation of interpolated solubilities between two measured values and facilitate computerized storage and retrieval of experimental data. Ochsner *et al.* (22) discussed the mathematical representation of solubility data using expressions based upon mixture response-surface methods, and Acree *et al.* (23,24) suggested representations based upon the Nearly Ideal Binary Solvent (NIBS) and Modified Wilson models. Readers are encouraged to read these articles for several interesting ideas and comparisons.

MOBILE ORDER THEORY FOR BINARY ALKANE + ALCOHOL SOLVENT MIXTURES

For many years one of the more challenging problems facing scientists in the field of solution thermodynamics has been prediction of phase equilibria in hydrogen-bonding systems containing either a self-associating alcohol or carboxylic acid cosolvent. Self-association decreases the vapor pressure and increases the boiling point temperature of the neat alcohol or carboxylic acid compared to the nonassociated hydrocarbon homomorph of comparable molecular size and mass. Moreover, the case of inert hydrocarbon + alcohol and inert hydrocarbon + carboxylic acid mixtures, hydrogen-bonding may give rise to liquid-liquid immiscibility caused by relatively large positive deviations from Raoult's law. Interpretation of solution nonideality in such nonelectrolyte solutions has historically followed two dissimilar lines, which are predicated upon long-range and short-range molecular forces. At one extreme are weakly bonded van der Waals complexes, characterized by weak, non-specific physical interactions and primarily stabilized by long-range dispersion forces. At the other extreme are hydrogen-bonded complexes that exhibit relatively strong, specific and highly directional binding of a primarily electrostatic nature.

Even in systems known to contain specific solute-solvent and/or solvent-solvent complexation, the need to properly account for nonspecific physical interactions has been recognized. Arnett *et al.* (25) with their "pure base" calorimetric method for determining enthalpies of hydrogen-bond formation attempted to separate specific and nonspecific interactions. The sensitivity of the numerical results to selection of "model" compound and inert solvent raised important doubts regarding the overall effectiveness of this particular method (26). Saluja *et al.* (27) used a somewhat similar rationale in their comparison of enthalpies of transfer of alkanes and alkenes from the vapor state to methanol, dimethylformamide, benzene and cyclohexane, with the more exothermic values for the alkenes in methanol and dimethylformamide attributed to dipole-induced dipole interactions between the solvent and the polarizable π-cloud. Bertrand (28) demonstrated that neglect of nonspecific interactions in the chloroform + triethylamine system can lead to an appreciable error in the enthalpy of complex formation determined with the Ideal Associated Solution (IAS) model.

McCargar and Acree (29-33) compared values for the carbazole-dibutyl ether association constant calculated from experimental carbazole solubilities in ten binary alkane + dibutyl ether solvent mixtures. A simple stoichiometric complexation model based entirely on specific solute-solvent interactions required two equilibrium constants to mathematically describe the solubility data. Calculated equilibrium constants in 2,2,4-trimethylpentane cosolvent were significantly different from values for the cyclooctane system. In comparison, expressions from the Extended Nearly Ideal Binary Solvent (NIBS) model described the experimental carbazole solubilities to within an average absolute deviation of 2 % using a single carbazole-dibutyl ether association constant. Variation of the calculated volume fraction-based equilibrium constant with inert hydrocarbon cosolvent was slight, with the numerical values ranging from a lower limit of $K_{AC}^{\phi} = 22$ for n-heptane to $K_{AC}^{\phi} = 30$ for both 2,2,4-trimethylpentane and t-butylcyclohexane. The success of the Extended NIBS model is even more remarkable if one realizes that the carbazole mole fraction solubilities covered a 25-fold range, and the inert cosolvents included both small (n-hexane, cyclohexane) and large (squalane, n-hexadecane) saturated hydrocarbons. The Extended NIBS model is discussed in greater detail in Volume 54 of the IUPAC *Solubility Data Series.*

Much of the earlier research concerning mixtures containing alcohols, as summarized by Pimental and McClellan (34), treated hydrogen-bonding as a stepwise polymerization process resulting in a continuum of species. Thus, at low alcohol concentrations dimers would be the predominant polymeric species, with larger polymer chains becoming significant with increasing alcohol concentrations. Van Ness *et al.* (35) compared infrared data with enthalpy of mixing data for n-heptane + ethanol and methylbenzene + ethanol, and concluded that the results were best explained by a model containing monomers, cyclic dimers and linear polymers having 20 or more units per chain. Tucker and Christian (36) noted that the simplest model (1-3-∞) that can adequately describe the vapor pressure data for n-hexadecane + ethanol systems contained two equilibrium constants, one for trimer formation and the other for the sequential addition of the monomer. Other studies have indicated that a simple polymer of definite size may dominate. Fletcher and Heller (37,38) explained the infrared data of 1-octanol dissolved in n-decane (from dilute solutions to the pure alcohol) in terms of a monomer-tetramer self-association model. Dixon (39) also found that the monomer-tetramer model gave the best correlations for his proton magnetic resonance data on the hydroxyl shift for methanol dissolved in cyclohexane. Anderson *et al.* (40,41) explained vapor pressures of several linear and branched alcohols in 2,2,4-trimethylpentane with a monomer-pentamer model.

The afore mentioned studies, along with many others too numerous to list, document the complexity of solutions containing a self-associating alcohol component, and the difficulty in developing an universal thermodynamic model applicable to all systems commonly encountered. During the past three decades many thermodynamic models have been suggested for both excess enthalpies and vapor-liquid equilibria for mixtures containing an alcohol with inert and with nonassociating active cosolvents. There has been little effort, however, devoted to developing descriptive models for crystalline solutes dissolved in alcoholic solvents. Scarcity of predictive methods for solid-liquid equilibria results, to a large extent, from the nature of solid solute isothermal solubility measurements. There is only a single data point associated with the solubility of a crystalline solute in each neat organic solvent or solvent mixture, from which the solvent self-association equilibrium constant as well as all nonspecific interaction parameters and any solute-solvent association constants must be deduced.

Of the published thermodynamic treatments found in the chemical and engineering literature, Mobile Order theory (42-50) has been one of the more successful models in describing the widest range of complexing systems. For purposes of this volume, discussion will be limited to expressions applicable to polycyclic aromatic compounds dissolved in binary alkane + alcohol and alcohol + alcohol solvent mixtures. As noted previously, predictive expressions provide a very convenient means to screen experimental data sets for possible outliers in need of redetermination. Close agreement between observed and predicted values would suggest that the measured solubilities are internally consistent.

Mobile Order Theory assumes that all molecular groups perpetually move, and that neighbors of a given external atom in a molecule constantly change identity. All molecules of a given kind dispose of the same volume, equal to the total volume V of the liquid divided by the number n_A molecules of the same kind, *ie.*, Dom A = V/n_A. The center of this domain perpetually moves. Highest mobile disorder is achieved whenever groups visit all parts of their domain without preference. Preferential contacts lead to deviations with respect to this "random" visiting. This is especially true in the case of hydrogen-bonding as specific interactions result in a specific orientation of the "donor" molecule with respect to an adjacent "acceptor" molecule.

In the case of an inert crystalline solute dissolved in a self-associating solvent, Mobile Order theory expresses the volume fraction saturation solubility (ϕ_A) as:

$$\ln \phi_A = \ln a_A(s) - 0.5\ (1 - V_{m,A}/V_{m,solvent})\ \phi_{solvent} + 0.5 \ln [\phi_A^{sat} + \phi_{solvent}(V_A/V_{solvent})]$$
$$- \phi_{solvent}^2\ V_{m,A}(\delta_A' - \delta_{solvent}')^2\ (RT)^{-1} - r_S\ (V_{m,A}/V_{m,solvent})\ \phi_{solvent} \qquad [26]$$

where the $r_S\ (V_{m,A}/V_{m,solvent})\ \phi_{solvent}$ term represents the contributions resulting from hydrogen-bond formation between the solvent molecules. For most of the published applications, r_S was assumed to be unity for strongly associated solvents with single hydrogen-bonded chains like alcohols, to be two for water or diols, and to equal zero for non-associated solvents such as saturated hydrocarbons. A more exact value for alcoholic solvents can be calculated based upon (46)

$$r_S = (K_S\ \phi_{solvent}/V_{m,solvent})/(1 + K_S\ \phi_{solvent}/V_{m,solvent}) \qquad [27]$$

with a numerical value of K_S = 5,000 $cm^3\ mol^{-1}$ used for monofunctional alcohols.

The symbols δ_A' and $\delta_{solvent}'$ denote the modified solubility parameters of the solute and solvent, respectively, and $a_A(s)$ is the activity of the solid solute defined previously by eqn. [9]. Modified solubility parameters account for only nonspecific interactions, and in the case of alcoholic cosolvents the hydrogen-bonding contributions have been removed. Numerical values of $\delta_{solvent}'$ are listed in Table IV for several of the common organic nonelectrolyte solvents. These values were obtained from published compilations, and were deduced either by regressing experimental solubility data in accordance with the configurational entropic model of Huyskens and Haulait-

TABLE IV. Solvent and Solute Molar Volumes and Modified Solubility Parameters Used in Mobile Order Predictions

Compound	$V_i/(cm^3 mole^{-1})$	$\delta_i'/(J^{1/2} cm^{-3/2})^a$
Solvents		
n-Hexane	131.51	14.56
n-Heptane	147.48	14.66
n-Octane	163.46	14.85
Cyclohexane	108.76	14.82
Methylcyclohexane	128.32	15.00
2,2,4-Trimethylpentane	166.09	14.30
1-Propanol	75.10	17.29
2-Propanol	76.90	17.60
1-Butanol	92.00	17.16
2-Butanol	92.4	16.60
1-Octanol	158.30	16.38
Solutes		
Anthracene[b]	150.0	20.32[c]

[a] Tabulated values are taken from a compilation given in Ruelle *et al.* (47,48).

[b] The numerical value of $a_A(s) = 0.01049$ was calculated from the molar enthalpy of fusion, ΔH^{fus}, at the normal melting point temperature of the solute, $T_{MP} = 515$ K.

[c] Numerical value was calculated using the measured anthracene mole fractions solubility in n-hexane, n-heptane and n-octane, in accordance with eqn. [26].

Pirson (51) or by making approximations based upon known values for similar compounds or homomorphic hydrocarbons.

Ruelle and coworkers (46-50) presented a very impressive set of comparisons between experimental and predicted solubilities for anthracene, biphenyl, carbazole, naphthalene, phenanthrene and methylparaben in a wide range of neat organic noncomplexing and self-associating solvents. In the case of alcoholic solvents, r_s was set equal to unity using the argument that the association constant, K_S, was sufficiently large so that $K_S\ \phi_{solvent}/V_{m,solvent} >> 1$ in the denominator of eqn. [27]. For binary hydrocarbon + alcohol solvent mixtures, the more exact expression will be required. At very low alcohol volume fractions, $K_{alcohol}\ \phi_{alcohol}/V_{m,alcohol}$ will not necessarily be large compared to one.

Extension of Mobile Order theory to binary alkane + alcohol, and later alcohol + alcohol solvents, requires that one assume a mathematical form for how $\delta'_{solvent}$ varies with mixture composition. The function assumed must reduce to $\delta'_{solvent} = \delta'_B$ and $\delta'_{solvent} = \delta'_C$ at $x_B^{(s)} = 1.0$ and $x_C^{(s)} = 1.0$, respectively, in order to give a correct thermodynamic description of solubilities in both pure solvents. Noting that the $(\delta'_A - \delta'_{solvent})^2$ term in eqn. [26] accounts for nonspecific physical interactions, and because of similarities between δ'_i and δ_i solubility parameters, we approximate $\delta'_{solvent}$ as a volume fraction average of the modified solubility parameters of the two pure solvents, *ie.*, $\delta'_{solvent} = \phi_B^{(s)}\ \delta'_B + \phi_C^{(s)}\ \delta'_C$. Superscript (s) denotes that the binary solvent volume fractions are calculated as if the solute were not present. Gordon and Scott (52) invoked a similar approximation, $\delta_{solvent} = \phi_B^{(s)}\ \delta_B + \phi_C^{(s)}\ \delta_C$, in using the Scatchard-Hildebrand solubility parameter theory to explain the solubility maximum observed in the phenanthrene-cyclohexane-methylene iodide system. The molar volume of the mixed solvent is given by $V_{m,solvent} = x_B^{(s)}V_{m,B} + x_C^{(s)}V_{m,C}$ and all $\phi_{solvent}$ terms in eqn. [26] are replaced by $1 - \phi_A$, except in the r_s term (see eqn. [27]) containing the equilibrium constant. Here, the last term should be replaced by $-\ (1 - \phi_A)\{\phi_C^{(s)}\ r_C(V_{m,A}/V_{m,C}) + \phi_B^{(s)}\ r_B(V_{m,A}/V_{m,B})\}$, with r_B being set equal to zero in the case of the inert hydrocarbon cosolvent (43,44). The reduction of the free energy of the system caused by specific solvent-solvent interactions depends upon the molar concentration of the "active hydrogen-bonding" sites in the alcohol.

The computational procedure can be simplified further by noting that the intended anthracene solute has only a very limited mole fraction solubility in the pure alcohols and saturated hydrocarbon cosolvents. The actual experimental solubilities of anthracene in binary alkane + alcohol solvent mixtures are tabulated in the data compilation portion of this volume, which immediately follows the survey of predictive methods. Each system contains solubility data for seven binary solvent compositions, in addition to the measured anthracene solubilities in both pure solvents. For all practical purposes, one can approximate $1 - \phi_A$ as equal to unity with no loss in predictive accuracy.

Performing the afore mentioned substitutions, and after suitable mathematical manipulations, eqn. [26] is rewritten as follows:

$$RT\ \{\ln\ [a_A(s)/\phi_A] - 0.5[1 - V_{m,A}/(x_B^{(s)}V_{m,B} + x_C^{(s)}V_{m,C})] + 0.5\ \ln\ [V_A/(x_B^{o}V_B + x_C^{o}V_C)]$$

$$- (V_{m,A}/V_{m,C})\ (K_C\phi^o{}_C{}^2/V_{m,C})/(1 + K_C\phi_C{}^o/V_{m,C})\} = V_{m,A}[\phi_B{}^{(s)}\ (\delta'_A - \delta'_B)^2$$

$$+ \phi_C{}^{(s)}\ (\delta'_A - \delta'_C)^2\ - \phi_B{}^{(s)}\ \phi_C{}^{(s)}\ (\delta'_B - \delta'_C)^2] \qquad [28]$$

whenever the saturation solubility is sufficiently low so that $1 - \phi_A \approx 1.0$. Component C is assumed to be the self-associating alcoholic cosolvent. Careful examination of eqn. [28] reveals that, for model systems obeying the Mobile Order theory, the $(\delta'_A - \delta'_B)^2$ and $(\delta'_A - \delta'_C)^2$ terms can be eliminated from the basic model *via*

$$RT\ \{\ln\ [a_A(s)/(\phi_A)_B] - 0.5(1- V_{m,A}/V_{m,B}) + 0.5\ \ln\ (V_{m,A}/V_{m,B})\} = V_{m,A}\ (\delta'_A - \delta'_B)^2 \qquad [29]$$

and

$$RT\ \{\ln\ [a_A(s)/(\phi_A)_C] - 0.5(1- V_{m,A}/V_{m,C}) + 0.5\ \ln\ (V_{m,A}/V_{m,C})$$

$$- (V_{m,A}\ K_C/V_{m,C}{}^2)/(1 + K_C/V_{m,C})\}\ = V_{m,A}\ (\delta'_A - \delta'_C)^2 \qquad [30]$$

where $(\phi_A)_B$ and $(\phi_A)_C$ denote the solubilities in the two pure solvents. Combining eqns. [28] - [30] one obtains a relatively simple mathematical expression for the solubility in a binary solvent mixture

$$\ln \phi_A = \phi_B{}^{(s)}\ \ln\ (\phi_A)_B + \phi_C{}^{(s)}\ \ln\ (\phi_A)_C\ - 0.5\ [\ln\ (x_B{}^{(s)}V_{m,B} + x_C{}^{(s)}V_{m,C}) - \phi_B{}^{(s)}\ \ln\ V_{m,B}$$

$$- \phi_C{}^{(s)}\ \ln\ V_{m,C}]\ + (V_{m,A}\ K_C\ \phi_C{}^{(s)}/V_C{}^2)(1 + K_C/V_{m,C})^{-1} - [V_{m,A}\ K_C\ \phi_C{}^{(s)2}/V_{m,C}{}^2]\ x$$

$$(1 + \phi_C{}^{(s)}\ K_C/V_{m,C})^{-1} + V_A\ \phi_B{}^{(s)}\ \phi_C{}^{(s)}\ (\delta'_B - \delta'_C)^2\ (RT)^{-1} \qquad [31]$$

which does not require *a prior* knowledge of the solute's enthalpy of fusion and melting point temperature. Elimination of the $a_A(s)$ term from the predictive equation can lead to better solubility estimates, particularly in the case of high melting point solutes such as anthracene. The two heat capacity terms in eqn. [9] become increasingly more important the further that the system temperature is removed from the solute's melting point temperature. In the case of anthracene, which melts at T_{MP} = 489 K, neglect of the two ΔC_p terms would mean that the enthalpy of fusion remained constant over the 200 K temperature range used in extrapolating the properties of the hypothetical supercooled liquid solute. More-over, the derived expression correctly describes the solubility in the pure complexing and noncomplexing solvents, and if one so desires, can be used to calculate the "optimum value" of the solvent-solvent self-association constant from measured solubility as a function of solvent composition.

Despite the complex appearance of eqn. [31] its application to solubilities in mixed solvents is relatively straightforward and is similar in concept to numerical examples presented previously [for example see McCargar and Acree (29)]. The quantities $(\phi_A)_B$ and $(\phi_A)_C$ are calculated from the measured mole fraction solubility of the solid in the pure solvents assuming that the excess molar volume (or alternatively the volume change upon mixing) is zero. These quantities, along with the molar volumes, modified solubility parameters, and an *assumed* value for the equilibrium constant, are then used in eqn. [31] to calculate ϕ_A at each binary solvent composition. If desired, the entire procedure can be repeated until the numerical value of K_C that "best" describes the experimental solubility in a particular binary solvent system is obtained. Alternatively, one could perhaps judiciously adjust the numerical value of $\delta'_{alcohol}$ in hope of improving the predictive accuracy of eqn. [31]. This latter possibility, however, was not explored as the primary interest was to critically evaluate the measured solubility data for possible outliers.

Table V lists the so-called "best" values of the K_C self-association constants for 1-propanol, 2-propanol, 1-butanol, 2-butanol and 1-octanol calculated *via* eqn. [31] for the 30 binary alkane + alcohol solvent systems for which experimental anthracene solubility data exists. Except for solvent mixtures containing 2-butanol, predicted solubilities differed from observed values by less than 5 %. Readers are reminded that in evaluating the applicability of Mobile Order theory one must realize that these particular systems are highly nonideal. Had an ideal solution been assumed, then the predicted mole fraction solubility would be $x_A = a_A(s) = 0.01049$ (53) at each binary solvent composition, which is between 5 and 25 times larger than the actual experimental values. During the course of these computations it was noted that eqn. [31] always underpredicted the observed anthracene solubilities in all six binary alkane + 2-butanol solvent mixtures. Adjustment of the modified solubility parameter of 2-butanol to $\delta'_{2\text{-butanol}} = 18.0\ J^{1/2}\ cm^{-3/2}$ was found to reduce the deviations considerably. For example, deviations between predicted and observed values were reduced to 2.1 % and 1.4 % in the case of n-hexane + 2-butanol and n-heptane + 2-butanol mixtures, respectively. Very close agreement between observed and calculated values suggests that each data set is internally consistent, which is further supported by the fact that plots of log x_A versus $x_B^{(s)}$ appear as smooth curves with no noticeable outliers.

Inspection of Table V further reveals that the so-called optimum value of the self-association constant for any given alcohol does vary somewhat from one hydrocarbon cosolvent to another. During the course of these computations it was noted that more than one local minima may exist in the K_C versus % deviation plots and that back-calculated mole fraction solubilities are not too sensitive to the numerical assumed for K_C, provided that one is not too far removed from the optimum value. For example, in the case of anthracene dissolved in n-heptane + 1-butanol mixtures the average deviation between observed and calculated values is essentially identical for values of K_C ranging from $K_C = 650\ cm^3\ mol^{-1}$ to $K_C = 750\ cm^3\ mol^{-1}$. Different numerical values of K_C for each of the six cosolvents studied give a nonunique description for the behavior of anthracene in the pure alcohols, thus violating the basic assumption used in deriving eqn. [31]. Mobile Order theory is viewed, therefore, as providing a very reasonable (though by no means perfect) thermodynamic description of anthracene dissolved in binary alkane + alcohol mixtures. While one cannot definitively state why K_C varies, it should be noted that molecular interactions in these systems are undoubtedly more complex than what is incorporated into this particular version of the Mobile Order theory. The aromatic hydrocarbon solute, anthracene, is assumed to be inert and is not permitted to form association complexes with either the monomeric alcohol or any of the *presumed* polymeric entities. Introduction of additional "curve-fit" association parameters for formation of anthracene-alcohol molecular complexes would lead to reduced deviations between observed and calculated values. At this time, however, the slight reduction in percent deviation does not necessarily warrant the increased calculational complexity whenever one realizes that it is possible to predict

TABLE V. Comparison Between Experimental Anthracene Solubilities and Predicted Values Based Upon Equation [31]

	Eqn. [31]		Eqn. [31]	
Component (B) + Component (C)	K_C	% Dev.[a]	K_C^{opt}	% Dev.[a]
n-Hexane + 1-Propanol	5000	2.2	1620	0.8
n-Heptane + 1-Propanol	5000	2.1	2075	1.3
n-Octane + 1-Propanol	5000	2.6	1405	0.8
Cyclohexane + 1-Propanol	5000	6.7	490	0.6
Methylcyclohexane + 1-Propanol	5000	6.3	560	0.8
2,2,4-Trimethylpentane + 1-Propanol	5000	2.8	5000	2.8
n-Hexane + 2-Propanol	5000	4.5	830	0.4
n-Heptane + 2-Propanol	5000	4.5	895	1.3
n-Octane + 2-Propanol	5000	5.9	520	1.5
Cyclohexane + 2-Propanol	5000	11.5	120	0.5
Methylcyclohexane + 2-Propanol	5000	10.9	180	0.5
2,2,4-Trimethylpentane + 2-Propanol	5000	1.9	5000	1.9
n-Hexane + 1-Butanol	5000	2.2	1600	1.3
n-Heptane + 1-Butanol	5000	1.0	3000	0.9
n-Octane + 1-Butanol	5000	2.1	1730	0.8
Cyclohexane + 1-Butanol	5000	4.4	750	0.9
Methylcyclohexane + 1-Butanol	5000	5.4	710	1.3
2,2,4-Trimethylpentane + 1-Butanol	5000	3.2	5000	3.2
n-Hexane + 2-Butanol	5000	10.2[b]	145	1.3
n-Heptane + 2-Butanol	5000	9.0[b]	95	0.7
n-Octane + 2-Butanol	5000	11.0[b]	126	2.1
Cyclohexane + 2-Butanol	5000	14.5[b]	140	5.6
Methylcyclohexane + 2-Butanol	5000	15.1[b]	145	6.3
2,2,4-Trimethylpentane + 2-Butanol	5000	6.4[b]	435	0.3
n-Hexane + 1-Octanol	5000	6.2	250	1.4
n-Heptane + 1-Octanol	5000	3.5	600	0.4
n-Octane + 1-Octanol	5000	2.1	1100	0.5
Cyclohexane + 1-Octanol	5000	3.5	750	0.3
Methylcyclohexane + 1-Octanol	5000	5.4	415	1.3
2,2,4-Trimethylpentane + 1-Octanol	5000	2.8	840	0.5

---

[a] Deviation (%) = $(100/N) \Sigma \left| \ln [x_A(cal)/x_A(exp)] \right|$.

[b] Average deviations were 2.1, 1.4, 3.6, 7.0, 8.3 and 2.7 % for n-hexane, n-heptane, n-octane, cyclohexane, methylcyclohexane and 2,2,4-trimethylpentane, respectively, $\delta'_{2\text{-butanol}} = 18.0\ MPa^{1/2}$.

anthracene solubilities at all 210 binary solvent compositions (seven compositions for each of the 30 binary solvents) to within an average deviation of *circa* 5.7 %, using a single association constant of $K_C = 5{,}000\ \mathrm{cm^3\ mol^{-1}}$.

MOBILE ORDER THEORY FOR BINARY ALCOHOL + ALCOHOL SOLVENT MIXTURES

The success of Mobile Order theory in describing the solubility behavior of anthracene in various alkane + alcohol mixtures prompted Acree and Zvaigzne (54) to extend the basic model to more complex systems having two self-associating alcoholic solvents. Monofunctional alcohols do form self-associated species, and there is no a prior experimental evidence or computational reason to preclude formation of heterogeneous B_iC_j complexes, particularly if a single equilibrium constant is used to describe every monofunctional alcohol's self-association characteristics. For each alcohol, the fraction of time that the alcohol is not involved in hydrogen-bond formation, $\gamma_{B:}$ and $\gamma_{C:}$, is calculated as:

$$\gamma_{B:} = 1/[1 + K_B\ \phi_B/V_{m,B} \quad + \quad K_{BC}\ \phi_C/V_{m,C}\ ] \qquad [32]$$

and

$$\gamma_{C:} = 1/[1 + K_{CB}\ \phi_B/V_{m,B} \quad + \quad K_C\ \phi_C/V_{m,C}\ ] \qquad [33]$$

where K_{BC} and K_{CB} refer to the two additional equilibrium constants needed to describe the formation of the new heterogeneous alcohol-alcohol complexes not found in either neat solvent. It can be readily shown that this set of conditions leads to the following expressions for the Gibbs free energy

$$G = n_A\ \mu_A^* + n_B\ \mu_B^* + n_C\ \mu_C^* + n_B\ RT\ \ln \gamma_{B:} + n_C\ RT\ \ln \gamma_{C:} + 0.5\ RT\ \{n_A \ln \phi_A + n_B \ln \phi_B \\ + n_C \ln \phi_C + n_A \ln x_A + n_B \ln x_B + n_C \ln x_C\ \} + (n_A V_{m,A} + n_B V_{m,B} + n_C V_{m,C}) \\ [\phi_A\ \phi_B\ (\delta_A' - \delta_B')^2 + \phi_A\ \phi_C\ (\delta_A' - \delta_C')^2 + \phi_B\ \phi_C\ (\delta_B' - \delta_C')^2] \qquad [34]$$

and saturation solubility of a sparingly soluble solute

$$RT\ \{\ln (a_A(s)/\phi_A) - 0.5[1 - V_{m,A}/(x_B^{(s)} V_{m,B} + x_C^{(s)} V_{m,C})] + 0.5 \ln [V_{m,A}/(x_B^{(s)} V_{m,B} + x_C^{(s)} V_{m,C})] \\ - (V_{m,A}/V_{m,B})\ RT\ \phi_B^{(s)}\ [\phi_B^{(s)}\ (K_B/V_{m,B}) + \phi_C^{(s)}\ (K_{BC}/V_{m,C})]/[1 + \phi_B^{(s)}\ (K_B/V_{m,B}) \\ + \phi_C^{(s)}\ (K_{BC}/V_{m,C})] - (V_{m,A}/V_{m,C})\ RT\ \phi_C^{(s)}\ [\phi_B^{(s)}\ (K_{CB}/V_{m,B}) + \phi_C^{(s)}\ (K_C/V_{m,C})] + \\ [1 + \phi_B^{(s)}\ (K_{CB}/V_{m,B}) + \phi_C^{(s)}\ (K_C/V_{m,C})]\} = V_{m,A}\ [\phi_B^{(s)}\ (\delta_A' - \delta_B')^2 + \phi_C^{(s)}\ (\delta_A' - \delta_C')^2 \\ - \phi_B^{(s)}\ \phi_C^{(s)}\ (\delta_B' - \delta_C')^2] \qquad [35]$$

To shorten the mathematical derivation, the approximation that $\delta_{solvent}' = \phi_B^{(s)}\ \delta_B' + \phi_C^{(s)}\ \delta_C'$ has been invoked at the outset, hence $V_{m,A}\ [\phi_B^{(s)}\ (\delta_A' - \delta_B')^2 + \phi_C^{(s)}\ (\delta_A' - \delta_C')^2 - \phi_B^{(s)}\ \phi_C^{(s)}\ (\delta_B' - \delta_C')^2]$, rather than $\phi_{solvent}^2\ V_{m,A}(\delta_A' - \delta_{solvent}')^2$ (see eqn. [26]), describes nonideality arising from nonspecific physical interactions.

Careful examination of eqn. [35] reveals that, for model systems obeying the Mobile Order theory, the $(\delta_A' - \delta_B')^2$ and $(\delta_A' - \delta_C')^2$ terms can be eliminated from the basic model *via*

$$RT\ \{\ln [a_A(s)/(\phi_A)_B] - 0.5(1 - V_{m,A}/V_{m,B}) + 0.5 \ln (V_{m,A}/V_{m,B}) \\ - (V_{m,A}\ K_B/V_{m,B}^2)/(1 + K_B/V_{m,B})\} = V_{m,A}\ (\delta_A' - \delta_B')^2 \qquad [36]$$

and

$$RT\ \{\ln [a_A(s)/(\phi_A)_C] - 0.5(1 - V_{m,A}/V_{m,C}) + 0.5 \ln (V_{m,A}/V_{m,C}) \\ - (V_{m,A}\ K_C/V_{m,C}^2)/(1 + K_C/V_{m,C})\} = V_{m,A}\ (\delta_A' - \delta_C')^2 \qquad [37]$$

where $(\phi_A^{sat})_B$ and $(\phi_A^{sat})_C$ denote the solubilities in the two pure solvents. After removal of the $(\delta_A' - \delta_B')^2$ and $(\delta_A' - \delta_C')^2$ terms, one obtains a relatively simple mathematical expression for the solubility in a binary solvent mixture

$$\begin{aligned}\ln \phi_A = {} & \phi_B{}^{(s)} \ln (\phi_A)_B + \phi_C{}^{(s)} \ln (\phi_A)_C - 0.5 [\ln (x_B{}^{(s)} V_{m,B} + x_C{}^{(s)} V_{m,C}) - \phi_B{}^{(s)} \ln V_{m,B} \\ & - \phi_C{}^{(s)} \ln V_{m,C}] - (V_{m,A}/V_{m,B}) \phi_B{}^{(s)} [\phi_B{}^{(s)} (K_B/V_{m,B}) + \phi_C{}^{(s)} (K_{BC}/V_{m,C})] \\ & + [1 + \phi_B{}^{(s)} (K_B/V_{m,B}) + \phi_C{}^{(s)} (K_{BC}/V_{m,C})] + (V_{m,A} K_B \phi_B{}^{(s)}/V_{m,B}{}^2)(1 + K_B/V_{m,B})^{-1} \\ & - (V_{m,A}/V_{m,C}) \phi_C{}^{(s)} [\phi_B{}^{(s)} (K_{CB}/V_{m,B}) + \phi_C{}^{(s)} (K_C/V_{m,C})]/[1 + \phi_B{}^{(s)} (K_{CB}/V_{m,B}) \\ & + \phi_C{}^{(s)} (K_C/V_{m,C})] + (V_{m,A} K_C \phi_C{}^{(s)}/V_{m,C}{}^2)(1 + K_C/V_{m,C})^{-1} \\ & + V_{m,A} \phi_B^{(s)} \phi_C^{(s)} (\delta_B' - \delta_C')^2 (RT)^{-1} \qquad [38]\end{aligned}$$

which like eqn. [31] correctly describes the solubility in both pure self-associating solvents.

The predictive ability of eqn. [38] is summarized in the last column of Table VI, in the form of the average absolute deviation between calculated and observed anthracene solubilities for the seven binary alcohol + alcohol systems studied. The algebraic sign indicates that all deviations for the given system had the same sign, as would be the case if eqn. [38] overestimated (or alternatively underestimated) the mole fraction solubility at each of the seven binary solvent compositions. All Mobile Order theory predictions assumed identical numerical values for the four hydrogen-bonded association constants of $K_B = K_C = K_{BC} = K_{CB} = 5{,}000$ cm^3 mol^{-1}. Careful examination of Table VI reveals that eqn. [38] does provide very reasonable solubility predictions, with the average absolute deviation between calculated and observed being on the order of 1.7 %.

Readers are reminded that it is fundamentally impossible to prove that a particular model is correct. One can demonstrate, however, that a model is consistent with a wide range of experimental observations. Similarly, it can be shown that a given model is inconsistent with experimental data so that the model must be either incorrect or incomplete. In the case of Mobile Order theory, one started with the prior knowledge that the basic model reasonably described experimental solubilities of anthracene, biphenyl, carbazole, naphthalene, phenanthrene, pyrene and methylparaben in a wide range of neat organic solvents. The expressions presented here document that Mobile Order theory provides a fairly accurately mathematical description of anthracene solubilities in binary alkane + alcohol and binary alcohol + alcohol solvent mixtures. The ability to accurately describe experimental solubility data with semi-empirical thermodynamic models ensures, in part, that the measured values are internally consistent with each other. Models, such as Mobile Order theory, do provide a convenient (and sometimes the only) means for assessing the reliability of measured solubility data in binary solvent mixtures, particularly in those many instances for which only a single set of measurements exist.

TABLE VI. Summarized Comparison Between Experimental Anthracene Solubilities and Predicted Values Based Upon Equation [37] Derived From Mobile Order Theory for Two Hydrogen-Bonding Alcohol Cosolvents

Solvent (B) + Solvent (C)	% Dev.[a]
1-Butanol + 1-Propanol	- 1.0
2-Butanol + 1-Propanol	0.5
2-Propanol + 1-Propanol	1.5
1-Octanol + 1-Propanol	- 2.9
1-Butanol + 2-Propanol	- 1.9
2-Butanol + 2-Propanol	0.3
1-Octanol + 2-Butanol	- 4.1
AVERAGE ABSOLUTE DEVIATION	1.7

[b] Deviation (%) = $(100/N)\ \Sigma\ |\ln [x_A(cal)/x_A(exp)]|$. The algebraic sign indicates that all deviations were of the same sign.

MATHEMATICAL REPRESENTATION OF SOLUBILITY DATA IN BINARY SOLVENTS

Expressions for predicting the thermodynamic properties of ternary nonelectrolyte systems have served as the point of departure for mathematical representation of experimental excess molar Gibbs energy, excess molar heat capacity, excess molar enthalpy and excess molar volume data. Differences between predicted and observed values are expressed as

$$(Z^E_{ABC})^{exp} - (Z^E_{ABC})^{calc} = x_A\ x_B\ x_C\ Q_{ABC} \qquad [39]$$

with Q-functions of varying complexity. For most systems encountered, the experimental data can be adequately represented by a power series expansion

$$Q_{ABC} = A_{ABC} + \Sigma\ B_{AB}^{(i)}\ (x_A - x_B)^i + \Sigma\ B_{AC}^{(j)}\ (x_A - x_C)^j + \Sigma\ B_{BC}^{(k)}\ (x_B - x_C)^k \qquad [40]$$

though rarely are experimental data determined with sufficient precision to justify more than a few parameters.

Conceptually, these ideas can be extended to solute solubilities in binary solvent mixtures, however, there has never been up until this volume a sufficiently large solid solute solubility data base to warrant computerized storage in equational form. With computerized data storage and retrieval becoming increasingly popular, it seems appropriate to review the various mathematical expressions that have been proposed in the chemical literature for describing the variation of solute solubility with binary solvent composition. Like the predictive expressions discussed in the preceding sections, mathematical representations provide not only a means to screen experimental data sets for possible outliers in need of redetermination, but also facilitate interpolation at solvent compositions falling between measured data points.

Acree and coworkers (23,24) suggested possible mathematical representations for isothermal solubility data based upon either a Combined NIBS/Redlich-Kister model

$$\ln x_A = x_B^{(s)} \ln (x_A)_B + x_C^{(s)} \ln (x_A)_C + x_B^{(s)} x_C^{(s)} \Sigma \; S_i \, (x_B^{(s)} - x_C^{(s)})^i \qquad [41]$$

or Modified Wilson equation

$$\begin{aligned}\ln (a_A(s)/x_A) \approx 1 &- x_B^{(s)} \{1 - \ln [a_A(s)/(x_A)_B]\}/(x_B^{(s)} + x_C^{(s)} \Lambda_{BC}^{adj}) \\ &- x_C^{(s)} \{1 - \ln [a_A(s)/(x_A)_C]\}/(x_B^{(s)} \Lambda_{CB}^{adj} + x_C^{(s)}) \qquad [42]\end{aligned}$$

where the various S_i and Λ_{ij}^{adj} "curve-fit" parameters can be evaluated via least squares analysis. A summarized comparison presenting the descriptive abilities of eqns. [42] and [41] is given in Tables VII and VIII, respectively. The actual solubilities are given in the data compilation portion of this volume. Careful examination of Tables VII and VIII reveals that both equations provide a reasonable mathematical representation of the anthracene solubility data in all systems considered. Back-calculated and observed values generally differ by less than ± 1 %, which is comparable to the quoted experimental uncertainty. There may be one or two individual data points with each system, however, for which deviations may exceed ± 2 %.

Both expressions describe the synergistic solubility behavior evidenced by the maxima in the anthracene mole fraction solubility versus solvent composition curves for such solvent mixtures as 3-methyl-1-butanol with hexane, cyclohexane, methylcyclohexane and 2,2,4-trimethylpentane. Synergistic behavior is in line with published studies (55-61) involving nonpolar and stable intramolecularly hydrogen-bonded solutes dissolved in binary hydrocarbon + alcohol, halohydrocarbon + alcohol, and cyclohexane + methylene iodide mixtures. Excellent agreement between experimental values and those back-calculated from the Combined NIBS/Redlich-Kister and Modified Wilson equations further document the internal consistency of the anthracene solubility data. For these systems there were no other convenient means to critically evaluate the published isothermal solubility data. In all of the computations performed to date, I failed to find any experimental data in need of redetermination.

TABLE VII. Mathematical Representation of Anthracene Solubilities in Select Binary Mixtures using the Modified Wilson Equation

Solvent (B) + Solvent (C)	Λ_{ij}^{adj}[a]	% Dev.[b]
t-Butylcyclohexane + 2,2,4-trimethylpentane	1.453 0.981	0.1
n-Hexane + 1-propanol	1.360 1.440	0.5
n-Heptane + 1-propanol	1.410 1.580	0.7
n-Octane + 1-propanol	1.240 1.880	0.6
Cyclohexane + 1-propanol	1.300 1.600	1.6
Methylcyclohexane + 1-propanol	1.344 1.667	1.4
2,2,4-Trimethylpentane + 1-propanol	1.100 1.500	0.6
t-Butylcyclohexane + 1-propanol	1.225 2.321	1.0
n-Hexane + 2-propanol	1.409 1.605	0.7
n-Heptane + 2-propanol	0.962 2.085	0.6
n-Octane + 2-propanol	0.913 2.365	0.3
Cyclohexane + 2-propanol	1.657 1.701	0.5
Methylcyclohexane + 2-propanol	1.689 1.801	0.6
2,2,4-Trimethylpentane + 2-propanol	0.956 1.797	0.3
t-Butylcyclohexane + 2-propanol	1.378 2.557	1.4
n-Hexane + 1-butanol	1.690 1.088	0.4
n-Heptane + 1-butanol	1.476 1.291	0.5
n-Octane + 1-butanol	1.460 1.500	0.5
Cyclohexane + 1-butanol	2.377 1.010	0.5
Methylcyclohexane + 1-butanol	2.387 1.080	0.9
2,2,4-Trimethylpentane + 1-butanol	2.600 0.680	1.8
t-Butylcyclohexane + 1-butanol	1.525 1.689	0.7
n-Hexane + 2-butanol	1.477 1.481	0.5
n-Heptane + 2-butanol	1.109 1.849	0.3
n-Octane + 2-butanol	0.949 2.205	0.4

TABLE VII. (Continued)

Cyclohexane + 2-butanol	2.157 1.345	0.5
Methylcyclohexane + 2-butanol	1.885 1.593	0.6
2,2,4-Trimethylpentane + 2-butanol	1.097 1.633	0.4
t-Butylcyclohexane + 2-butanol	1.325 2.225	0.5
n-Hexane + 1-octanol	2.501 0.601	0.6
n-Heptane + 1-octanol	2.201 0.685	0.3
n-Octane + 1-octanol	1.901 0.801	0.2
Cyclohexane + 1-octanol	4.733 0.213	0.4
Methylcyclohexane + 1-octanol	9.568 0.102	0.2
2,2,4-Trimethylpentane + 1-octanol	2.009 0.493	0.3
t-Butylcyclohexane + 1-octanol	3.097 0.577	0.3
n-Hexane + 2-methyl-1-propanol	1.557 1.417	0.6
n-Heptane + 2-methyl-1-propanol	1.265 1.721	0.5
n-Octane + 2-methyl-1-propanol	1.141 1.969	0.5
Cyclohexane + 2-methyl-1-propanol	2.197 1.249	0.6
Methylcyclohexane + 2-methyl-1-propanol	1.961 1.501	0.9
2,2,4-Trimethylpentane + 2-methyl-1-propanol	1.133 1.525	0.9
t-Butylcyclohexane + 2-methyl-1-propanol	1.345 2.017	0.5
n-Hexane + 3-methyl-1-butanol	1.709 1.149	0.3
n-Heptane + 3-methyl-1-butanol	1.437 1.341	0.3
n-Octane + 3-methyl-1-butanol	1.477 1.529	0.2
Cyclohexane + 3-methyl-1-butanol	2.449 0.977	0.3
Methylcyclohexane + 3-methyl-1-butanol	2.453 1.061	0.4
2,2,4-Trimethylpentane + 3-methyl-1-butanol	1.449 1.121	0.2
t-Butylcyclohexane + 3-methyl-1-butanol	1.701 1.561	0.4
1-Butanol + 1-propanol	1.293 0.857	0.2
2-Propanol + 1-propanol	0.953 1.073	0.5

TABLE VII. (Continued)

2-Butanol + 1-propanol	1.000 1.000	0.3
1-Octanol + 1-propanol	0.453 2.213	0.4
1-Butanol + 2-propanol	1.169 0.989	0.5
2-Butanol + 2-propanol	0.689 1.429	0.1
1-Octanol + 2-butanol	0.505 1.937	0.6

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[a] Adjustable parameters for the Modified Wilson equation are ordered as Λ_{BC}^{adj} and then Λ_{CB}^{adj}.

[b] % Dev. = $(100/N) \Sigma \mid \ln [x_A(\text{cal})/x_A(\text{exp})] \mid$.

TABLE VIII. Mathematical Representation of Anthracene Solubilities in Select Binary Solvent Mixtures using the Combined NIBS/Redlich-Kister Equation

Solvent (B) + Solvent (C)	S_i	% Dev^a	S_i	% Dev^a
t-Butylcyclohexane + 2,2,4-trimethylpentane	0.225	0.2	1.453	0.1
	0.042		0.981	
			4.024	
n-Hexane + 1-propanol	1.033	0.5	0.982	0.2
	- 0.121		- 0.075	
			0.186	
n-Heptane + 1-propanol	1.184	1.0	1.098	0.4
	- 0.182		- 0.106	
			0.324	
n-Octane + 1-propanol	1.340	0.9	1.275	0.3
	- 0.361		- 0.290	
			0.250	
Cyclohexane + 1-propanol	1.207	1.0	1.121	0.5
	0.015		0.040	
			0.256	
Methylcyclohexane + 1-propanol	1.291	0.8	1.235	0.5
	0.047		0.088	
			0.204	
2,2,4-Trimethylpentane + 1-propanol	0.892	0.9	0.825	0.4
	- 0.192		- 0.103	
			0.291	
t-Butylcyclohexane + 1-propanol	1.725	2.5	1.519	1.0
	- 0.807		- 0.526	
			0.841	
n-Hexane + 2-propanol	1.466	1.4	1.367	0.3
	- 0.324		- 0.239	
			0.372	
n-Heptane + 2-propanol	1.639	1.9	1.491	0.3
	- 0.735		- 0.587	
			0.566	
n-Octane + 2-propanol	1.838	1.9	1.687	0.6
	- 1.002		- 0.787	
			0.645	
Cyclohexane + 2-propanol	1.659	1.0	1.589	0.3
	- 0.176		- 0.143	
			0.248	
Methylcyclohexane + 2-propanol	1.812	1.6	1.703	0.4
	- 0.252		- 0.182	
			0.386	
2,2,4-Trimethylpentane + 2-propanol	1.277	1.1	1.193	0.3
	- 0.471		- 0.369	
			0.333	
t-Butylcyclohexane + 2-propanol	2.346	3.9	2.030	0.9
	- 1.209		- 0.746	
			1.343	
n-Hexane + 1-butanol	0.703	0.5	0.737	0.4
	0.183		0.165	
			- 0.124	
n-Heptane + 1-butanol	0.779	0.8	0.723	0.2
	- 0.032		0.004	
			0.201	

TABLE VIII. (Continued)

n-Octane + 1-butanol	0.933	0.6	0.909	0.4
	- 0.033		- 0.014	
			0.088	
Cyclohexane + 1-butanol	0.810	0.9	0.741	0.5
	0.336		0.345	
			0.223	
Methylcyclohexane + 1-butanol	0.948	1.1	0.850	1.0
	0.282		0.146	
			0.295	
2,2,4-Trimethylpentane + 1-butanol	0.576	0.5	0.536	0.3
	0.121		0.151	
			0.142	
t-Butylcyclohexane + 1-butanol	1.134	1.2	1.039	0.4
	- 0.210		- 0.109	
			0.372	
n-Hexane + 2-butanol	1.165	0.3		
	- 0.081			
n-Heptane + 2-butanol	1.225	0.2		
	- 0.292			
n-Octane + 2-butanol	1.458	1.3		
	- 0.618			
Cyclohexane + 2-butanol	1.260	0.6		
	0.206			
Methylcyclohexane + 2-butanol	1.447	1.2		
	- 0.009			
2,2,4-Trimethylpentane + 2-butanol	1.070	0.8		
	- 0.213			
t-Butylcyclohexane + 2-butanol	1.718	1.7	1.588	0.3
	- 0.612		- 0.493	
			0.497	
n-Hexane + 1-octanol	0.748	1.9	0.607	0.8
	0.488		0.448	
			0.479	
n-Heptane + 1-octanol	0.488	0.6	0.442	0.3
	0.231		0.229	
			0.159	
n-Octane + 1-octanol	0.330	0.1		
	0.135			
Cyclohexane + 1-octanol	0.518	1.6	0.400	0.7
	0.421		0.358	
			0.431	
Methylcyclohexane + 1-octanol	0.574	2.4	0.397	1.0
	0.594		0.549	
			0.614	
2,2,4-Trimethylpentane + 1-octanol	0.469	0.3		
	0.247			
t-Butylcyclohexane + 1-octanol	0.428	0.9		
	0.236			
n-Hexane + 2-methyl-1-propanol	1.267	1.2	1.177	0.5
	- 0.080		- 0.032	
			0.322	

TABLE VIII. (Continued)

n-Heptane + 2-methyl-1-propanol	1.356	1.1	1.284	0.7
	- 0.350		- 0.301	
			0.266	
n-Octane + 2-methyl-1-propanol	1.540	1.4	1.422	0.4
	- 0.570		- 0.464	
			0.447	
Cyclohexane + 2-methyl-1-propanol	1.214	1.3	1.116	0.3
	0.148		0.172	
			0.341	
Methylcyclohexane +	1.462	1.8	1.342	0.6
2-methyl-1-propanol	- 0.070		0.121	
			0.430	
2,2,4-Trimethylpentane +	1.090	1.5	0.972	0.4
2-methyl-1-propanol	- 0.221		- 0.100	
			0.462	
t-Butylcyclohexane +	1.688	1.4	1.576	0.1
2-methyl-1-propanol	- 0.549		- 0.435	
			0.432	
n-Hexane + 3-methyl-1-butanol	0.857	0.8		
	0.186			
n-Heptane + 3-methyl-1-butanol	0.802	0.3		
	0.021			
n-Octane + 3-methyl-1-butanol	1.014	0.6		
	- 0.112			
Cyclohexane + 3-methyl-1-butanol	0.786	1.1		
	0.378			
Methylcyclohexane + 3-methyl-1-butanol	0.880	0.9		
	0.358			
2,2,4-Trimethylpentane +	0.663	0.3		
3-methyl-1-butanol	0.095			
t-Butylcyclohexane +	1.092	0.5		
3-methyl-1-butanol	- 0.087			
1-Butanol + 1-propanol	0.117	0.3		
	0.015			
2-Propanol + 1-propanol	0.068	0.7		
	0.058			
2-Butanol + 1-propanol	0.000	0.3		
	0.000			
1-Octanol + 1-propanol	1.025	1.2		
	- 0.575			
1-Butanol + 2-propanol	0.243	0.6		
	- 0.011			
2-Butanol + 2-propanol	0.097	0.1		
	- 0.013			
1-Octanol + 2-butanol	0.871	1.1		
	- 0.335			

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[a] % Dev. = $(100/N) \Sigma \left| \ln [x_A(\text{cal})/x_A(\text{exp})] \right|$.

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ACENAPHTHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-octadecane
cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,2,3,4-tetrahydronaphthalene
1,2-dimethylbenzene
1,2,4,5-tetramethylbenzene
naphthalene
2-methylnaphthalene
2,6-dimethylnaphthalene
2,7-dimethylnaphthalene
anthracene
phenanthrene
fluorene
chrysene
fluoranthene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

trichloromethane
tetrachloromethane

G. Alcohols

methanol
ethanol
1-propanol
1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene
1,2,3,5-tetranitrobenzene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) n-Octadecane; $C_{18}H_{38}$; [593-45-3]

ORIGINAL MEASUREMENTS:

Djordjevic, N.M.

Thermochim. Acta 1991, *177*, 109-118.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
352.4	0.3075	0.6925	363.5	0.0792	0.9208
356.2	0.2410	0.7590			
359.0	0.1815	0.8185			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter.

Mixtures (1.5 - 2.0 mg) of known concentration were weighed into aluminum pans, which were then crimped to preclude sample loss during the heating process. Solubilities determined by measuring melting points of binary mixtures using a Perkin-Elmer DSC-2 differential scanning calorimeter and scan rate of 5 K/min.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (compiler).
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 3854-3857.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
308.7	0.9120	0.0880	330.2	0.7188	0.2812
323.2	0.7923	0.2077	334.0	0.6547	0.3453

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.

(2) Purity, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.

J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
303.35	0.9147	0.0853	329.95	0.7016	0.2984
307.35	0.8969	0.1031	334.65	0.6303	0.3697
312.05	0.8726	0.1274	339.85	0.5355	0.4645
316.45	0.8435	0.1565	346.45	0.4008	0.5992
320.95	0.8069	0.1931	354.45	0.2258	0.7742
325.65	0.7579	0.2421			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.7	0.8761	0.1239	327.8	0.6698	0.3302
310.9	0.8127	0.1873	336.0	0.5523	0.4477
318.7	0.7504	0.2496	348.3	0.3403	0.6597

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.
(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.

J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.55	0.7747	0.2253	335.95	0.4899	0.5101
312.95	0.7276	0.2724	345.75	0.3502	0.6498
319.85	0.6691	0.3309			
328.05	0.5842	0.4158			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
303.8	0.8185	0.1815
314.6	0.7460	0.2540
336.4	0.5269	0.4731
342.6	0.4448	0.5552

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Gesellschaft fur Teerverwertung, passed over an alumina column with benzene eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Speyers, C.L.

Am. J. Sci. 1902, *14*, 293-302.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9212	0.0788	314.8	0.7071	0.2929
283.5	0.8924	0.1076	334.7	0.5492	0.4508
297.3	0.8347	0.1653			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.

(2) Purity not given, Kahlbaum, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 8 % (relative error, compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
308.1	0.7479	0.2521	343.7	0.3825	0.6175
312.6	0.7151	0.2849	351.9	0.2539	0.7461
322.2	0.6359	0.3641			
331.9	0.5305	0.4695			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 1,2-Dimethylbenzene; C_8H_{10}; [95-47-6]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
247.2	1.000	0.000
246.7	0.978	0.022
246.2	0.956	0.044
245.4	0.945	0.055
253.3	0.935	0.065
261.0	0.917	0.083
271.2	0.886	0.114
287.3	0.821	0.179
302.2	0.739	0.261
313.8	0.653	0.347
324.7	0.564	0.436
332.2	0.488	0.512
342.7	0.362	0.638
351.7	0.249	0.751
359.6	0.136	0.864
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,2,4,5-Tetramethylbenzene; $C_{10}H_{14}$; [95-93-2]	Kravchenko, V.M.; Pastukhova, I.S. *Zhur. Fiz. Khim.* 1957, *31*, 1802-1811.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
352.2	1.000	0.000
347.9	0.918	0.082
344.3	0.856	0.146
338.2	0.769	0.231
332.1	0.689	0.311
323.6	0.577	0.423
324.6	0.562	0.438
325.7	0.553	0.447
328.2	0.525	0.475
331.6	0.487	0.513
338.9	0.410	0.590
347.4	0.303	0.697
354.5	0.207	0.793
363.7	0.072	0.928
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Naphthalene; $C_{10}H_8$; [91-20-3]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
353.2	1.000	0.000
343.3	0.849	0.151
334.1	0.718	0.282
329.2	0.654	0.346
325.0	0.604	0.396
323.2	0.583	0.417
327.0	0.541	0.459
335.7	0.450	0.550
344.7	0.344	0.656
351.3	0.257	0.743
361.8	0.107	0.893
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
307.3	1.000	0.000
300.2	0.901	0.099
297.2	0.860	0.140
292.7	0.807	0.193
290.9	0.788	0.212
293.0	0.773	0.227
301.9	0.724	0.276
309.0	0.681	0.319
318.7	0.615	0.385
328.7	0.524	0.476
337.0	0.435	0.565
345.9	0.320	0.680
353.5	0.216	0.784
358.4	0.148	0.852
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
383.2	1.000	0.000
374.5	0.846	0.154
366.9	0.728	0.272
360.2	0.626	0.374
349.0	0.504	0.496
344.4	0.440	0.560
339.7	0.402	0.598
342.9	0.365	0.635
348.2	0.294	0.706
356.1	0.183	0.817
363.5	0.076	0.924
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 2,7-Dimethylnaphthalene; $C_{12}H_{12}$; [582-16-1]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
370.2	1.000	0.000
364.4	0.904	0.096
361.0	0.858	0.142
354.4	0.756	0.244
347.3	0.650	0.350
340.2	0.555	0.445
335.3	0.496	0.504
333.9	0.469	0.531
334.8	0.449	0.551
338.7	0.420	0.580
344.3	0.348	0.652
352.9	0.214	0.786
360.7	0.100	0.900
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Anthracene; $C_{14}H_{10}$; [120-12-7]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
489.7	1.000	0.000
477.2	0.822	0.178
466.2	0.706	0.294
456.2	0.590	0.410
443.2	0.484	0.516
434.2	0.397	0.603
418.2	0.294	0.706
402.5	0.216	0.784
387.5	0.156	0.844
368.2	0.104	0.896
361.2	0.086	0.914
362.7	0.071	0.929
364.4	0.051	0.949
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Phenanthrene; $C_{14}H_{10}$; [85-01-8]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M.; Pastukhova, I.S. *Zhur. Fiz. Khim.* 1957, *31*, 1802-1811.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
372.5	1.000	0.000
357.4	0.801	0.199
347.7	0.707	0.293
338.7	0.614	0.386
329.0	0.508	0.492
334.5	0.459	0.541
339.1	0.401	0.599
346.7	0.314	0.686
355.0	0.204	0.796
362.0	0.099	0.901
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Fluorene; $C_{16}H_{10}$; [86-73-7]	Kravchenko, V.M.; Pastukhova, I.S. *Zhur. Fiz. Khim.* 1957, *31*, 1802-1811.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
387.2	1.000	0.000
379.6	0.889	0.111
367.9	0.746	0.254
356.0	0.619	0.381
348.1	0.528	0.472
339.3	0.438	0.562
337.8	0.418	0.582
340.9	0.382	0.618
348.2	0.293	0.707
355.6	0.194	0.806
361.7	0.103	0.897
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) Chrysene; $C_{18}H_{12}$; [218-01-9]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M.; Pastukhova, I.S. *Proc. Acad. Sci. U.S.S.R., Sect. Chem.* 1956, *111*, 667-669 (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
528.2	1.000	0.000
513.2	0.853	0.147
500.2	0.722	0.278
477.8	0.613	0.387
471.5	0.501	0.499
457.0	0.404	0.596
437.4	0.296	0.704
416.2	0.204	0.796
378.5	0.101	0.899
364.2	0.072	0.928
366.4	0.034	0.966
368.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Fluoranthene; $C_{16}H_{10}$; [206-44-0]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

J. Gen. Chem. U.S.S.R. 1959, *29*, 29-34.
(English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
383.2	1.000	0.000
368.8	0.815	0.185
363.4	0.752	0.248
350.7	0.606	0.394
340.8	0.492	0.508
335.0	0.438	0.562
335.3	0.429	0.571
339.4	0.388	0.612
348.2	0.293	0.707
358.1	0.163	0.837
362.3	0.092	0.908
368.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Trichloromethane; $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Speyers, C.L.

Am. J. Sci. 1902, *14*, 293-302.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
273.0	0.8728	0.1272
284.4	0.8346	0.1654
325.9	0.5783	0.4219

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.

(2) Purity unknown, several sources listed, washed with water, sulfuric acid, dried over calcium chloride and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 8 % (relative error, compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

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

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 2485-2488.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
303.2	0.8195	0.1805	325.2	0.6415	0.3585
314.6	0.7373	0.2627			
318.6	0.7013	0.2987			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.

(2) AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Speyers, C.L.

Am. J. Sci. 1902, *14*, 293-302.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9961	0.0039	319.2	0.9845	0.0155
285.6	0.9962	0.0038	335.5	0.9754	0.0246
303.9	0.9927	0.0073			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.

(2) Marked "Acetonfrei", from Kahlbaum, dried over calcium oxide and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 8 % (relative error, compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Speyers, C.L.

Am. J. Sci. 1902, *14*, 293-302.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9943	0.0057	323.0	0.9614	0.0386
283.2	0.9916	0.0084	344.8	0.8706	0.1294
303.5	0.9830	0.0170			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.

(2) Marked absolute, from Eimer and Amend and Chas. Cooper and Co., dried over calcium oxide and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 8 % (relative error, compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Speyers, C.L.

Am. J. Sci. 1902, *14*, 293-302.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
273.2	0.9912	0.0088	323.5	0.9563	0.0437
283.7	0.9903	0.0097	346.6	0.801	0.199
304.3	0.9812	0.0188			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Experimental procedure only marginally described by author. Excess solute and solvent were equilibrated in a constant temperature water bath for between 10-30 minutes. Saturated solution was withdrawn through a coarse filter and analyzed by specific gravity. Author noted that evaporation to dryness and weighing the residue was subject to too much decomposition.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Kahlbaum, was recrystallized from alcohol to a melting point temperature of 93.5 °C.

(2) Purity not given, Kahlbaum, was dried over calcium oxide and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 8 % (relative error, compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.2561

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.7	0.7898	0.2102	343.7	0.3890	0.6110
320.0	0.6834	0.3166			
332.9	0.5408	0.4592			
337.5	0.4809	0.5191			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.3	0.7416	0.2584	344.8	0.3572	0.6428
319.6	0.6458	0.3542			
328.4	0.5593	0.4407			
335.7	0.4776	0.5224			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.2 %, British Drug Houses, United Kingdom, was recrystallized and then zone refined.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Acenaphthene; $C_{12}H_{10}$; [83-32-9] (2) 1,2,3,5-Tetranitrobenzene; $C_6H_2N_4O_8$; [3698-53-1]	Shinomiya, C. *J. Chem. Soc. Japan* 1940, *15*, 259-270.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
399.2	1.000	0.000
388.2	0.802	0.198
382.2	0.706	0.296
381.7	0.572	0.428
383.2	0.470	0.530
381.2	0.429	0.571
372.2	0.290	0.710
362.7	0.235	0.765
348.2	0.118	0.882
361.7	0.099	0.901
369.2	0.000	1.000

Author reports formation of a 1:1 acenaphthene - 1,2,3,5-tetranitrobenzene molecular compound having a melting point temperature of 383.7 K. Two eutectic points occur at x_1 = 0.358 and T/K = 375.2, and at x_1 = 0.810 and T/K = 349.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

ACRIDINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
1,2,3,4-tetrahydronaphthalene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Acridine; $C_{13}H_9N$; [260-94-6]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.3	0.9791	0.0209	353.3	0.7550	0.2450
320.3	0.9697	0.0303	356.1	0.7029	0.2971
330.9	0.9508	0.0492			
345.4	0.8931	0.1069			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acridine; $C_{13}H_9N$; [260-94-6]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.0	0.9705	0.0295	354.7	0.6791	0.3209
320.7	0.9537	0.0463	358.1	0.6037	0.3963
335.0	0.9031	0.0969			
345.7	0.8150	0.1850			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to a purity of 99.87 %.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acridine; $C_{13}H_9N$; [260-94-6]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
296.3	0.8996	0.1004	330.3	0.7122	0.2878
304.7	0.8680	0.1320	335.6	0.6559	0.3441
317.2	0.8002	0.1998			
324.2	0.7587	0.2413			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Acridine; $C_{13}H_9N$; [260-94-6]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.2	0.8517	0.1483	331.3	0.6956	0.3044
306.9	0.8409	0.1591	336.7	0.6537	0.3463
316.3	0.8023	0.1977			
322.4	0.7608	0.2392			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was vacuum sublimed to a final purity of 99.87 %.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Acridine; $C_{13}H_9N$; [260-94-6]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.7	0.8385	0.1615	339.1	0.5899	0.4101
309.3	0.7986	0.2014	339.9	0.5616	0.4384
322.9	0.7209	0.2791			
328.5	0.6600	0.3400			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Acridine; $C_{13}H_9N$; [260-94-6]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
302.1	0.8203	0.1797	331.6	0.6497	0.3503
304.1	0.8024	0.1976	337.9	0.6115	0.3885
314.2	0.7563	0.2437			
325.0	0.7056	0.2944			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Kodak Chemical Company, Rochester, New York, USA, was purified by vacuum sublimation to purity of 99.87 %.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
n-hexadecane
n-octadecane
cyclohexane
methylcyclohexane
cyclooctane
2,2,4-trimethylpentane
t-butylcyclohexane
squalane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,4-dimethylbenzene
4-isopropyl methylbenzene
acenaphthene
chrysene
fluoranthene
1,2,3,4-tetrahydronaphthalene

D. Esters

ethyl ethanoate
butyl ethanoate
dimethyl hexanedioate
diethyl hexanedioate
dibutyl oxalate

E. Ethers

1,1-oxybisethane
1,1-oxybisbutane
tetrahydrofuran
tetrahydropyran
1,4-dioxane

F. Haloalkanes and Haloaromatic Hydrocarbons

trichloromethane
tetrachloromethane
iodoethane
1-chlorobutane
1,4-dichlorobutane
trichloroethylene
iodobenzene
bromobenzene
chlorobenzene

G. Alcohols

methanol
1-propanol
2-propanol
1-butanol
2-butanol
2-methyl-1-propanol
3-methyl-1-butanol
1-octanol
phenol
1-hydroxy-2-methylbenzene

H. Ketones

2-propanone
2-butanone

I. Miscellaneous Pure Solvents

acetonitrile
carbon disulfide
acetic anhydride
dimethyl sulfoxide
nitrobenzene
aniline
pyridine
quinoline
thiophene
methoxybenzene
1-methyl-2-pyrrolidinone
N,N-dimethylacetamide
N,N-dimethylformamide
tetramethylene sulfone
tributyl phosphate
1,2,3,5-tetranitrobenzene
2,4,6-trinitrophenol

J. Binary Solvent Mixtures

t-butylcyclohexane + 2,2,4-trimethylpentane
n-hexane + 1-propanol
n-heptane + 1-propanol
n-octane + 1-propanol
cyclohexane + 1-propanol
methylcyclohexane + 1-propanol
2,2,4-trimethylpentane + 1-propanol
t-butylcyclohexane + 1-propanol
n-hexane + 2-propanol
n-heptane + 2-propanol
n-octane + 2-propanol
cyclohexane + 2-propanol
methylcyclohexane + 2-propanol
2,2,4-trimethylpentane + 2-propanol
t-butylcyclohexane + 2-propanol
n-hexane + 1-butanol
n-heptane + 1-butanol

n-octane + 1-butanol
cyclohexane + 1-butanol
methylcyclohexane + 1-butanol
2,2,4-trimethylpentane + 1-butanol
t-butylcyclohexane + 1-butanol
n-hexane + 2-butanol
n-heptane + 2-butanol
n-octane + 2-butanol
cyclohexane + 2-butanol
methylcyclohexane + 2-butanol
2,2,4-trimethylpentane + 2-butanol
t-butylcyclohexane + 2-butanol
n-hexane + 2-methyl-1-propanol
n-heptane + 2-methyl-1-propanol
n-octane + 2-methyl-1-propanol
cyclohexane + 2-methyl-1-propanol
methylcyclohexane + 2-methyl-1-propanol
2,2,4-trimethylpentane + 2-methyl-1-propanol
t-butylcyclohexane + 2-methyl-1-propanol
n-hexane + 3-methyl-1-butanol
n-heptane + 3-methyl-1-butanol
n-octane + 3-methyl-1-butanol
cyclohexane + 3-methyl-1-butanol
methylcyclohexane + 3-methyl-1-butanol
2,2,4-trimethylpentane + 3-methyl-1-butanol
t-butylcyclohexane + 3-methyl-1-butanol
n-hexane + 1-octanol
n-heptane + 1-octanol
n-octane + 1-octanol
cyclohexane + 1-octanol
methylcyclohexane + 1-octanol
2,2,4-trimethylpentane + 1-octanol
t-butylcyclohexane + 1-octanol
1-butanol + 1-propanol
2-butanol + 1-propanol
2-propanol + 1-propanol
1-octanol + 1-propanol
1-butanol + 2-propanol
2-butanol + 2-propanol
1-octanol + 2-butanol
acetonitrile + water
methanol + water
2-propanol + water
dimethyl sulfoxide + water

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Rytting, J.H.

J. Pharm Sci. 1983, *72*, 292-296.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9987	0.001290

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$x_2{}^a$	$x_1{}^a$
25.0	0.99853	0.00150

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Rytting, J.H.

J. Pharm Sci. 1983, *72*, 292-296.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9984	0.001571

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$c_1/(\text{mol dm}^{-3})$
20.0	0.0040

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifugation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming that the dilute solution behavior extrapolates up to saturation point.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Rytting, J.H.

J. Pharm Sci. 1983, *72*, 292-296.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9982	0.001850

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexadecane; $C_{16}H_{34}$; [544-76-3]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Pharm. Sci. 1987, *76*, 572-574.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9962	0.00380

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetrachloromethane. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) n-Octadecane; $C_{18}H_{38}$; [593-45-3]	**ORIGINAL MEASUREMENTS:** Djordjevic, N.M. *Thermochim. Acta* <u>1991</u>, *177*, 109-118.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
466.5	0.4423	0.5577	477.5	0.2000	0.8000
468.0	0.4091	0.5909	478.5	0.1857	0.8143
472.6	0.3226	0.6774	480.8	0.1487	0.8513
477.0	0.2385	0.7615	483.0	0.0989	0.9011

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Differential scanning calorimeter.

Mixtures (1.5 - 2.0 mg) of known concentration were weighed into aluminum pans, which were then crimped to preclude sample loss during the heating process. Solubilities determined by measuring melting points of binary mixtures using a Perkin-Elmer DSC-2 differential scanning calorimeter and scan rate of 5 K/min.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99 %, Aldrich Chemical Company, was vacuum-distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (compiler).
x_1: ± 0.0003 (compiler).

COMPONENTS: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	**ORIGINAL MEASUREMENTS:** Acree, W.E., Jr.; Rytting, J.H. *J. Pharm Sci.* <u>1983</u>, *72*, 292-296.
VARIABLES: $T/K = 298$	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9984	0.001574

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99.5 %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. *J. Solution Chem.* 1988, *16*, 519-534.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
346.8	0.9905	0.0095	391.2	0.9625	0.0375
358.5	0.9857	0.0143	402.4	0.9500	0.0500
366.8	0.9810	0.0190			
378.3	0.9745	0.0255			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	Mahieu, J. *Bull. Soc. Chim. Belgique* 1936, *45*, 667-677.
VARIABLES:	**PREPARED BY:**
T/K = 313	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2^a	x_1^a
40.0	0.9969	0.00306

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

ORIGINAL MEASUREMENTS:

Tucker, S.A.; Acree, W.E., Jr.

Phys. Chem. Liq. 1989, *20*, 31-38.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.9984	0.00165

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Cyclooctane; C_8H_{16}; [292-64-8]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Rytting, J.H.

J. Pharm Sci. 1983, *72*, 292-296.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.9977	0.002258

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Rytting, J.H.

J. Pharm Sci. 1983, *72*, 292-296.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9989	0.001087

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
25.0	0.00660

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99.7 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99+ %, Phillips Petroleum, Bartlesville, Oklahoma, USA, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$;
[3178-22-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 117-118.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9980	0.001978

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,6,10,15,19,23-Hexamethyltetracosane (squalane); $C_{30}H_{64}$; [111-01-3]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Pharm. Sci. 1987, *76*, 572-574.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9953	0.00472

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetrachloromethane. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
323.6	0.9921	0.0079	362.9	0.9701	0.0299
327.1	0.9913	0.0087	385.6	0.9413	0.0587
342.5	0.9849	0.0151			
351.0	0.9796	0.0204			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Rytting, J.H.

J. Pharm Sci. 1983, *72*, 292-296.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9926	0.007418

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Spectroanalyzed, 99.9+ %, Fisher Chemical Company, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Benzene; C_6H_6; [71-43-2]	Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* <u>1967</u>, *32*, 931-943.
VARIABLES: *T*/K = 293 and 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
20.0	0.9940	0.00595
25.0	0.9929	0.00711

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Benzene; C_6H_6; [71-43-2]	Somayajulu, G.R.; Palit, S.R. *J. Phys. Chem.* <u>1954</u>, *58*, 417-421.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
305.2	0.9909	0.00912	320.2	0.9856	0.01437
310.2	0.9894	0.01059	325.2	0.9830	0.01698
315.2	0.9875	0.01245	330.2	0.9807	0.01934
			340.2	0.9744	0.02558

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Reported values computed from variation of mole fraction solubility with temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, J. T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate. tallized from toluene.
(2) AR Grade, thiophene free, source not specified, was dried over calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3.
x_1: ± 0.00001 (compilier).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
308.9	0.9899	0.0101	353.9	0.9607	0.0393
330.6	0.9797	0.0203	364.3	0.9501	0.0499
338.2	0.9743	0.0257			
344.6	0.9697	0.0303			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2^a	x_1^a
25.0	0.9926	0.00740

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).

x_1: ± 5 % (relative error; compiler).

COMPONENTS:	EVALUATOR:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Benzene; C_6H_6; [71-43-2]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) June, 1994

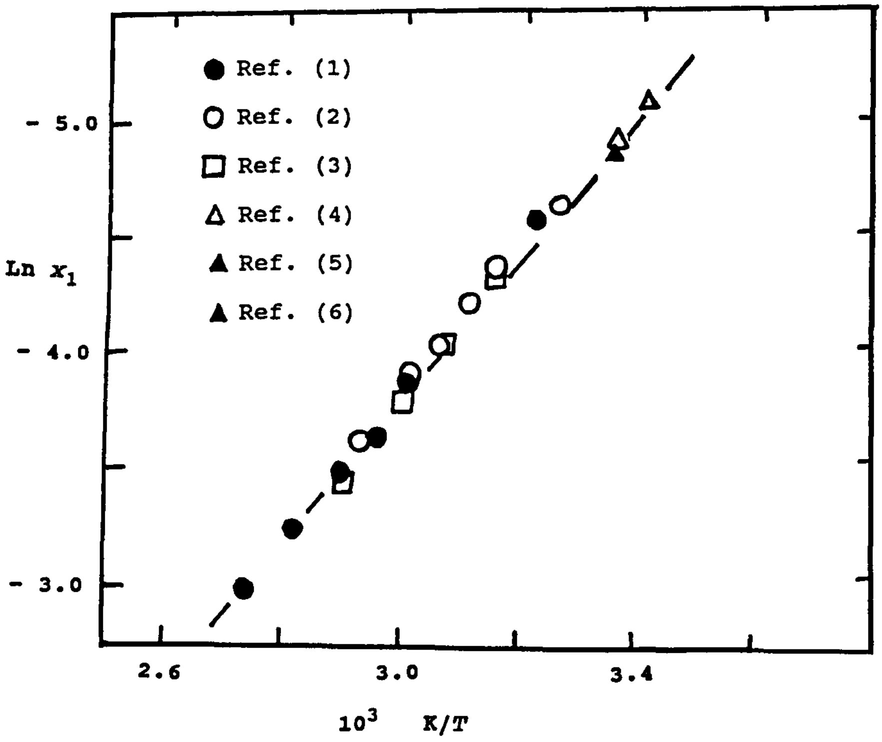
CRITICAL EVALUATION:

Anthracene solubilities in benzene were retrieved from papers by Coon *et al.* (1), Somayajulu and Palit (2), McLaughlin and Zainal (3), Smutek *et al.* (4), Acree and Rytting (5) and Mahieu (6). The first three studies report observed values at several temperatures, Smutek *et al.* report values at 293 and 298 K, and the latter two papers report the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the six studies from the critical evaluation.

Regressional analysis of the experimental data as Ln x_1 versus $1/T$ yielded the following mathematical relationship: < >

$$\text{Ln}\ x_1 = -3200.1\ (1/T) + 5.7899 \qquad (r = 0.9987)$$ nr >

for variation of anthracene solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.00713$, and differs by less than 4 % from experimental values of $x_1 = 0.00711$ (4), $x_1 = 0.007418$ (5) and $x_1 = 0.00740$ (6).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. *J. Solution Chem.* 1988, *16*, 519-534.
2. Somayajulu, G.R.; Palit, S.R. *J. Phys. Chem.* 1954, *58*, 417-421.
3. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1959, 863-867.
4. Smutek, M.; Fris, M.; Fohl, J. *Coll. Czech. Chem. Commun.* 1967, *32*, 931-943.
5. Acree, W.E., Jr.; Rytting, J.H. *J. Pharm. Sci.* 1983, *72*, 292-296.
6. Mahieu, J. *Bull. Soc. Chim. Belgique* 1936, *45*, 667-677.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.0	0.9897	0.0103	343.4	0.9685	0.0315
315.6	0.9870	0.0130			
323.8	0.9827	0.0173			
332.8	0.9775	0.0225			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedure not specified.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Tucker, S.A.; Murral, D.J.; Oswalt, B.M.; Halmi, J.L.; Acree, W.E., Jr.

Phys. Chem. Liq. 1988, *18*, 279-286.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9926	0.00736

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 293, 313 and 333

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1	t/°C	x_2	x_1
20.0	0.9935	0.00645	60.0	0.9770	0.0230
40.0	0.9876	0.0124			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]

ORIGINAL MEASUREMENTS:

Tucker, S.A.; Acree, W.E., Jr.

Phys. Chem. Liq. 1989, *20*, 31-38.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9927	0.00733

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.5+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]	Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.*, 1967, *32*, 931-943.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9923	0.00770

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 4-Isopropyl methylbenzene; $C_{10}H_{14}$; [99-87-6]	Wheeler, A.S. *J. Am. Chem. Soc.* 1920, *42*, 1842-1846.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
298.2	0.9883	0.0117	373.2	0.9349	0.0651
303.2	0.9872	0.0128			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Acenaphthene; $C_{12}H_{10}$; [83-32-9]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Zhur. Fiz. Khim. 1957, *31*, 1802-1811.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
368.3	1.000	0.000
364.4	0.949	0.051
362.7	0.929	0.071
361.2	0.914	0.086
368.2	0.896	0.104
387.5	0.844	0.156
402.5	0.784	0.216
418.2	0.706	0.294
434.2	0.603	0.397
443.2	0.516	0.484
456.2	0.410	0.590
466.2	0.294	0.706
477.2	0.178	0.822
489.7	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Chrysene; $C_{18}H_{12}$; [218-01-9]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M.; Pastukhova, I.S. *Proc. Acad. Sci. U.S.S.R., Sect. Chem.* 1956, *111*, 667-669 (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
528.2	1.000	0.000
519.2	0.896	0.104
509.5	0.788	0.212
499.7	0.693	0.307
490.9	0.603	0.397
480.4	0.496	0.504
470.5	0.402	0.598
466.2	0.365	0.635
467.2	0.303	0.697
469.7	0.260	0.740
473.7	0.202	0.798
481.7	0.103	0.897
489.7	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use. **ESTIMATED ERRORS:** T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Fluoranthene; $C_{16}H_{10}$; [206-44-0]	Kravchenko, V.M.; Pastukhova, I.S. *J. Gen. Chem. U.S.S.R.* 1959, *29*, 29-34. (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
383.2	1.000	0.000
377.8	0.930	0.070
376.5	0.906	0.094
375.0	0.884	0.116
374.2	0.860	0.140
380.2	0.859	0.141
387.3	0.830	0.170
395.7	0.804	0.196
419.9	0.671	0.329
435.2	0.566	0.434
449.4	0.456	0.544
459.7	0.355	0.645
467.4	0.269	0.731
475.1	0.178	0.822
489.7	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
299.6	0.9900	0.0100	343.4	0.9592	0.0408
319.5	0.9801	0.0199	346.2	0.9567	0.0433
327.6	0.9741	0.0259			
333.0	0.9697	0.0303			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

Phys. Chem. Liq. 1991, *24*, 31-42.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9952	0.00484

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99.5+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Butyl ethanoate; $C_6H_{12}O_2$;
[123-86-4]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

J. Chem. Soc. Faraday Trans. 1991, *87*, 461-464.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9934	0.00661

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Dimethyl hexanedioate; $C_8H_{14}O_4$;
[627-93-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr.

Phys. Chem. Liq. 1992, *25*, 51-58.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9913	0.00871

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Diethyl hexanedioate; $C_{10}H_{18}O_4$; [141-28-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

Phys. Chem. Liq. 1991, *24*, 31-42.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9897	0.01033

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Dibutyl Oxalate; $C_{10}H_{18}O_4$; [2050-60-4]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Smith, B.; Cordero, Y.; Acree, W.E., Jr.

Phys. Chem. Liq. 1992, *25*, 51-58.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9896	0.01043

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,1-Oxybisethane; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2[a]	x_1[a]
25.0	0.9965	0.00353

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

Marthandan, M.V.; Acree, W.E., Jr.

J. Chem. Eng. Data 1987, *32*, 301-303.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9964	0.003609

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	McCargar, J.W.; Acree, W.E., Jr. *J. Pharm. Sci.* 1987, *76*, 572-574.
VARIABLES:	**PREPARED BY:**
$T/K = 298$	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9965	0.00354

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetrachloromethane. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]	Anderson, B.D. Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	**PREPARED BY:**
$T/K = 298$	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
25.0	0.0210

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99.7 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Tetrahydrofuran; C_4H_8O; [109-99-9]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.991	0.009

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Tetrahydropyran; $C_5H_{10}O$; [142-68-7]

ORIGINAL MEASUREMENTS:

Bissell, M.; Chittick, C.E.; Acree, W.E., Jr.

Fluid Phase Equilibr. 1988, *41*, 187-194.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9898	0.01024

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9904	0.0096

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Procyk, A.D.; Bissell, M.; Street, K.W., Jr.; Acree, W.E., Jr.

J. Pharm. Sci. 1987, *76*, 621-626.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9916	0.008381

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.8 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.0756

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Trichloromethane; $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9895	0.0105

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Trichloromethane; $CHCl_3$;
[67-66-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2[a]	x_1[a]
25.0	0.9893	0.0107

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Tucker, S.A.; Acree, W.E., Jr.

Phys. Chem. Liq. 1989, *19*, 73-79.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9954	0.00464

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

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

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 293, 298, 313 and 333

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1	t/°C	x_2	x_1
20.0	0.9959	0.00411	40.0	0.9916	0.00836
25.0	0.9952	0.00483	60.0	0.9844	0.0156

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Iodoethane; C_2H_5I; ~~[74-88-4]~~ 75-03-6

ORIGINAL MEASUREMENTS:

Somayajulu, G.R.; Palit, S.R.

J. Phys. Chem. 1954, *58*, 417-421.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
310.2	0.9881	0.01189	340.2	0.9713	0.02867
320.2	0.9839	0.01612			
330.2	0.9783	0.02175			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by visunoting the temperature at which the last trace of solid solute disappeared. Reported values computed from variation of mole fraction solubility with temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, J. T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate. tallized from toluene.

(2) Purity not specified, prepared by authors, dried over calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3.
x_1: ± 0.00001 (compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Chlorobutane; C_4H_9Cl; [109-69-3]	Acree, W.E., Jr. *J. Solution Chem.* 1991, *20*, 307-318.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9941	0.00586

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) HPLC Grade, 99.5+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** *T*/K: ± 0.05. x_1: ± 1.5 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1,4-Dichlorobutane; $C_4H_8Cl_2$; [110-56-5]	Acree, W.E., Jr.; Zvaigzne, A.I. *Phys. Chem. Liq.* 1991, *23*, 225-237.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9895	0.01053

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.	(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received. (2) puriss, 99+ %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** *T*/K: ± 0.05. x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Trichloroethylene; C_2HCl_3; [79-01-6]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

$T/K = 296$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	$c_1/(\text{mol dm}^{-3})$
23.0	0.0705

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.

c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Iodobenzene; C_6H_5I; [591-50-4]

ORIGINAL MEASUREMENTS:

Somayajulu, G.R.; Palit, S.R.

J. Phys. Chem. 1954, *58*, 417-421.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.2	0.9854	0.01462	320.2	0.9766	0.02344
310.2	0.9827	0.01728			
315.2	0.9799	0.02014			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Reported values computed from variation of mole fraction solubility with temperature.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, J. T. Baker, USA, was recrystallized several times from ethanol and ethyl ethanoate. tallized from toluene.

(2) Purity not specified, Columbia Organic Chemicals, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.3.

x_1: ± 0.00001 (compilier).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Bromobenzene; C_6H_5Br; [108-86-1]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2[a]	x_1[a]
25.0	0.9881	0.0119

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2[a]	x_1[a]
25.0	0.9897	0.0103

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

$T/K = 296$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
23.0	0.0628

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
20.0	0.9998	0.000202

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2[a]	x_1[a]
25.0	0.9997	0.000252

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methanol; CH_4O; [67-56-1]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.00477

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2[a]	x_1[a]
25.0	0.9996	0.000371

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9994	0.000591

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9996	0.000411

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.00950

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99.7 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) puriss, 99.5 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9992	0.000801

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.8+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 114-116.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9994	0.000585

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 541-543.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9995	0.000470

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9993	0.000727

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
25.0	0.0140

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99.7 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
25.0	0.0118

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.0117

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.

c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9978	0.002160

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

EVALUATOR:

W.E. Acree, Jr.
Department of Chemistry
University of North Texas
Denton, Texas 76203-5068 (USA)
June, 1994

CRITICAL EVALUATION:

Anthracene solubilities in 1-octanol were retrieved from papers by Pinal *et al.* (1), Miller *et al.* (2), Acree *et al.* (3), and Anderson (4). All four studies report the solubility at only a single temperature, either 296 K (1) or 298 K (2-4). In the case of both Miller *et al.* and Anderson, the published molarity solubilities were converted to mole fraction values of x_1 = 0.00222 and x_1 = 0.00187 using molar volumes of V_1 = 150 cm^3 mol^{-1} and V_2 = 158.30 cm^3 mol^{-1} for anthracene and 1-octanol, respectively. The arithmetic average of the three reported solubilities at 298.15 K, x_1 = 0.00208 ± 0.00019 is the recommended value for the mole fraction solubility of anthracene in 1-octanol.

REFERENCES

1. Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639.
2. Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay D. *Environ. Sci. Technol.* 1985, *19*, 522.
3. Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A. *Fluid Phase Equilibr.* **1994**, *92*, 233.
4. Anderson, B.D., Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, 1978.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Phenol; C_6H_6O; [108-95-2]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
40.0	0.9951	0.00487

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Hydroxy-2-methylbenzene; C_7H_8O; [95-48-7]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

$T/K = 296$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
23.0	0.0308

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
20.0	0.9969	0.00313

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Propanone; C_3H_8O; [67-64-1]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$x_2{}^a$	$x_1{}^a$
25.0	0.9957	0.00432

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.954	0.046

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) 2-Butanone; C_4H_8O; [78-93-3]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9953	0.0047

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Acetonitrile; C_2H_3N; [75-05-8]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.00973

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun., 1967, *32*, 931-943.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
20.0	0.9913	0.00872

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Doane, E.P.; Drickamer, H.G.

J. Phys. Chem. 1955, *59*, 454-457.

VARIABLES:

T/K = 298, Pressure

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

P/atm	x_2	x_1	*P*/atm	x_2	x_1
1	0.9916	0.0084	2000	0.9973	0.0027
240	0.9930	0.0070	4000	0.9987	0.0013
500	0.9941	0.0059			
1000	0.9959	0.0041			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, analytical balance and high pressure equipment.

Excess solute and solvent allowed to equilibrate in a specially designed high pressure cell at constant temperature temperature for 20-24 hours. Known amount of saturated solution removed, solvent evaporated to dryness, and contration determined from weight of solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purest grade, Eastman Kodak Chemical Company, Rochester, New York, USA, was used as received.

(2) C.P. grade, J.T. Baker, was dried over phosphorous pentoxide and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 1-3 % at atmospheric pressure, and ± 10 % at the higher pressures.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Acetic anhydride; $C_4H_6O_3$; [108-24-7]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9972	0.0028

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Dimethylsulfoxide; C_2H_6OS; [67-68-5]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9979	0.0021

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Dimethyl sulfoxide; C_2H_6SO;
[67-68-5]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
23.0	0.0315

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2[a]	x_1[a]
25.0	0.9897	0.01032

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

VARIABLES:

T/K = 296

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	c_1/(mol dm^{-3})
23.0	0.0738

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an HPLC equipped with uv absorption and fluorescence detection.

Excess solute and solvent were placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at a minimum of 300 RCF for 15 minutes. The clear supernatant solution was analyzed by reversed-phase liquid chromatography with either fluorescence or uv detection.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 1.
c_1: ± 5% (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Srivastava, R.D.; Gupta, P.D.

J. Indian Chem. Soc. 1967, *44*, 960-963.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
286.2	0.9931	0.00688	307.4	0.9846	0.01545
289.8	0.9908	0.00916	308.2	0.9839	0.01614
296.2	0.9890	0.01104	313.0	0.9811	0.01892
298.2	0.9885	0.01152			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was recrystallized and sublimed.

(2) Purity not given, British Drug Houses, was dried and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Aniline; C_6H_7N; [62-53-3]

ORIGINAL MEASUREMENTS:

Mahieu, J.

Bull. Soc. Chim. Belgique 1936, *45*, 667-677.

VARIABLES:

T/K = 298 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2[a]	x_1[a]
25.0	0.9961	0.00390
40.0	0.9923	0.00773

[a] computed by compiler from published solvent compositions and solute solubilities, which were expressed as weight percent and grams of solute per 100 grams of solvent.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass containers and allowed to equilibrate for several hours at constant temperature. Aliquots of saturatured solutions transferred into tared containers and weighed. Solubiliites calculated from weight of solid residue which remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and source not given.

(2) Purity and source not given.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (compiler).
x_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
313.5	0.9833	0.0167	353.1	0.9470	0.0530
326.7	0.9758	0.0242	359.0	0.9415	0.0585
337.4	0.9674	0.0326			
344.5	0.9603	0.0397			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 293 and 333

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
20.0	0.9917	0.00834
60.0	0.9716	0.0284

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) 95 % initial purity, Urxovy Zavady, Czech., was recrystallized several times from pyridine and cyclohexane to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.989	0.011

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Quinoline; C_9H_7N; [91-22-5]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.989	0.011

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
297.4	0.9895	0.0105	351.8	0.9506	0.0494
317.9	0.9798	0.0202	358.1	0.9430	0.0570
332.9	0.9697	0.0303			
337.0	0.9659	0.0341			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Methoxybenzene; C_7H_8O; [100-66-3]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9898	0.0102

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) 1-Methyl-2-pyrrolidinone; C_5H_9NO; [872-50-4]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.975	0.025

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.986	0.014

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) N,N-Dimethylformamide; C_3H_7NO; [68-12-2]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.991	0.009

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Tetramethylene sulfone; $C_4H_8O_2S$; [126-33-0]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9964	0.0036

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-17-7]

(2) Tributyl phosphate; $C_{12}H_{27}O_4P$; [126-73-8]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.989	0.011

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1,2,3,5-Tetranitrobenzene; $C_6H_2N_4O_8$; [3698-53-1]

ORIGINAL MEASUREMENTS:

Shinomiya, C.

J. Chem. Soc. Japan 1940, *15*, 259-270.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
399.2	1.000	0.000
398.2	0.935	0.065
418.2	0.842	0.158
436.2	0.693	0.307
442.2	0.604	0.396
444.2	0.487	0.513
441.7	0.430	0.570
449.2	0.354	0.646
459.2	0.301	0.699
462.2	0.271	0.729
490.2	0.000	1.000

Author reports formation of a 1:1 anthracene - 1,2,3,5-tetranitrobenzene molecular compound having a melting point temperature of 444.2 K. Two eutectic points occur at x_1 = 0.055 and T/K = 393.7, and at x_1 = 0.605 and T/K = 436.2.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details given in paper.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper.

(2) Purity and chemical source were not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,4,6-Trinitrophenol; $C_6H_3N_3O_7$; [88-89-1]

ORIGINAL MEASUREMENTS:

Singh, N.P.; Shukla, B.M.

Cryst. Res. Technol. 1985, *20*, 345-349.

VARIABLES:

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

Phase equilibrium data not given in cited paper. Authors report formation of a 1:1 anthracene - 2,4,6-trinitrophenol molecular compound having a melting point temperature of 413.2 K. Two eutectic points occur at $x_1 = 0.1017$ and $T/\text{K} = 382.7$, and at $x_1 = 0.6250$ and $T/\text{K} = 403.2$.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Binary mixtures were prepared by weight. Melting and thaw point temperatures determined by the method of Rastogi *et al.* (see *J. Cryst. Growth* 1977, *40*, 329).

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: precision ± 0.3 (Compiler).
x_1: ± 0.0002 (Compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 117-118.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1093	0.1091	0.001899
0.2115	0.2111	0.001809
0.3862	0.3856	0.001651
0.5049	0.5041	0.001536
0.6142	0.6133	0.001429
0.8099	0.8089	0.001249
0.8961	0.8951	0.001163
1.0000	0.9989	0.001074

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) HPLC Grade, 99.7 %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1751	0.1749	0.001288
0.3162	0.3158	0.001237
0.5447	0.5441	0.001071
0.6331	0.6325	0.000990
0.7297	0.7290	0.000898
0.8712	0.8706	0.000740
0.9411	0.9435	0.000661
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) n-Heptane; C_7H_{16}; [142-82-5] (3) 1-Propanol; C_3H_8O; [71-23-8]	Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1993, *38*, 389-392.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1719	0.1716	0.001566
0.3272	0.3267	0.001456
0.5674	0.5667	0.001182
0.6622	0.6615	0.001077
0.7444	0.7437	0.000953
0.8824	0.8817	0.000762
0.9398	0.9392	0.000681
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1908	0.1905	0.001779
0.3483	0.3477	0.001632
0.5892	0.5884	0.001300
0.6806	0.6798	0.001145
0.7661	0.7653	0.001013
0.8939	0.8932	0.000784
0.9477	0.9471	0.000682
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1335	0.1333	0.001576
0.2567	0.2563	0.001543
0.4886	0.4880	0.001288
0.5890	0.5883	0.001150
0.6893	0.6886	0.001010
0.8511	0.8504	0.000795
0.9226	0.9220	0.000699
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 1-Propanol; C_3H_8O; [71-23-8]	Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1993, *38*, 389-392.

VARIABLES:	PREPARED BY:
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1539	0.1536	0.001697
0.2943	0.2938	0.001578
0.5326	0.5319	0.001294
0.6305	0.6298	0.001154
0.7206	0.7199	0.001018
0.8687	0.8680	0.000781
0.9328	0.9322	0.000687
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1] (3) 1-Propanol; C_3H_8O; [71-23-8]	Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1993, *38*, 389-392.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.2141	0.2139	0.001089
0.3510	0.3506	0.001057
0.5891	0.5886	0.000929
0.6884	0.6878	0.000862
0.7911	0.7905	0.000783
0.8968	0.8962	0.000693
0.9454	0.9448	0.000649
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 117-118.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.2089	0.2085	0.001958
0.3695	0.3688	0.001792
0.6061	0.6052	0.001423
0.7002	0.6993	0.001250
0.7780	0.7771	0.001100
0.9021	0.9014	0.000824
0.9537	0.9530	0.000706
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1739	0.1737	0.001271
0.3076	0.3072	0.001201
0.5342	0.5337	0.000987
0.6314	0.6308	0.000873
0.7185	0.7179	0.000767
0.8700	0.8695	0.000581
0.9391	0.9386	0.000490
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1851	0.1848	0.001499
0.3256	0.3252	0.001371
0.5575	0.5569	0.001102
0.6607	0.6601	0.000956
0.7381	0.7375	0.000836
0.8861	0.8856	0.000603
0.9416	0.9411	0.000509
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.2157	0.2153	0.001690
0.3580	0.3574	0.001540
0.5840	0.5833	0.001206
0.6874	0.6867	0.001025
0.7670	0.7663	0.000868
0.8928	0.8922	0.000622
0.9478	0.9473	0.000515
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1430	0.1428	0.001568
0.2666	0.2662	0.001474
0.4882	0.4876	0.001213
0.5897	0.5891	0.001051
0.6817	0.6811	0.000899
0.8463	0.8458	0.000639
0.9239	0.9234	0.000519
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

$x_3^{(s)}$: ± 0.0001.

x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1518	0.1515	0.001683
0.2965	0.2960	0.001536
0.5234	0.5228	0.001226
0.6234	0.6227	0.001055
0.7170	0.7164	0.000887
0.8649	0.8644	0.000631
0.9375	0.9370	0.000508
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1997	0.1995	0.001054
0.3535	0.3532	0.000988
0.5865	0.5860	0.000839
0.6809	0.6804	0.000751
0.7676	0.7671	0.000664
0.8932	0.8927	0.000535
0.9492	0.9488	0.000471
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

$x_3^{(s)}$: ± 0.0001.

x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 117-118.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.2154	0.2150	0.001978
0.3666	0.3660	0.001760
0.5948	0.5940	0.001335
0.6912	0.6904	0.001152
0.7744	0.7737	0.000948
0.8963	0.8957	0.000660
0.9537	0.9532	0.000526
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1460	0.1458	0.001316
0.2668	0.2665	0.001310
0.4876	0.4870	0.001218
0.5800	0.5793	0.001162
0.6804	0.6797	0.001068
0.8479	0.8471	0.000931
0.9247	0.9239	0.000857
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1562	0.1560	0.001576
0.2876	0.2872	0.001511
0.5171	0.5164	0.001333
0.6174	0.6166	0.001230
0.7033	0.7025	0.001142
0.8622	0.8614	0.000972
0.9315	0.9307	0.000886
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) n-Octane; C_8H_{18}; [111-65-9] (3) 1-Butanol; $C_4H_{10}O$; [71-36-3]	Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1993, *38*, 389-392.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]
t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1645	0.1642	0.001828
0.3070	0.3065	0.001725
0.5368	0.5360	0.001467
0.6389	0.6380	0.001336
0.7313	0.7304	0.001207
0.8738	0.8729	0.000998
0.9365	0.9357	0.000892
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1151	0.1149	0.001622
0.2108	0.2105	0.001586
0.4380	0.4374	0.001414
0.5390	0.5383	0.001291
0.6811	0.6803	0.001152
0.8255	0.8247	0.000978
0.9086	0.9078	0.000895
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1358	0.1356	0.001710
0.2675	0.2671	0.001671
0.4783	0.4776	0.001453
0.5740	0.5732	0.001329
0.6764	0.6756	0.001193
0.8449	0.8441	0.000995
0.9221	0.9213	0.000892
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: $\pm$ 0.05.
$x_3^{(s)}$: $\pm$ 0.0001.
x_1: $\pm$ 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Teng, I.-L.; Martinez, E.; Trejo, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1993, *38*, 389-392.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1567	0.1565	0.001125
0.3031	0.3028	0.001121
0.5376	0.5370	0.001051
0.6387	0.6381	0.000996
0.7330	0.7323	0.000956
0.8819	0.8811	0.000870
0.9443	0.9435	0.000838
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 1-Butanol; $C_4H_{10}O$; [71-36-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data <u>1994</u>, *39*, 117-118.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1882	0.1878	0.001977
0.3325	0.3319	0.001855
0.5540	0.5531	0.001561
0.6547	0.6538	0.001405
0.7426	0.7417	0.001265
0.8842	0.8833	0.001010
0.9413	0.9404	0.000918
1.0000	0.9992	0.000801

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) n-Hexane; C_6H_{14}; [110-54-3] (3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]	Zvaigzne, A.I.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1994, *39*, 114-116.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1432	0.1430	0.001311
0.2657	0.2654	0.001282
0.4851	0.4845	0.001169
0.5863	0.5857	0.001070
0.6820	0.6813	0.000969
0.8497	0.8490	0.000770
0.9249	0.9243	0.000676
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data <u>1994</u>, *39*, 114-116.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1599	0.1597	0.001541
0.2887	0.2883	0.001476
0.5182	0.5175	0.001280
0.6157	0.6150	0.001163
0.7059	0.7052	0.001041
0.8693	0.8686	0.000784
0.9328	0.9322	0.000685
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 114-116.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1724	0.1721	0.001783
0.3201	0.3196	0.001658
0.5408	0.5400	0.001412
0.6384	0.6376	0.001263
0.7265	0.7257	0.001111
0.8791	0.8784	0.000826
0.9353	0.9346	0.000717
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]	Zvaigzne, A.I.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1994, *39*, 114-116.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1266	0.1264	0.001618
0.2285	0.2281	0.001565
0.4422	0.4416	0.001370
0.5429	0.5422	0.001247
0.6425	0.6418	0.001088
0.8210	0.8203	0.000829
0.9089	0.9083	0.000699
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 114-116.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1460	0.1457	0.001725
0.2585	0.2581	0.001647
0.4740	0.4733	0.001413
0.5832	0.5825	0.001262
0.6743	0.6735	0.001117
0.8541	0.8534	0.000821
0.9234	0.9227	0.000705
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 114-116.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1574	0.1572	0.001116
0.3118	0.3115	0.001091
0.5396	0.5391	0.001000
0.6365	0.6359	0.000935
0.7292	0.7286	0.000863
0.8766	0.8760	0.000720
0.9475	0.9469	0.000646
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data <u>1994</u>, *39*, 117-118.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1795	0.1791	0.001977
0.3264	0.3258	0.001833
0.5520	0.5512	0.001513
0.6528	0.6519	0.001343
0.7394	0.7385	0.001167
0.8794	0.8786	0.000854
0.9348	0.9341	0.000735
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 541-543.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1473	0.1471	0.001299
0.2688	0.2685	0.001236
0.4807	0.4802	0.001063
0.5889	0.5883	0.000947
0.6846	0.6840	0.000838
0.8524	0.8519	0.000645
0.9250	0.9245	0.000560
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 541-543.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1644	0.1642	0.001514
0.2825	0.2821	0.001435
0.5123	0.5117	0.001181
0.6094	0.6088	0.001031
0.7105	0.7099	0.000899
0.8567	0.8561	0.000680
0.9294	0.9289	0.000575
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 541-543.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1786	0.1783	0.001742
0.3077	0.3072	0.001601
0.5373	0.5366	0.001278
0.6371	0.6364	0.001111
0.7281	0.7274	0.000955
0.8741	0.8735	0.000693
0.9385	0.9380	0.000581
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1994, *39*, 541-543.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1267	0.1265	0.001565
0.2262	0.2259	0.001488
0.4297	0.4292	0.001232
0.5441	0.5435	0.001073
0.6400	0.6394	0.000928
0.8155	0.8149	0.000692
0.9131	0.9126	0.000575
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Methylcyclohexane; C_7H_{14}; [108-87-2] (3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]	Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr. *J. Chem. Eng. Data* 1994, *39*, 541-543.
VARIABLES:	**PREPARED BY:**
$T/K = 298$, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1438	0.1436	0.001697
0.2568	0.2564	0.001568
0.4769	0.4763	0.001265
0.5837	0.5831	0.001100
0.6739	0.6733	0.000963
0.8428	0.8422	0.000693
0.9143	0.9138	0.000590
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 541-543.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1859	0.1857	0.001087
0.3227	0.3224	0.001019
0.5402	0.5397	0.000880
0.6451	0.6446	0.000805
0.7334	0.7329	0.000730
0.8780	0.8775	0.000591
0.9413	0.9408	0.000536
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 2-Methyl-1-propanol; $C_4H_{10}O$; [78-83-1]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Wolfe, J.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 541-543.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1860	0.1856	0.001892
0.3238	0.3232	0.001716
0.5548	0.5541	0.001336
0.6531	0.6523	0.001150
0.7351	0.7344	0.000990
0.8806	0.8800	0.000699
0.9449	0.9444	0.000574
1.0000	0.9995	0.000470

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.1275	0.1273	0.001341
0.2355	0.2352	0.001312
0.4384	0.4379	0.001221
0.5447	0.5441	0.001146
0.6401	0.6394	0.001064
0.8269	0.8262	0.000890
0.9115	0.9108	0.000813
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1431	0.1429	0.001554
0.2545	0.2541	0.001500
0.4751	0.4745	0.001337
0.5713	0.5706	0.001234
0.6681	0.6674	0.001128
0.8383	0.8375	0.000916
0.9151	0.9143	0.000823
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) n-Octane; C_8H_{18}; [111-65-9] (3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]	**ORIGINAL MEASUREMENTS:** Zvaigzne, A.I.; Acree, W.E., Jr. *J. Chem. Eng. Data*, in press.
VARIABLES: T/K = 298, Solvent composition	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1537	0.1534	0.001814
0.2672	0.2667	0.001728
0.4914	0.4907	0.001488
0.5939	0.5931	0.001345
0.6958	0.6950	0.001199
0.8537	0.8529	0.000952
0.9265	0.9257	0.000844
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.1048	0.1046	0.001607
0.2011	0.2008	0.001561
0.3923	0.3918	0.001389
0.4977	0.4971	0.001277
0.5993	0.5986	0.001153
0.7958	0.7951	0.000934
0.8896	0.8889	0.000836
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.1290	0.1288	0.001709
0.2350	0.2346	0.001633
0.4367	0.4361	0.001422
0.5422	0.5415	0.001299
0.6437	0.6430	0.001153
0.8247	0.8239	0.000923
0.9137	0.9129	0.000821
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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SOURCE AND PURITY OF MATERIALS:

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(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1476	0.1474	0.001114
0.2838	0.2835	0.001103
0.4998	0.4993	0.001042
0.6038	0.6032	0.000990
0.6973	0.6966	0.000937
0.8537	0.8530	0.000831
0.9196	0.9189	0.000782
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 3-Methyl-1-butanol; $C_5H_{12}O$; [123-51-3]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data, in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1685	0.1682	0.001938
0.2866	0.2861	0.001843
0.5168	0.5160	0.001545
0.6089	0.6080	0.001400
0.7072	0.7063	0.001217
0.8650	0.8642	0.000944
0.9274	0.9266	0.000852
1.0000	0.9993	0.000727

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

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SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.3 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Hexane; C_6H_{14}; [110-54-3]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001274
0.0774	0.0773	0.001469
0.1758	0.1755	0.001608
0.3536	0.3530	0.001827
0.4524	0.4515	0.001917
0.5528	0.5517	0.001979
0.7728	0.7712	0.002101
0.8747	0.8728	0.002138
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ mole %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Heptane; C_7H_{16}; [142-82-5]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, A.I.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001571
0.1018	0.1016	0.001738
0.1925	0.1921	0.001835
0.3897	0.3889	0.002002
0.4808	0.4798	0.002057
0.5865	0.5853	0.002098
0.7841	0.7824	0.002135
0.8958	0.8939	0.002163
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) n-Octane; C_8H_{18}; [111-65-9]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001838
0.1090	0.1088	0.001948
0.2110	0.2106	0.002040
0.4021	0.4012	0.002138
0.5071	0.5060	0.002169
0.6139	0.6126	0.002182
0.8015	0.7998	0.002175
0.9021	0.9001	0.002167
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001553
0.0815	0.0814	0.001730
0.1521	0.1518	0.001804
0.3128	0.3122	0.001937
0.4106	0.4098	0.002002
0.5153	0.5142	0.002048
0.7254	0.7239	0.002120
0.8499	0.8481	0.002143
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.9+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001649
0.0884	0.0882	0.001885
0.1712	0.1709	0.001966
0.3497	0.3490	0.002058
0.4438	0.4429	0.002090
0.5454	0.5442	0.002119
0.7623	0.7607	0.002147
0.8752	0.8733	0.002154
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.; Tucker, S.A.

Fluid Phase Equilibr. 1994, *92*, 233-253.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001074
0.1236	0.1234	0.001261
0.2128	0.2125	0.001378
0.4069	0.4062	0.001608
0.5092	0.5083	0.001719
0.6123	0.6112	0.001809
0.8054	0.8038	0.001987
0.8992	0.8973	0.002065
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.7 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

(3) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Zvaigzne, A.I.; Acree, W.E., Jr.

J. Chem. Eng. Data 1994, *39*, 117-118.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.001978
0.1124	0.1122	0.002151
0.2170	0.2165	0.002198
0.4191	0.4181	0.002274
0.5221	0.5209	0.002274
0.6185	0.6171	0.002249
0.8152	0.8134	0.002219
0.9127	0.9107	0.002180
1.0000	0.9978	0.002160

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

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(2) 99 %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.

Fluid Phase Equilibr., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1331	0.1330	0.000783
0.2419	0.2417	0.000762
0.4468	0.4465	0.000716
0.5538	0.5534	0.000692
0.6472	0.6468	0.000674
0.8289	0.8284	0.000631
0.9043	0.9037	0.000616
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

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(2) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Butanol; $C_4H_{10}O$; [15892-23-6]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.

Fluid Phase Equilibr., in press.

VARIABLES:

T/K = 298, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1310	0.1309	0.000586
0.2470	0.2469	0.000584
0.4461	0.4458	0.000586
0.5495	0.5492	0.000586
0.6514	0.6510	0.000588
0.8243	0.8238	0.000593
0.9065	0.9060	0.000592
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

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(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Propanol; C_3H_8O; [67-63-0]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.

Fluid Phase Equilibr., in press.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^\circ C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000411
0.1092	0.1092	0.000436
0.2068	0.2067	0.000449
0.4016	0.4014	0.000478
0.5073	0.5070	0.000497
0.6105	0.6102	0.000516
0.7955	0.7951	0.000553
0.8882	0.8877	0.000572
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

(3) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.

Fluid Phase Equilibr., in press.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES^a

$t = 25.0\ ^{\circ}C$

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.2116	0.2112	0.001873
0.3583	0.3577	0.001655
0.5747	0.5739	0.001322
0.6793	0.6785	0.001145
0.7689	0.7681	0.000996
0.8921	0.8914	0.000782
0.9481	0.9474	0.000688
1.0000	0.9994	0.000591

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 1-Butanol; $C_4H_{10}O$; [71-36-3]

(3) 2-Propanol; C_3H_8O; [67-63-0]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Zvaigzne, A.I.

Fluid Phase Equilibr., in press.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000801
0.1362	0.1361	0.000757
0.2456	0.2454	0.000710
0.4369	0.4366	0.000630
0.5448	0.5445	0.000584
0.6427	0.6423	0.000548
0.8193	0.8189	0.000482
0.9061	0.9057	0.000449
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) HPLC Grade, 99.8+ %, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 2-Butanol; $C_4H_{10}O$; [15892-23-6] (3) 2-Propanol; C_3H_8O; [67-63-0]	Acree, W.E., Jr.; Zvaigzne, A.I. *Fluid Phase Equilibr.*, in press.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.000585
0.1355	0.1354	0.000564
0.2441	0.2440	0.000545
0.4403	0.4401	0.000512
0.5429	0.5426	0.000495
0.6486	0.6483	0.000476
0.8169	0.8165	0.000445
0.9008	0.9004	0.000430
1.0000	0.9996	0.000411

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5] (3) 2-Butanol; $C_4H_{10}O$; [15892-23-6]	Acree, W.E., Jr.; Zvaigzne, A.I. *Fluid Phase Equilibr.*, in press.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$x_3^{(s)}$	x_3	x_1
0.0000	0.0000	0.002160
0.1773	0.1770	0.001911
0.3041	0.3036	0.001698
0.5351	0.5344	0.001314
0.6328	0.6321	0.001164
0.7235	0.7228	0.001012
0.8703	0.8696	0.000787
0.9308	0.9302	0.000696
1.0000	0.9994	0.000585

[a] $x_3^{(s)}$: initial mole fraction of binary solvent mixture; x_1: mole fraction solubility of the solute; x_3: mole fraction of component 3 in the ternary solution.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Binary solvent mixtures were prepared by weight. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium was verified by several repetitive measurements and by approaching equilibrium from supersaturation. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Gold Label, 99.9+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, used as received.

(2) 99+ %, anhydrous, Aldrich Chemical Company.

(3) 99+ %, anhydrous, Aldrich Chemical Company.

Components 2 and 3 were stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
$x_3^{(s)}$: ± 0.0001.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Acetonitrile; C_2H_3N; [75-05-8] (3) Water; H_2O; [7732-18-5]	Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639-646. (Numerical values obtained from L.S. Lee in a private communication.)
VARIABLES:	**PREPARED BY:**
T/K = 296, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 23.0 °C

$\phi_2^{(s)}$	c_1/(mol dm^{-3})
0.00	4.16×10^{-7}
0.10	1.30×10^{-6}
0.20	7.46×10^{-6}
0.30	2.83×10^{-5}
0.40	1.94×10^{-4}
0.50	6.51×10^{-4}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile-methanol-water mobile phase were used in the chromatographic analysis.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in the paper.

(2) Purity and chemical source were not specified in the paper.

(3) Purity and chemical source were not specified in the paper.

ESTIMATED ERRORS:

T/K: ± 1.
$\phi_2^{(s)}$: ± 0.01 (compiler).
c_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) Methanol; CH_4O; [67-56-1]

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

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

(Numerical values obtained from L.S. Lee in a private communication.)

VARIABLES:

T/K = 296, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 23.0 °C

$\phi_2^{(s)}$	c_1/(mol dm^{-3})
0.00	4.16×10^{-7}
0.10	7.41×10^{-7}
0.20	1.17×10^{-6}
0.30	2.88×10^{-6}
0.40	1.02×10^{-5}
0.50	4.34×10^{-5}
0.60	1.12×10^{-4}
0.80	1.03×10^{-3}
0.90	2.28×10^{-3}
1.00	4.82×10^{-3}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile-methanol-water mobile phase were used in the chromatographic analysis.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in the paper.

(2) Purity and chemical source were not specified in the paper.

(3) Purity and chemical source were not specified in the paper.

ESTIMATED ERRORS:

T/K: ± 1.
$\phi_2^{(s)}$: ± 0.01 (compiler).
c_1: ± 5 % (relative error; compiler).

COMPONENTS:

(1) Anthracene; $C_{14}H_{10}$; [120-12-7]

(2) 2-Propanol; C_3H_8O; [67-63-0]

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

ORIGINAL MEASUREMENTS:

Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H.

Environ. Sci. Technol. 1990, *24*, 639-646.

(Numerical values obtained from L.S. Lee in a private communication.)

VARIABLES:

T/K = 296, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 23.0 °C

$\phi_2^{(s)}$	c_1/(mol dm^{-3})
0.00	4.16×10^{-7}
0.10	7.69×10^{-7}
0.20	4.57×10^{-6}
0.30	2.47×10^{-5}
0.40	1.03×10^{-4}
0.50	5.49×10^{-4}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile-methanol-water mobile phase were used in the chromatographic analysis.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in the paper.

(2) Purity and chemical source were not specified in the paper.

(3) Purity and chemical source were not specified in the paper.

ESTIMATED ERRORS:

T/K: ± 1.
$\phi_2^{(s)}$: ± 0.01 (compiler).
c_1: ± 5 % (relative error; compiler).

COMPONENTS: (1) Anthracene; $C_{14}H_{10}$; [120-12-7] (2) Dimethyl sulfoxide; C_2H_6OS; [67-68-5] (3) Water; H_2O; [7732-18-5]	**ORIGINAL MEASUREMENTS:** Pinal, R.; Rao, P.S.C.; Lee, L.S.; Cline, P.V.; Yalkowsky, S.H. *Environ. Sci. Technol.* 1990, *24*, 639-646. (Numerical values obtained from L.S. Lee in a private communication.)
VARIABLES: T/K = 296, Solvent composition	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 23.0 °C

$\phi_2^{(s)}$	c_1/(mol dm^{-3})
0.00	4.16×10^{-7}
0.10	6.06×10^{-7}
0.20	2.29×10^{-6}
0.30	6.73×10^{-6}
0.40	2.10×10^{-5}
0.50	5.89×10^{-5}
0.60	2.13×10^{-4}
0.70	8.86×10^{-4}
0.80	3.76×10^{-3}
0.90	1.35×10^{-2}
1.00	4.23×10^{-2}

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: molar solubility (mol dm^{-3}) of the solute.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an HPLC equipped with fluorescence detection.

Binary solvent mixtures were prepared by volume. Excess solute and solvent placed in glass vials and allowed to equilibrate with rotation for 12-24 hours in a constant temperature bath. Prior to analysis samples were centrifuged at 300 RCF for 15 minutes. The clear supernatant solutions were analyzed by reversed-phase liquid chromatography with fluorescence detection. Excitation and emission filters employed were 350 nm and 420 nm, respectively. An octadecylsilanized stationary phase and a acetonitrile-methanol-water mobile phase were used in the chromatographic analysis.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in the paper.

(2) Purity and chemical source were not specified in the paper.

(3) Purity and chemical source were not specified in the paper.

ESTIMATED ERRORS:

T/K: ± 1.
$\phi_2^{(s)}$: ± 0.01 (compiler).
c_1: ± 5 % (relative error; compiler).

BENZ[a]ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

n-heptane

B. <u>Alkenes</u>

C. <u>Aromatic Hydrocarbons</u>

D. <u>Esters</u>

E. <u>Ethers</u>

F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>

G. <u>Alcohols</u>

H. <u>Ketones</u>

I. <u>Miscellaneous Pure Solvents</u>

J. <u>Binary Solvent Mixtures</u>

COMPONENTS:

(1) Benz[a]anthracene; $C_{18}H_{12}$;
[56-55-3]
(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
20.0	0.0133

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: $\pm$ 2.
c_1: unknown.

BENZO[b]FLUORENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS: (1) Benzo[b]fluorene; $C_{17}H_{12}$; [243-17-4] (2) 1-Octanol; $C_8H_{18}O$; [111-87-5]	**ORIGINAL MEASUREMENTS:** Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D. *Environ. Sci. Technol.* 1985, *19*, 522-529.
VARIABLES: T/K = 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.01563

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection. Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.	(1) Highest available commercial purity, specific chemical supplier not given, was used as received. (2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.
	ESTIMATED ERRORS: T/K: ± 0.1 (compiler). c_1: ± 3 % (relative error; compiler).

BENZO[ghi]PERYLENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane
cyclohexane

B. Alkenes

C. Aromatic Hydrocarbons

methylbenzene

D. Esters

ethyl butyrate

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

acetone
cyclohexanone
acetophenone

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2] (2) n-Heptane; C_7H_{16}; [142-82-5]	Lissi, E.A.; Abuin, E.B. *Bol. Soc. Chil. Quim.* 1981, *26*, 19-34.
VARIABLES:	**PREPARED BY:**
T/K = 293	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.0012

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured fluorescence emission intensity.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2] (2) Cyclohexane; C_6H_{12}; [110-82-7]	Carre, O.R.; Phillips, D.J.; Brennecke, J.F. *Ind. Eng. Chem. Res.* 1994, *33*, 1255-1262.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 294 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9999	0.000149

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) HPLC Grade, 99+ %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 9.5 % (relative error).

COMPONENTS:

(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2]
(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, *33*, 1355-1362.

VARIABLES:

T/K = *Circa* 294 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9980	0.00204

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) ACS Grade, 99 %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 1.4 % (relative error).

COMPONENTS:

(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2]
(2) Ethyl butyrate; $C_6H_{12}O_2$; [105-54-4]

ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, *33*, 1355-1362.

VARIABLES:

T/K = *Circa* 294 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9988	0.00116

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 6.5 % (relative error).

COMPONENTS:

(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2]
(2) Acetone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, *33*, 1355-1362.

VARIABLES:

T/K = *Circa* 294 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
21.0	0.9994	0.000634

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) ACS Grade, 99.5 %, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 0.7 % (relative error).

COMPONENTS:

(1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2]
(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

ORIGINAL MEASUREMENTS:

Carre, O.R.; Phillips, D.J.; Brennecke, J.F.

Ind. Eng. Chem. Res. 1994, *33*, 1255-1262.

VARIABLES:

T/K = *Circa* 294 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
21.0	0.9960	0.00400

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and diluted quantitatively for subsequent spectrophotometric analysis. Attainment of equilibrium was verified by repetitive measurements taken at 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) 99.8 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 5.1 % (relative error).

COMPONENTS: (1) Benzo[ghi]perylene; $C_{22}H_{12}$; [191-24-2] (2) Acetophenone; C_8H_8O; [98-86-2]	**ORIGINAL MEASUREMENTS:** Carre, O.R.; Phillips, D.J.; Brennecke, J.F. *Ind. Eng. Chem. Res.* 1994, *33*, 1355-1362.
VARIABLES: *T*/K = *Circa* 294 (Ambient Room)	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
21.0	0.9936	0.00640

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Ultraviolet/visible spectrophotometer and centrifugal automatic particle analyzer.

Excess solute and solvent were allowed to equilibrate under vigorous agitation at ambient temperature (presumed). Sample was centrifuged at 3000 rpms to remove solid particles in suspension. Samples of 2 mLs of saturated liquid were then removed and the solvent evaporated. Residue dissolved in cyclohexane and diluted quantitatively for spectrophotometric analysis. Attainement of equilibrium was verified by repetitive measurements after 24 hour intervals.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received from manufacturer.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 2 (Compiler).
x_1: ± 4.6 % (relative error).

BENZO[a]PYRENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

benzene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8] (2) n-Heptane; C_7H_{16}; [142-82-5]	Lissi, E.A.; Abuin, E.B. *Bol. Soc. Chil. Quim.* 1981, *26*, 19-34.
VARIABLES:	**PREPARED BY:**
T/K = 293	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.0034

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifugation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming that the dilute solution behavior extrapolates up to saturation point.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Benzo[a]pyrene; $C_{20}H_{12}$; [50-32-8] (2) Benzene; C_6H_6; [71-43-2]	Mishra, D.S.; Yalkowsky, S.H. *Ind. Eng. Chem. Res.*, 1990, *29*, 2278-2283.
VARIABLES:	**PREPARED BY:**
T/K = 296	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
23.0	0.9646	0.0354

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent placed in screw-capped test tube and allowed to equilibrate for 3 days with gentle agitation in a constant temperature bath. Samples centrifuged for 30 minutes and concentrations were determined spectrophotometrically. Attainment of equilibrium verified by repetitive measurements 4 days later.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent grade, source not specified, was used as received.

(2) Reagent grade, source not specified, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 5 % (relative error; compiler).

BIPHENYL SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
tetracosane
octacosane
cyclohexane
methylcyclohexane
cis-1,2-dimethylcyclohexane
trans-1,2-dimethylcyclohexane
trans-1,4-dimethylcyclohexane
cis-1,4-dimethylcyclohexane
cis-1,3-dimethylcyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
ethylbenzene
naphthalene
2-methylnaphthalene
2,6-dimethylnaphthalene
1,2-diphenylethane
1,2,3,4-tetrahydronaphthalene

D. Esters

E. Ethers

1,4-dioxane
diphenyl ether

F. Haloalkanes and Haloaromatic Hydrocarbons

dichloromethane
trichloromethane
tetrachloromethane
1,2-dibromoethane
1,1-dichloroethane
1,2-dichloroethane
chlorobenzene
1,4-dichlorobenzene
hexafluorobenzene

G. Alcohols

1-octanol
1-octadecanol

H. Ketones

benzophenone

I. Miscellaneous Pure Solvents

carbon disulfide
pyridine
thiophene
indole
diphenylamine
nitrobenzene
1-octadecanoic acid

J. Binary Solvent Mixtures

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.8767	0.1233

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.876	0.124

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) n-Hexane; C_6H_{14}; [110-54-3]	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* <u>1986</u>, *31*, 225-230.
VARIABLES:	**PREPARED BY:**
T/K = 303, 308 and 313	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.8392	0.1608	40.0	0.7369	0.2631
35.0	0.7994	0.2006			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) n-Heptane; C_7H_{16}; [142-82-5]	Acree, W.E., Jr. *Int. J. Pharm.* <u>1984</u>, *18*, 47-52.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.8619	0.1381

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Warner, J.C.; Scheib, R.C.; Svirbely, W.J.

J. Chem. Phys. 1934, *2*, 590-594.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
299.7	0.860	0.140
308.4	0.784	0.216
313.1	0.726	0.274
316.3	0.665	0.335
319.9	0.591	0.409
322.2	0.532	0.468
322.3	0.525	0.475
328.5	0.335	0.665
330.7	0.284	0.726
332.7	0.197	0.803
333.7	0.194	0.806
334.8	0.164	0.836
335.7	0.143	0.857
337.2	0.108	0.892
339.2	0.066	0.934
341.3	0.028	0.972

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Solubilities were measured using a dynamic method. Mixtures of known concentrations were sealed in thick-walled glass tubes and placed in a constant temperature to equilibrate with gentle rotation to thoroughly mix contents. Bath temperature was slowly increased and solubility visually determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized three times from alcohol.

(2) Purity not specified, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.002. (compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.45

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Solubility determined indirectly from measured aqueous solubility and solute partition coefficient between n-heptane and water. Solute concentration in both phases, after equilibration and centrifugation, determined from the fluorescence intensity. This indirect method computes the solubility that is expected assuming that the dilute solution behavior extrapolates up to saturation point.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. 1986, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1	t/° C	x_2	x_1
30.0	0.8250	0.1750	40.0	0.7227	0.2773
35.0	0.7786	0.2214			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**EVALUATOR:**
(1) Biphenyl; $C_{12}H_{10}$; [120-12-7] (2) n-Heptane; C_7H_{16}; [110-54-3]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) June, 1994

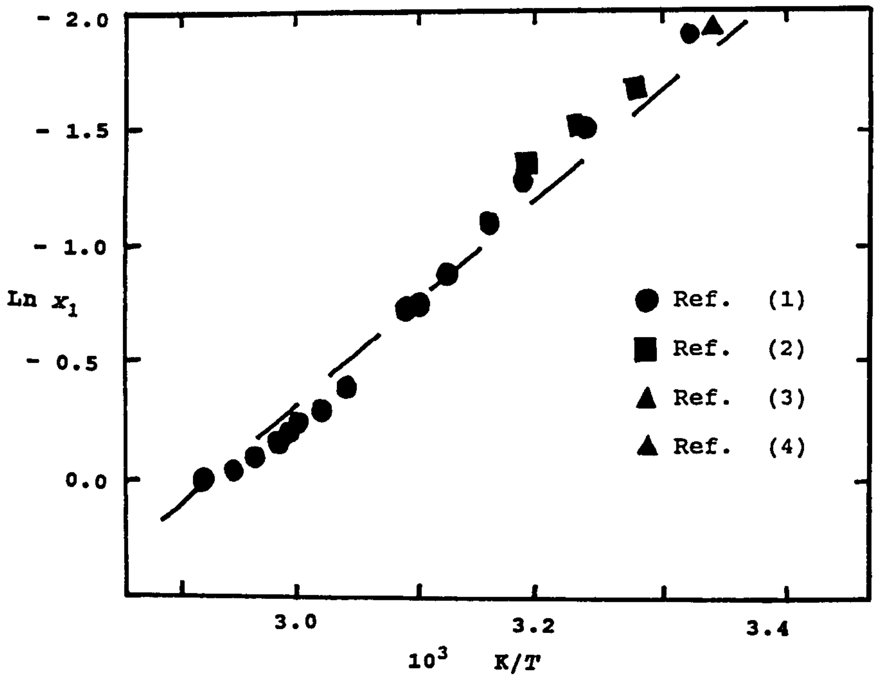
CRITICAL EVALUATION:

Biphenyl solubilities in n-heptane were retrieved from papers by Warner *et al.* (1), Acree *et al.* (2), Acree (3), Chang (4), and Lissi and Abuin (5). The first study reports observed values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and the latter three studies give the mole fraction solubility at either 298 K or 293 K. The value of Lissi was excluded from the critical evaluation since the n-heptane solvent was saturated with water, rather than a dried solvent.

Regressional analysis of the experimental data as Ln x_1 versus $1/T$ yielded the following mathematical relationship:

$$\text{Ln } x_1 = -5153.7\ (1/T) + 15.229 \qquad (r = 0.9982)$$

for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is x_1 = 0.1279, and differs by about 8 - 10 % from experimental values of x_1 = 0.1381 (3) and x_1 = 0.138 (4).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. *J. Chem. Phys.* 1934, *2*, 590-594.
2. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
3. Acree, W.E., Jr. *Int. J. Pharm.* 1984, *18*, 47-52.
4. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.
5. Lissi, E.A.; Abuin, E.B. *Bol Soc. Chil. Quin.* 1981, *26*, 19-34.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.862	0.138

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) n-Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.8520	0.1480

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) n-Octane; C_8H_{18}; [111-65-9]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.853	0.147

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) n-Octane; C_8H_{18}; [111-65-9]	Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
VARIABLES:	**PREPARED BY:**
T/K = 303, 308 and 313	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1	t/°C	x_2	x_1
30.0	0.8164	0.1836	40.0	0.7109	0.2891
35.0	0.7707	0.2293			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Tetracosane; $C_{24}H_{50}$; [646-31-1]	Vitali, G. *Int. DATA Ser., Ser. A* 1984, 94.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
323.8	1.000	0.000
323.4	0.980	0.020
323.3	0.972	0.028
322.8	0.942	0.058
321.8	0.882	0.118
320.6	0.804	0.196
319.8	0.718	0.282
319.1	0.641	0.359
318.7	0.623	0.377
318.0	0.586	0.414
318.6	0.568	0.432
319.7	0.544	0.456
320.8	0.534	0.466
321.6	0.512	0.488
323.9	0.477	0.523
326.0	0.436	0.564
327.8	0.395	0.605
328.8	0.383	0.617
330.5	0.339	0.661
333.9	0.253	0.747
336.1	0.183	0.817
337.4	0.132	0.868
337.6	0.120	0.880
338.7	0.087	0.913
339.5	0.068	0.932
340.3	0.045	0.955
340.8	0.044	0.956
341.5	0.022	0.978
341.9	0.012	0.988
342.0	0.007	0.993
342.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Ega, Steinheim, Germany, was used as received.

(2) 97 %, Baker, Deventer, The Netherlands, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.25.
x_1: ± 0.001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Octacosane; $C_{28}H_{58}$; [630-02-4]

ORIGINAL MEASUREMENTS:

Vitali, G.

Int. DATA Ser., Ser. A 1984, 95.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
334.7	1.000	0.000
334.5	0.986	0.014
334.3	0.971	0.029
334.0	0.952	0.048
333.5	0.922	0.078
332.3	0.853	0.147
331.0	0.767	0.233
329.5	0.670	0.330
329.0	0.585	0.415
327.3	0.505	0.495
326.2	0.460	0.540
326.2	0.399	0.601
331.1	0.306	0.694
333.4	0.250	0.750
335.7	0.187	0.813
337.5	0.128	0.872
339.9	0.072	0.928
341.2	0.033	0.967
341.4	0.023	0.977
341.9	0.011	0.989
342.1	0.003	0.997
342.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Ega, Steinheim, Germany, was used as received.

(2) 98 %, Ega, Steinheim, Germany, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.25.
x_1: ± 0.001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.

Int. J. Pharm. 1984, *18*, 47-52.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.8079	0.1921

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.

x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E.

J. Chem. Eng. Data 1985, *30*, 403-409.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
302.35	0.7652	0.2348	326.95	0.3071	0.6929
310.45	0.6460	0.3540	333.05	0.1748	0.8252
314.65	0.5681	0.4319			
320.85	0.4384	0.5616			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Eastman Kodak Chemical Company, Rochester, New York, USA, was passed over activated alumina and recrystallized from toluene

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.810	0.190

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 3854-3857.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
299.5	0.7987	0.2013	331.2	0.2186	0.7814
310.4	0.6503	0.3497			
318.3	0.4978	0.5022			
325.2	0.3473	0.6527			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.

(2) Purity, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:	**EVALUATOR:**
(1) Biphenyl; $C_{12}H_{10}$; [120-12-7] (2) Cyclohexane; C_6H_{12}; [110-82-7]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) June, 1994

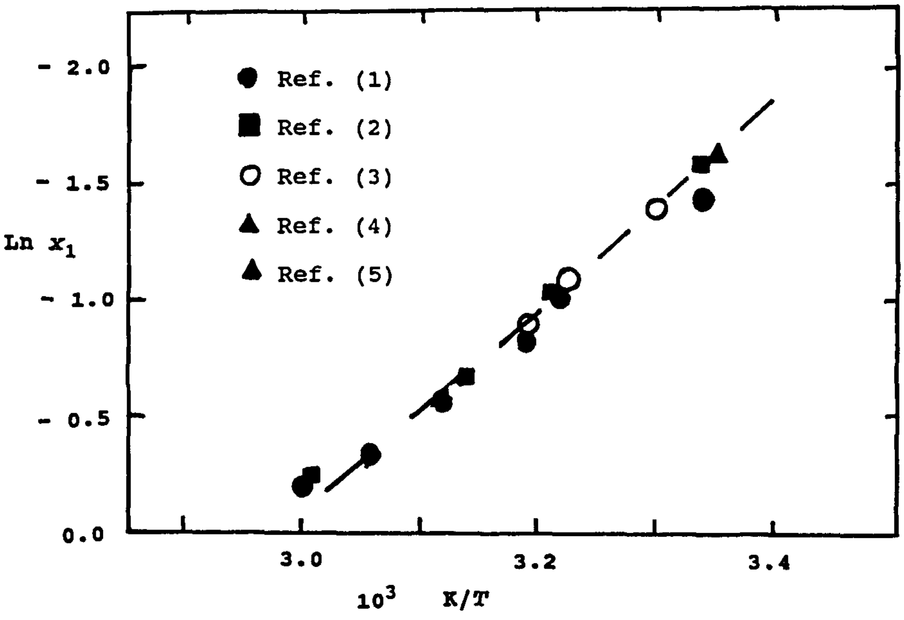
CRITICAL EVALUATION:

Biphenyl solubilities in cyclohexane were retrieved from papers by Choi *et al.* (1), McLaughlin and Zainal (2), Acree *et al.* (3), Acree (4) and Chang (5). The first two studies report observed values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and the latter two studies give the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the five studies from the critical evaluation.

Regressional analysis of the experimental data as Ln x_1 versus 1/T yielded the following mathematical relationship:

$$\text{Ln } x_1 = -4295.7\ (1/T) + 12.770 \qquad (r = 0.9975)$$

for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is x_1 = 0.1944, and differs by about 1 - 2 % from experimental values of x_1 = 0.1921 (4) and x_1 = 0.190 (5).



Graphical plot of Ln x_1 versus 1/T

REFERENCES

1. Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin *J. Chem. Eng. Data* 1985, *30*, 403-409.
2. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 3854-3857.
3. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
4. Acree, W.E., Jr. *Int. J. Pharm.* 1984, *18*, 47-52.
5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. 1986, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1	t/°C	x_2	x_1
30.0	0.7529	0.2471	40.0	0.6052	0.3948
35.0	0.6825	0.3175			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.817	0.183

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) cis-1,2-Dimethylcyclohexane; C_8H_{16}; [2207-01-4]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.805	0.195

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) trans-1,2-Dimethylcyclohexane; C_8H_{16}; [6876-23-9]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.817	0.183

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) trans-1,4-Dimethylcyclohexane; C_8H_{16}; [2207-04-7]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.827	0.173

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) cis-1,4-Dimethylcyclohexane; C_8H_{16}; [624-29-3]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.818	0.182

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) cis-1,3-Dimethylcyclohexane; C_8H_{16}; [638-04-0]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.828	0.172

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.0	0.6389	0.3611	328.2	0.4477	0.7385
316.0	0.5260	0.4740			
318.2	0.4820	0.5180			
324.3	0.3594	0.6406			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Benzene; C_6H_6; [71-43-2]	Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. *J. Chem. Eng. Data* <u>1985</u>, *30*, 403-409.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.95	0.5167	0.4833	328.95	0.2289	0.7711
313.85	0.4439	0.5561	333.15	0.1578	0.8422
316.85	0.4068	0.5932			
323.65	0.3103	0.6897			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Eastman Kodak Chemical Company, Rochester, New York, USA, was passed over activated alumina and recrystallized from toluene

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Benzene; C_6H_6; [71-43-2]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.619	0.381

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Spectroanalyzed, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
310.2	0.4882	0.5118
320.8	0.3522	0.6478
332.4	0.1805	0.8195
336.4	0.1084	0.8916

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Gesellschaft fur Teerverwertung, passed over an alumina column with benzene eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Warner, J.C.; Scheib, R.C.; Svirbely, W.J.

J. Chem. Phys. 1934, *2*, 590-594.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.1	0.590	0.410	318.7	0.374	0.626
316.3	0.415	0.585	322.6	0.323	0.677
317.5	0.395	0.605	325.5	0.187	0.713

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from alcohol.
(2) Thiophene free, Eastman Kodak Company, was dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.002. (compiler).

COMPONENTS:	**EVALUATOR:**
(1) Biphenyl; $C_{12}H_{10}$; [120-12-7] (2) Benzene; C_6H_6; [71-43-2]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) June, 1994

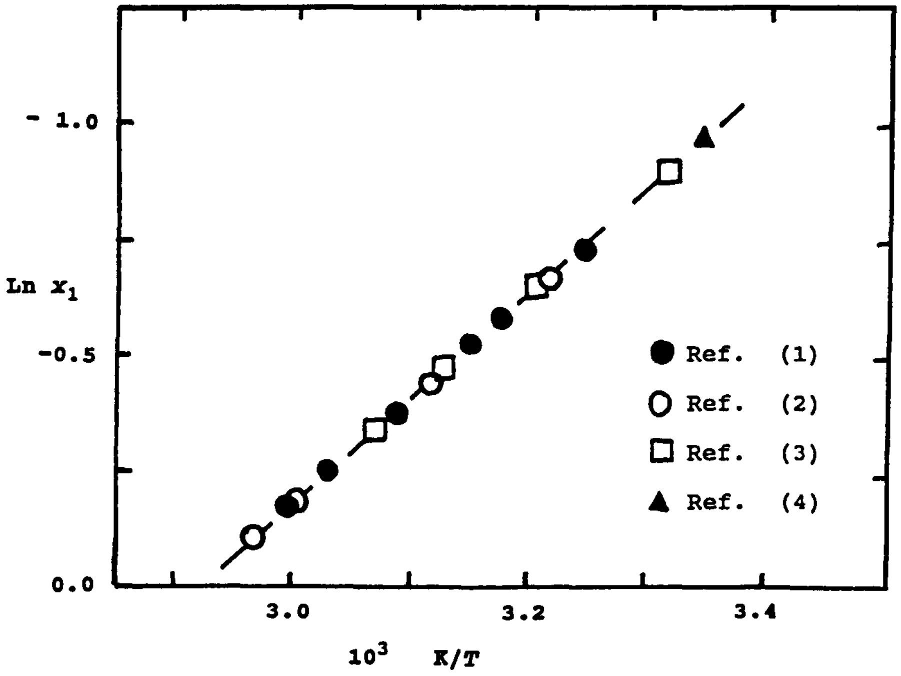
CRITICAL EVALUATION:

Biphenyl solubilities in benzene were retrieved from papers by Choi *et al.* (1), McLaughlin and Zainal (2), Warner *et al.* (3) and Chang (4). The first three studies report observed values at several temperatures, whereas Chang determined only a single mole fraction solubility for 298 K. There is no a prior reason to exclude any of the four studies from the critical evaluation.

Regressional analysis of the experimental data as Ln x_1 versus $1/T$ yielded the following mathematical relationship:

$$\text{Ln } x_1 = -2233.1\ (1/T) + 6.5272 \qquad (r = 0.9998)$$

for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.3819$, and differs by less than 1 % from experimental value of $x_1 = 0.381$ (4).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. Choi, P.B.; Williams, C.P.; Buehring, K.G.; McLaughlin, E. *J. Chem. Eng. Data* 1985, *30*, 403-409.
2. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1959, 863-867.
3. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. *J. Chem. Phys.* 1934, *2*, 590-594.
4. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.623	0.377

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.637	0.363

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

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COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Naphthalene; $C_{10}H_8$; [91-20-3]	Lee, H.H.; Warner, J.C. *J. Am. Chem. Soc.* 1935, *57*, 318-321.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
353.3	1.000	0.000
339.3	0.770	0.230
334.0	0.700	0.300
334.3	0.697	0.303
327.5	0.607	0.393
326.8	0.600	0.400
322.8	0.551	0.449
318.6	0.500	0.500
315.7	0.474	0.526
314.2	0.459	0.541
313.0	0.450	0.550
313.2	0.448	0.552
312.9	0.447	0.553
312.8	0.445	0.555
313.0	0.444	0.556
315.7	0.427	0.573
316.1	0.400	0.600
321.0	0.343	0.657
323.5	0.300	0.700
331.0	0.194	0.806
336.7	0.102	0.898
342.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.	(1) Highest Purity, Eastman Chemicals, was recrystallized. (2) Highest Purity, Eastman Chemicals, was recrystallized. **ESTIMATED ERRORS:** *T*/K: precision ± 0.1. x_1: ± 0.001.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2-Methylnaphthalene; $C_{11}H_{10}$; [91-57-6]	Szafranski, A.M.; Wyrzykowska-Stankiewicz, D. *Int. DATA Ser., Ser. A* 1984, 41.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
307.70	1.0000	0.0000
304.95	0.9071	0.0929
302.35	0.8127	0.1873
301.35	0.7649	0.2351
301.15	0.7489	0.2511
300.85	0.7328	0.2672
300.65	0.7167	0.2833
300.75	0.6974	0.3026
300.75	0.6844	0.3156
300.95	0.6780	0.3220
301.10	0.6682	0.3318
301.75	0.6519	0.3481
302.75	0.6356	0.3644
304.05	0.6193	0.3807
311.75	0.5203	0.4797
319.00	0.4196	0.5804
325.65	0.3173	0.6827
331.75	0.2133	0.7867
337.15	0.1075	0.8925
342.05	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly increased. Solubility determined by visual noting the temperature at which the last trace of solid solute disappeared.	(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined. (2) Pure Grade, Inst. Chem. Przerobki Wegla, Zabre, Poland, was recrystallized thrice from methanol.
	ESTIMATED ERRORS:
	T/K: precision ± 0.1. x_1: ± 0.0005.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 2,6-Dimethylnaphthalene; $C_{12}H_{12}$; [581-42-0]	Szafranski, A.M.; Wyrzykowska-Stankiewicz, D. *Int. DATA Ser., Ser. A* 1984, 42.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
383.35	1.0000	0.0000
375.65	0.8483	0.1517
369.45	0.7476	0.2524
351.75	0.4968	0.5032
342.95	0.3969	0.6031
331.65	0.2973	0.7027
329.55	0.2807	0.7193
328.15	0.2724	0.7276
327.15	0.2641	0.7359
328.15	0.2476	0.7524
331.35	0.1979	0.8021
326.95	0.0988	0.9012
342.05	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.

(2) Pure Grade, Schuchardt, Munchen, GFR, was sodium-refined and fractionally crystallized.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0005.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1,2-Diphenylethane; $C_{14}H_{14}$; [103-29-7]	Lee, H.H.; Warner, J.C. *J. Am. Chem. Soc.* 1935, *57*, 318-321.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
324.5	1.000	0.000
320.1	0.900	0.100
316.0	0.800	0.200
313.3	0.750	0.250
310.7	0.700	0.300
308.1	0.650	0.350
305.6	0.600	0.400
304.1	0.577	0.423
305.5	0.567	0.433
303.1	0.560	0.440
303.0	0.558	0.442
302.9	0.557	0.443
303.0	0.555	0.445
303.2	0.553	0.447
303.1	0.550	0.450
308.0	0.500	0.500
317.0	0.400	0.600
324.0	0.300	0.700
330.7	0.200	0.800
336.8	0.100	0.900
342.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Highest Purity, Eastman Chemicals, was recrystallized

(2) Highest Purity, Eastman Chemicals, was recrystallized.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
305.6	0.5472	0.4528	322.7	0.3292	0.6708
310.5	0.4940	0.5060	326.9	0.2661	0.7339
314.6	0.4444	0.5556			
319.2	0.3815	0.6185			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was passed over an activated alumina column and then recrystallized from solution.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Warner, J.C.; Scheib, R.C.; Svirbely, W.J.

J. Chem. Phys. 1934, *2*, 590-594.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
299.6	0.602	0.398	328.2	0.248	0.752
305.6	0.543	0.457	330.9	0.204	0.796
312.5	0.465	0.535	336.6	0.104	0.896
320.5	0.362	0.638	340.9	0.031	0.969
326.3	0.275	0.725			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from alcohol.

(2) Purity not given, Eastman Kodak Company, was refluxed over metallic sodium and distilled from phosphorous pentoxide.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.002. (compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Diphenyl ether; $C_{12}H_{10}O$; [101-84-8]	Szafranski, A.M.; Wyrzykowska-Stankiewicz, D. *Int. DATA Ser., Ser. A* 1984, 43.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
300.00	1.0000	0.0000
294.35	0.8908	0.1092
289.75	0.7837	0.2163
286.75	0.7310	0.2690
286.05	0.7153	0.2847
289.45	0.6789	0.3211
301.45	0.5761	0.4239
310.95	0.4753	0.5247
318.75	0.3766	0.6234
325.65	0.2797	0.7203
331.95	0.1847	0.8153
337.25	0.0915	0.9085
341.99	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.

(2) Pure Grade, Fabryka Odczynnikov Chem., Gliwice, Poland, was distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0005.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Dichloromethane; CH_2Cl_2; [75-09-2]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
$T/K = 298$	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.588	0.412

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, J. T. Baker Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Trichloromethane; $CHCl_3$; [67-66-3]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES:	**PREPARED BY:**
$T/K = 298$	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.578	0.422

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Tetrachloromethane; CCl_4; [56-23-5]	Acree, W.E., Jr. *Int. J. Pharm.* 1984, *18*, 47-52.
VARIABLES: *T*/K = 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.6579	0.3421

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol. (2) 99.8+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use. **ESTIMATED ERRORS:** *T*/K: ± 0.05. x_1: ± 1 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Tetrachloromethane; CCl_4; [56-23-5]	Chang, W. Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).
VARIABLES: *T*/K = 298	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.658	0.342

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/*T* graph.	(1) Purity, source and purification procedures not specified. (2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received. **ESTIMATED ERRORS:** *T*/K: precision ± 0.1. x_1: ± 2 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Tetrachloromethane; CCl_4; [56-23-5]	Warner, J.C.; Scheib, R.C.; Svirbely, W.J. *J. Chem. Phys.* 1934, *2*, 590-594.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.3	0.628	0.372	326.8	0.286	0.714
303.9	0.599	0.401	330.6	0.218	0.782
313.2	0.482	0.518	337.5	0.094	0.906
314.5	0.466	0.534	339.2	0.061	0.939

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from alcohol.
(2) Purity not given, Eastman Kodak Company, was dried over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.002. (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Tetrachloromethane; CCl_4; [56-23-5]	McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 2485-2488.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
303.2	0.6037	0.3963
311.6	0.5054	0.4946
318.6	0.4002	0.5998
326.8	0.1721	0.8279

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with benzene as eluant.

(2) AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:	EVALUATOR:
(1) Biphenyl; $C_{12}H_{10}$; [120-12-7] (2) Tetrachloromethane; CCl_4; [56-23-5]	W.E. Acree, Jr. Department of Chemistry University of North Texas Denton, Texas 76203-5068 (USA) June, 1994

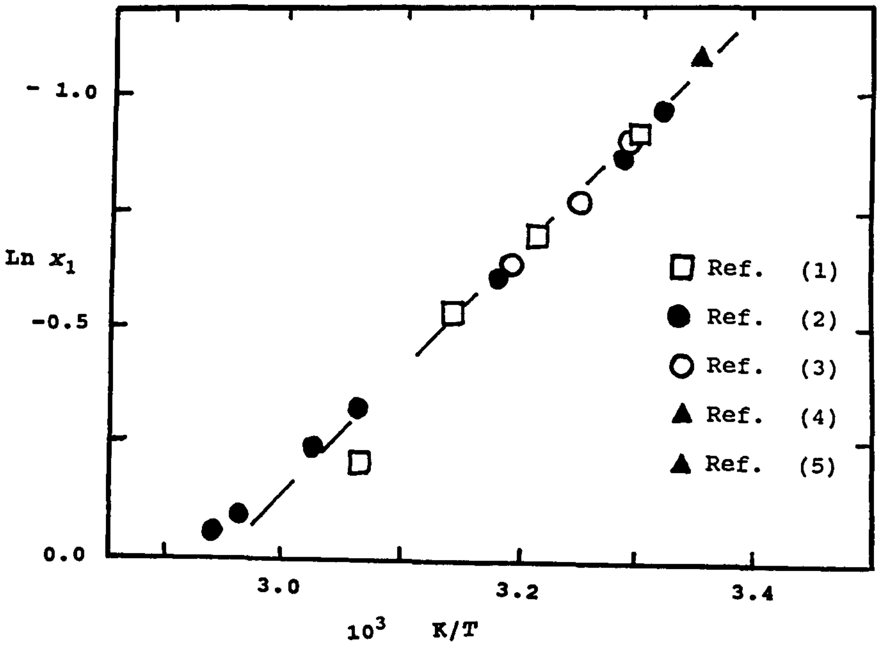
CRITICAL EVALUATION:

Biphenyl solubilities in tetrachloromethane were retrieved from papers by McLaughlin and Zainal (1), Warner *et al.* (2), Acree *et al.* (3), Acree (4) and Chang (5). The first two studies report observed values at several temperatures, Acree *et al.* determined values at 303, 308 and 313 K, and Acree and Chang measured only the mole fraction solubility at 298 K. There is no a prior reason to exclude any of the five studies from the critical evaluation.

Regressional analysis of the experimental data as Ln x_1 versus $1/T$ yielded the following mathematical relationship:

$$\text{Ln } x_1 = -2555.1\ (1/T) + 7.5025 \qquad (r = 0.9947)$$

for variation of biphenyl solubility with absolute temperature (see graph below). Back-calculated solubility at 298 K is $x_1 = 0.3438$, and differs by less than 1 % from experimental values of $x_1 = 0.3421$ (4) and $x_1 = 0.342$ (5).



Graphical plot of Ln x_1 versus $1/T$

REFERENCES

1. McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 2485-2488.
2. Warner, J.C.; Scheib, R.C.; Svirbely, W.J. *J. Chem. Phys.* 1934, *2*, 590-594.
3. Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L. *Int. J. Pharm.* 1986, *31*, 225-230.
4. Acree, W.E., Jr. *Int. J. Pharm.* 1984, *18*, 47-52.
5. Chang, W., Ph.D. Dissertation, North Dakota State University, North Dakota, 1969.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

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

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; Pontikos, N.M.; Judy, C.L.

Int. J. Pharm. 1986, *31*, 225-230.

VARIABLES:

T/K = 303, 308 and 313

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1	t/°C	x_2	x_1
30.0	0.6044	0.3956	40.0	0.4802	0.5198
35.0	0.5426	0.4574			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with cyclohexane. Concentrations determined spectrophotometrically at 250 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from methanol.

(2) 99.8+ %, Spectroanalyzed, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1 % (relative error).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,2-Dibromoethane; $C_2H_4Br_2$;
[106-93-4]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.611	0.389

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,1-Dichloroethane; $C_2H_4Cl_2$; [75-34-3]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.619	0.381

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,2-Dichloroethane; $C_2H_4Cl_2$; [107-06-2]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.603	0.397

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Matheson, Coleman and Bell, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.603	0.397

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus $1/T$ graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade, Eastman Organic Chemical Company, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]

ORIGINAL MEASUREMENTS:

Warner, J.C.; Scheib, R.C.; Svirbely, W.J.

J. Chem. Phys. 1934, *2*, 590-594.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
300.9	0.575	0.425	330.6	0.198	0.802
307.3	0.504	0.496	334.6	0.141	0.859
314.4	0.425	0.575	338.2	0.077	0.923
323.0	0.308	0.692			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from alcohol.

(2) Purity not given, Eastman Kodak Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.002. (compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1,4-Dichlorobenzene; $C_6H_4Cl_2$; [106-46-7]

ORIGINAL MEASUREMENTS:

Morris, R.E.; Cook, W.A.

J. Am. Chem. Soc. 1935, *57*, 2403-2406.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
326.4	1.000	0.000
322.6	0.931	0.069
318.2	0.849	0.151
314.4	0.788	0.212
308.4	0.690	0.310
304.0	0.630	0.370
300.1	0.575	0.425
302.6	0.540	0.460
308.2	0.480	0.520
312.3	0.440	0.560
317.3	0.379	0.621
324.0	0.292	0.708
331.9	0.177	0.823
336.4	0.106	0.894
339.5	0.050	0.950
342.3	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) C.P. grade, Eastman Chemicals, was recrystallized from alcohol to give a melting point temperature of 69.1 °C.

(2) Purity and chemical source were not specified, was purified by distillation.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Hexafluorobenzene; C_6F_6; [392-56-3]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Messer, C.E.

J. Chem. Soc., Sect. A 1966, 1106-1110.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.45	0.5954	0.4046	331.35	0.2097	0.7903
310.95	0.5528	0.4472	331.75	0.2025	0.7975
314.85	0.5031	0.4969	336.55	0.1077	0.8923
321.30	0.3992	0.6008	337.30	0.0934	0.9066
326.70	0.3018	0.6982			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, passed over alumina column, recrystallized and sublimed.

(2) Purity not given, Imperial Smelting, Ltd, Avonmouth, Bristol, was dried over anhydrous calcium sulfate.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.6913

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) 1-Octadecanol; $C_{18}H_{38}O$; [112-92-5]	Berchiesi, G. *Int. DATA Ser., Ser. A* <u>1985</u>, 95.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
331.2	1.0000	0.0000
330.3	0.9793	0.0207
329.3	0.9366	0.0634
328.2	0.8786	0.1214
327.6	0.8013	0.1987
325.9	0.7006	0.2994
324.4	0.5880	0.4120
325.0	0.5019	0.4981
329.8	0.3892	0.6108
332.3	0.3192	0.6808
334.3	0.2477	0.7523
336.4	0.1649	0.8351
338.6	0.0967	0.9033
340.8	0.0344	0.9656
342.3	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, C. Erba, Milano, Italy, was used as received.

(2) 99 %, Analytical Reagent, Fluka, St. Gallen, Switzerland, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Benzophenone; $C_{13}H_{10}O$; [119-61-9]	Lee, H.H.; Warner, J.C. *J. Am. Chem. Soc.* 1933, *55*, 209-214.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
326.0	1.000	0.000
308.2	0.772	0.228
303.5	0.693	0.307
299.1	0.628	0.372
298.4	0.607	0.393
301.2	0.575	0.425
305.5	0.530	0.470
311.7	0.458	0.542
319.3	0.362	0.638
329.4	0.220	0.780
342.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Highest Purity, Eastman Chemicals, was recrystallized from alcohol.

(2) Highest Purity, Eastman Chemicals, was distilled under reduced pressure.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Chang, W.

Ph.D Dissertation, North Dakota State University, North Dakota, USA (1969).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/° C	x_2	x_1
25.0	0.631	0.369

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Solubilities at 298 K interpolated from experimental values using ln x_1 versus 1/T graph.

SOURCE AND PURITY OF MATERIALS:

(1) Purity, source and purification procedures not specified.

(2) Reagent Grade or better, source not specified, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 2 % (relative error; compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Warner, J.C.; Scheib, R.C.; Svirbely, W.J.

J. Chem. Phys. 1934, *2*, 590-594.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.6	0.596	0.404	317.3	0.405	0.595
309.8	0.502	0.498	320.8	0.363	0.637
310.9	0.486	0.514	322.7	0.326	0.674
311.4	0.480	0.520	324.5	0.306	0.694
313.9	0.447	0.553	331.5	0.190	0.810

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass tubes and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared. Measurements repeated several times to verify results.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not specified, Eastman Kodak Company, Rochester, New York, USA, was recrystallized several times from alcohol.

(2) Purity not given, Eastman Kodak Company, was dried over calcium chloride and distilled twice from mercury.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.002. (compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
297.3	0.6258	0.3742	323.7	0.3116	0.6884
300.9	0.5915	0.4085	331.7	0.1830	0.8170
307.1	0.5257	0.4743			
312.4	0.4673	0.5327			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.1.
x_1: $\pm$ 0.0003.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Choi, P.B.; McLaughlin, E.

Ind. Eng. Chem. Fundam. 1983, *22*, 46-51.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
295.9	0.6149	0.3851	329.5	0.2347	0.7653
298.4	0.5929	0.4071	334.8	0.1302	0.8698
309.7	0.4782	0.5218			
317.0	0.3940	0.6060			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision $\pm$ 0.1.
x_1: $\pm$ 0.0003.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Biphenyl; $C_{12}H_{10}$; [92-52-4] (2) Indole; C_8H_7N; [120-72-9]	Yokoyama, C.; Ebina, T.; Takahashi, S. *J. Chem. Eng. Data* 1993, *38*, 583-586.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
326.26	1.0000	0.0000
317.55	0.8978	0.1022
310.08	0.8002	0.1998
306.45	0.7530	0.2470
301.76	0.6995	0.3005
301.45	0.6826	0.3174
304.01	0.6538	0.3462
308.08	0.6098	0.3902
312.57	0.5565	0.4435
318.19	0.4637	0.5363
323.66	0.3709	0.6291
328.51	0.2864	0.7136
335.36	0.1436	0.8564
343.13	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.8 %, Wako Pure Chemical Ind Ltd., was used as received.

(2) 99.9 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.02.
x_1: ± 0.0001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Indole; C_8H_7N; [120-72-9]

ORIGINAL MEASUREMENTS:

Szafranski, A.M.; Wyrzykowska-Stankiewicz, D.

Int. DATA Ser., Ser. A 1984, 46.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
324.95	1.0000	0.0000
318.75	0.9222	0.0778
312.65	0.8404	0.1596
306.45	0.7544	0.2456
302.05	0.6945	0.3055
302.70	0.6638	0.3362
310.95	0.5683	0.4317
317.65	0.4674	0.5326
323.85	0.3607	0.6393
329.75	0.2476	0.7524
333.90	0.1644	0.8356
335.75	0.1276	0.8724
337.00	0.1027	0.8973
341.99	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Pure Grade, Glovkhimreaktiv, Kharkov, USSR, was recrystallized thrice from methanol and zone refined.

(2) Pure Grade, Inst. Chem. Przerobki Wegla, Zabre, Poland, was recrystallized thrice from methanol.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0005.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Diphenylamine; $C_{12}H_{11}N$; [122-39-4]

ORIGINAL MEASUREMENTS:

Lee, H.H.; Warner, J.C.

J. Am. Chem. Soc. <u>1933</u>, *55*, 209-214.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
326.0	1.000	0.000
317.7	0.820	0.180
309.2	0.695	0.305
306.8	0.646	0.354
303.5	0.603	0.397
302.8	0.587	0.417
304.0	0.565	0.435
307.3	0.533	0.467
308.2	0.422	0.478
312.2	0.477	0.523
316.9	0.425	0.575
321.8	0.354	0.646
326.9	0.268	0.732
334.1	0.155	0.845
342.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Highest Purity, Eastman Chemicals, was recrystallized from alcohol.

(2) Highest Purity, Eastman Chemicals, was distilled under reduced pressure.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Srivastava, R.D.; Gupta, P.D.

J. Indian Chem. Soc. 1967, *44*, 960-963.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
281.4	0.7858	0.2142	302.2	0.6056	0.3944
291.4	0.6988	0.3012	305.0	0.5808	0.4192
296.0	0.6586	0.3414	311.2	0.5093	0.4907
298.4	0.6399	0.3601			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was recrystallized and sublimed.

(2) Purity not given, British Drug Houses, was dried and distilled.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) Biphenyl; $C_{12}H_{10}$; [92-52-4]

(2) 1-Octadecanoic acid; $C_{18}H_{36}O_2$; [57-11-4]

ORIGINAL MEASUREMENTS:

Berchiesi, G.

Int. DATA Ser., Ser. A 1985, 96.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
339.3	1.0000	0.0000
338.7	0.9726	0.0274
338.0	0.9333	0.0667
335.5	0.7873	0.2127
334.4	0.7249	0.2751
332.4	0.6373	0.3627
330.7	0.5570	0.4430
329.9	0.5100	0.4900
328.3	0.4478	0.5522
327.7	0.4106	0.5894
329.3	0.3783	0.6217
331.0	0.3425	0.6575
332.8	0.3019	0.6981
334.6	0.2544	0.7456
336.4	0.2000	0.8000
337.7	0.1553	0.8447
339.2	0.1054	0.8946
341.3	0.0371	0.9629
342.3	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations put in open containers and placed in constant temperature to equilibrate. Samples were rocked while bath temperature slowly decreased. Solubility determined by visual noting the temperature at which the first trace of solid solute appeared.

SOURCE AND PURITY OF MATERIALS:

(1) 98 %, C. Erba, Milano, Italy, was used as received.

(2) 99 %, Schuchardt, Hohenbrunn, Germany, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.001.

2,2'-BIPYRIDINE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

methanol + water
ethanol + water
2-methyl-2-propanol + water

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) 2,2'-Bipyridine; $C_{10}H_8N_2$; [366-18-7] (2) Methanol; CH_4O; [67-56-1] (3) Water; H_2O; [7732-18-5]	Burgess, J.; Haines, R.I. *Chem. Ind. (London)* 1980, 289.
VARIABLES:	**PREPARED BY:**
T/K = 298, Solvent composition	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

t = 25.0 °C

$\phi_2^{(s)}$	c_1/(mol dm^{-3})
0.00	0.037
0.10	0.063
0.20	0.116
0.30	0.240
0.40	0.60

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: solubility of the solute expressed in terms of molarity.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified, was recrystallized from aqueous-ethanol.

(2) Purity and chemical source not specified in paper.

(3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: ± 0.1 (Compiler).
$\phi_2^{(s)}$: ± 0.01 (Compiler).
c_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) 2,2'-Bipyridine; $C_{10}H_8N_2$; [366-18-7]

(2) Ethanol; C_2H_6O; [64-17-5]

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

ORIGINAL MEASUREMENTS:

Burgess, J.; Haines, R.I.

Chem. Ind. (London) 1980, 289.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0$ °C

$\phi_2^{(s)}$	$c_1/(\text{mol dm}^{-3})$
0.00	0.037
0.10	0.114
0.20	0.240
0.30	0.76

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: solubility of the solute expressed in terms of molarity.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified, was recrystallized from aqueous-ethanol.

(2) Purity and chemical source not specified in paper.

(3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: ± 0.1 (Compiler).
$\phi_2^{(s)}$: ± 0.01 (Compiler).
c_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) 2,2'-Bipyridine; $C_{10}H_8N_2$; [366-18-7]

(2) 2-Methyl-2-propanol; $C_4H_{10}O$; [75-65-0]

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

ORIGINAL MEASUREMENTS:

Burgess, J.; Haines, R.I.

Chem. Ind. (London) 1980, 289.

VARIABLES:

$T/K = 298$, Solvent composition

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

$t = 25.0\ ^{\circ}C$

$\phi_2^{(s)}$	$c_1/(\text{mol dm}^{-3})$
0.00	0.037
0.05	0.078
0.10	0.120
0.15	0.195
0.20	0.33
0.25	0.92

[a] $\phi_2^{(s)}$: initial volume fraction of binary solvent mixture; c_1: solubility of the solute expressed in terms of molarity.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, and an ultraviolet/visible spectrophotometer.

Excess solute and binary solvent equilibrated in a constant temperature vessel. Aliquots of saturated solution withdrawn and concentrations determined spectrometrically at 283 nm. Attainment of equilibrium verified by several repetitive measurements.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified, was recrystallized from aqueous-ethanol.

(2) Purity and chemical source not specified in paper.

(3) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: ± 0.1 (Compiler).
$\phi_2^{(s)}$: ± 0.01 (Compiler).
c_1: ± 3 % (relative error, Compiler).

BUCKMINSTERFULLERENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-pentane
n-hexane
n-octane
n-decane
n-dodecane

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
ethylbenzene
n-propylbenzene
iso-propylbenzene
n-butylbenzene
sec-butylbenzene
t-butylbenzene
1,2-dimethylbenzene
1,3-dimethylbenzene
1,4-dimethylbenzene
1,2,3-trimethylbenzene
1,2,4-trimethylbenzene
1,3,5-trimethylbenzene
1,2,3,4-tetramethylbenzene
1,2,3,5-tetramethylbenzene
1,2,3,4-tetrahydronaphthalene
1-methylnaphthalene

D. Esters

E. Ethers

1,4-dioxane
methoxybenzene

F. Haloalkanes and Haloaromatic Hydrocarbons

dichloromethane
trichloromethane
tetrachloromethane
1,2-dibromoethane
tetrachloroethylene
1,1,2,2-tetrachloroethane
bromobenzene
chlorobenzene
1,2-dibromobenzene
1,3-dibromobenzene
1,2-dichlorobenzene
1,3-dichlorobenzene
1,2,4-trichlorobenzene
fluorobenzene

iodobenzene
1-bromo-2-methylnaphthalene

G. Alcohols

2-hydroxymethylbenzene

H. Ketones

I. Miscellaneous Pure Solvents

carbon disulfide
benzonitrile
nitrobenzene
pyridine
quinoline
thiophene
2-methylthiophene
tetrahydrothiophene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Pentane; C_5H_{12}; [109-66-0]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	5.55×10^{-6}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Pentane; C_5H_{12}; [109-66-0]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	8×10^{-7}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	5.55×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Hexane; C_6H_{14}; [110-54-3]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	7.3×10^{-6}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	3.47×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Decane; $C_{10}H_{22}$; [124-18-5]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	9.71×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Decane; $C_{10}H_{22}$; [124-18-5]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. <u>1993</u>, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_1
22	1.9×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Dodecane; $C_{12}H_{26}$; [112-40-3]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. <u>1992</u>, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
30.0	1.26×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	2.00×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	2.1×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.1×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	2.98×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	4.0×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	4.0×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Ethylbenzene; C_8H_{10}; [100-41-4]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	3.6×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Propylbenzene; C_9H_{12}; [103-65-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.1×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) iso-Propylbenzene; C_9H_{12}; [98-82-8]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	1.7×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) n-Butylbenzene; $C_{10}H_{14}$; [104-51-8]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.6×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) sec-Butylbenzene; $C_{10}H_{14}$; [135-98-8]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
22	1.5×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) t-Butylbenzene; $C_{10}H_{14}$; [98-06-6]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
22	1×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,2-Dimethylbenzene; C_8H_{10}; [95-47-6]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	1.2×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,3-Dimethylbenzene; C_8H_{10}; [108-38-3]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	1.9×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]	Scrivens, W.A.; Tour, J.M. *J. Chem. Soc., Chem. Commun.* 1993, 1207-1209.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	8.2×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) 1,2,3-Trimethylbenzene; C_9H_{12}; [526-73-8]	Scrivens, W.A.; Tour, J.M. *J. Chem. Soc., Chem. Commun.* 1993, 1207-1209.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	6.5×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,2,4-Trimethylbenzene; C_9H_{12}; [95-63-6]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.48×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,3,5-Trimethylbenzene; C_9H_{12}; [108-67-8]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	1.38×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,3,5-Trimethylbenzene; C_9H_{12}; [108-67-8]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	3.1×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,3,5-Trimethylbenzene; C_9H_{12}; [108-67-8]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.4×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) 1,2,3,4-Tetramethylbenzene; $C_{10}H_{14}$; [488-23-3]	Scrivens, W.A.; Tour, J.M. *J. Chem. Soc., Chem. Commun.* <u>1993</u>, 1207-1209.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	8.0×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.	(1) Purity and chemical source were not given in the paper. (2) Purity and chemical source were not given in the paper. **ESTIMATED ERRORS:** *T*/K: ± 3 (Compiler). c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) 1,2,3,5-Tetramethylbenzene; $C_{10}H_{14}$; [527-53-7]	Scrivens, W.A.; Tour, J.M. *J. Chem. Soc., Chem. Commun.* <u>1993</u>, 1207-1209.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.89×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Analytical balance and centrifuge. Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.	(1) Purity and chemical source were not given in the paper. (2) Purity and chemical source were not given in the paper. **ESTIMATED ERRORS:** *T*/K: ± 3 (Compiler). c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	3.1×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	6.8×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1-Methylnaphthalene; $C_{11}H_{10}$; [90-12-0]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\mathrm{mol\ dm^{-3}})$
22	4.61×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol $\mathrm{dm^{-3}}$.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\mathrm{mol\ dm^{-3}})$
30.0	5.69×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was with- and the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Methoxybenzene; C_7H_8O; [100-66-3]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	8.4×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	3.52×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Dichloromethane; CH_2Cl_2; [75-09-2]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_1
22	2.7×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Trichloromethane; $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_1
22	2.2×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer. Reported to contain 1 % ethanol as a stabilizer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
30.0	6.20×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	4.0×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60};
[99685-96-8]
(2) 1,2-Dibromoethane; $C_2H_4Br_2$;
[106-93-4]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	6.0×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60};
[99685-96-8]
(2) Tetrachloroethylene; C_2Cl_4;
[127-18-4]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	1.7×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,1,2,2-Tetrachloroethane; $C_2H_2Cl_4$; [79-34-5]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	7.7×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Bromobenzene; C_6H_5Br; [108-86-1]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	4.8×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Bromobenzene; C_6H_5Br; [108-86-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$c_1/(\text{mol dm}^{-3})$
22	3.9×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_1
22	9.9×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60};
[99685-96-8]
(2) Chlorobenzene; C_6H_5Cl; [108-90-7]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$c_1/(\text{mol dm}^{-3})$
22	7.9×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60};
[99685-96-8]
(2) 1,2-Dibromobenzene; $C_6H_4Br_2$;
[583-53-9]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	$c_1/(\text{mol dm}^{-3})$
22	1.9×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,3-Dibromobenzene; $C_6H_4Br_2$; [108-36-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	1.9 x 10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	5.3 x 10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) 1,2-Dichlorobenzene; $C_6H_4Cl_2$; [95-50-1]	Scrivens, W.A.; Tour, J.M. *J. Chem. Soc., Chem. Commun.* <u>1993</u>, 1207-1209.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
22	3.41×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) 1,3-Dichlorobenzene; $C_6H_4Cl_2$; [541-73-1]	Scrivens, W.A.; Tour, J.M. *J. Chem. Soc., Chem. Commun.* <u>1993</u>, 1207-1209.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
22	3.3×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	1.5×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili-for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1,2,4-Trichlorobenzene; $C_6H_3Cl_3$; [120-82-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	1.44×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Fluorobenzene; C_6H_5F; [462-06-6]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_1
22	7.8×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly-(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Fluorobenzene; C_6H_5F; [462-06-6]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
22	1.7×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Iodobenzene; C_6H_5I; [591-50-4]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	2.9×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 1-Bromo-2-methylnaphthalene; $C_{11}H_9Br$; [2586-62-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	4.83×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 2-Hydroxymethylbenzene; C_7H_8O; [95-48-7]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_1
22	2.9×10^{-6}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Sivaraman, N.; Dhamodaran, R.; Kaliappan, I., Srinivasan, R.G.; Vasudeva Rao, P.R.; Mathews, C.K.
J. Org. Chem. 1992, *57*, 6077-6079.

VARIABLES:

T/K = 303

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
30.0	7.16×10^{-3}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, stirrer, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass tube and allowed to equilibrate for 5 hours at constant temperature with stirring. Tube was then centrifuged and aliquots of saturated solution was withand the absorbance measured at 328 nm after appropriate dilution with spectroscopic grade n-hexane.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, fullerenes recovered by soxhlet extraction with toluene, and sample purified by chromatographic separation on alumina column.

(2) HPLC grade or AR grade solvent, chemical source not given, aromatic impurities removed by chromatography if necessary.

ESTIMATED ERRORS:

T/K: ± 0.1.
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Carbon disulfide; CS_2; [75-15-0]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	6.6×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Benzonitrile; C_7H_5N; [100-47-0]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	7.1×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Nitrobenzene; $C_6H_5NO_2$; [98-95-3]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	1.1×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	9.9×10^{-5}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equili- for 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, Baxter Scientific Products, McGaw Park, Illinois, USA, was used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	4×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent allowed to equilibrate in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Quinoline; C_9H_7N; [91-22-5]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	1.0×10^{-2}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent sonicated and equilibrated in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 μm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Scrivens, W.A.; Tour, J.M.

J. Chem. Soc., Chem. Commun. 1993, 1207-1209.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
22	6×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Analytical balance and centrifuge.

Excess solute and solvent sonicated and equilibrated in a room temperature bath for 30 minutes. Solution centrifuged for about 5 minutes and filtered through a 0.45 µm HPLC syringe filtered. Three 1.0 mls were removed and placed in tared vials, which were then placed in a heated oil bath to facilitate solvent evaporation. Concentrations determined gravimetrically from the weight of the solid residue.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not given in the paper.

(2) Purity and chemical source were not given in the paper.

ESTIMATED ERRORS:

T/K: ± 3 (Compiler).
c_1: ± 0.0007 mol dm^{-3}.

COMPONENTS:

(1) Buckminsterfullerene; C_{60}; [99685-96-8]
(2) 2-Methylthiophene; C_5H_6S; [554-14-3]

ORIGINAL MEASUREMENTS:

Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C.

J. Phys. Chem. 1993, *97*, 3379-3383.

VARIABLES:

T/K = *Circa* 295 (Ambient Room)

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_1
22	9.1×10^{-4}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 98 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Buckminsterfullerene; C_{60}; [99685-96-8] (2) Tetrahydrothiophene; C_4H_8S; [110-01-0]	Ruoff, R.S.; Tse, D.S.; Malhotra, R.; Lorents, D.C. *J. Phys. Chem.* 1993, *97*, 3379-3383.
VARIABLES:	**PREPARED BY:**
T/K = *Circa* 295 (Ambient Room)	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_1
22	3.6×10^{-6}

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

High performance liquid chromatograph system equipped with an ultraviolet detector aned integrator.

Excess solute and solvent placed in 1-dram glass bottle and allowed to equilifor 24 hours at ambient room temperature with agitation. Saturated solution was filtered through a 0.45 micrometer poly(tetrafluoroethylene) filter. Concentrations determined via HPLC with uv detection at 340 nm. Stationary phase was a dinitroanilinopropyl column, and a binary toluene/hexane (20:80 by volume) mobile phase was used.

SOURCE AND PURITY OF MATERIALS:

(1) Graphite soot obtained by passing an ac discharge between spectroscopic grade graphite, and sample purified by chromatographic separation on alumina column. Final purity of 99.95 % as determined by mass spectrometry.

(2) Reagent grade, 99 % (or better), chemical source not given, used as received from manufacturer.

ESTIMATED ERRORS:

T/K: ± 3.
x_1: ± 8 % (relative error; compiler).

CARBAZOLE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-hexane
n-heptane
n-octane
n-decane
n-dodecane
n-hexadecane
cyclohexane
methylcyclohexane
cyclooctane
2,2,4-trimethylpentane
t-butylcyclohexane
squalane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
methylbenzene
1,4-dimethylbenzene
chrysene
1,2,3,4-tetrahydronaphthalene

D. Esters

ethyl ethanoate
butyl butyrate

E. Ethers

tetrahydropyran
tetrahydrofuran
1,1-oxybisethane
1,1-oxybisbutane
1,1-oxybispentane
1,4-dioxane
methoxybenzene

F. Haloalkanes and Haloaromatic Hydrocarbons

trichloromethane
tetrachloromethane
1-chlorohexane
1-chlorooctane
1-chlorotetradecane
chlorocyclohexane

G. Alcohols

methanol
ethanol
1,2-ethanediol

1-propanol
2-propanol
1-butanol
1-octanol
phenol

H. Ketones

2-propanone
2-butanone
cyclohexanone
acetophenone

I. Miscellaneous Pure Solvents

carbon disulfide
pyridine
quinoline
thiophene
dimethyl sulfoxide
nitromethane
acetic anhydride
1-methyl-2-pyrrolidinone
N,N-dimethylacetamide
N,N-dimethylformamide
tetramethylene sulfone
tributyl phosphate
dibenzofuran

J. Binary Solvent Mixtures

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) n-Hexane; C_6H_{14}; [110-54-3]	McCargar, J.W.; Acree, W.E., Jr. *Phys. Chem. Liq.* <u>1987</u>, *17*, 123-138.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9999	0.000139

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) n-Hexane; C_6H_{14}; [110-54-3]	Fung, H.-L.; Higuchi, T. *J. Pharm. Sci.* <u>1987</u>, *60*, 1782-1788.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9999	0.00017

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) ACS Reagent Grade, source not specified, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *17*, 123-138.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9998	0.000173

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9998	0.00023

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Octane; C_8H_{18}; [111-65-9]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *17*, 123-138.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9998	0.000198

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Decane; $C_{10}H_{22}$; [142-18-5]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9997	0.00029

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Dodecane; $C_{12}H_{26}$; [112-40-3]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9997	0.00032

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was passed through a silica gel column.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Hexadecane; $C_{16}H_{34}$; [544-76-3]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Pharm. Sci. 1987, *76*, 572-574.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9996	0.000414

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetrachloromethane. Concentrations determined spectrophotmetrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) n-Hexadecane; $C_{16}H_{34}$; [544-76-3]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9996	0.00059

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was passed through a silica gel column and distilled over sodium.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *17*, 123-138.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9998	0.000183

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.9 %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 293 and 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
20.0	0.999+	0.000153
25.0	0.999+	0.000224

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9998	0.00018

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was distilled over phosphorous pentoxide.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
320.6	0.9993	0.00066
321.1	0.9992	0.00083
325.1	0.9989	0.00106
357.2	0.9971	0.00293

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Methylcyclohexane; C_7H_{14}; [108-87-2]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *17*, 123-138.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9998	0.000196

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Cyclooctane; C_8H_{16}; [292-64-8]	McCargar, J.W.; Acree, W.E., Jr. *Phys. Chem. Liq.* 1987, *17*, 123-138.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9997	0.000309

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]	McCargar, J.W.; Acree, W.E., Jr. *Phys. Chem. Liq.* 1987, *17*, 123-138.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9999	0.000126

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) HPLC Grade, 99.7+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9998	0.00018

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was distilled over sodium.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2,2,4-Trimethylpentane; C_8H_{18}; [540-84-1]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
25.0	0.00077

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.

(2) 99 %, Phillips Petroleum Company, Bartlesville, Oklahoma, USA, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) t-Butylcyclohexane; $C_{10}H_{20}$; [3178-22-1]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Solution Chem. 1988, *17*, 1081-1091.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9997	0.000250

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2,6,10,15,19,23-Hexamethyltetracosane (squalane); $C_{30}H_{62}$; [111-01-3]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Pharm. Sci. 1987, *76*, 572-574.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9993	0.000671

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with tetrachloromethane. Concentrations determined spectrophotmetrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 2 % (relative error).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]	**ORIGINAL MEASUREMENTS:** Coon, J.E.; Auwaerter, J.E.; McLaughlin, E. *Fluid Phase Equilibr.* <u>1989</u>, *44*, 305-345.
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
333.3	0.9974	0.00263
348.7	0.9959	0.00414
357.6	0.9946	0.00544
361.6	0.9944	0.00557
376.0	0.9890	0.01098
388.2	0.9812	0.01880
402.2	0.9719	0.02811
416.2	0.9503	0.04967
438.2	0.9047	0.09527
473.2	0.7009	0.29909
491.7	0.4945	0.50551
502.2	0.3085	0.69153

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 293 and 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
20.0	0.996	0.00352
25.0	0.996	0.00412

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
307.1	0.9946	0.0054	326.8	0.9891	0.0109
310.3	0.9932	0.0068	340.3	0.9866	0.0134
313.2	0.9937	0.0063			
324.1	0.9907	0.0093			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Carbazole; $C_{12}H_{10}N$; [86-74-8]

(2) Methylbenzene; C_7H_8; [108-88-3]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 293, 313$ and 333

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1	$t/°C$	x_2	x_1
20.0	0.996	0.00374	60.0	0.989	0.0111
40.0	0.993	0.00666			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,4-Dimethylbenzene; C_8H_{10}; [106-42-3]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
20.0	0.995	0.00483

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Chrysene; $C_{18}H_{12}$; [218-01-9]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M.; Pastukhova, I.S. *Proc. Acad. Sci. U.S.S.R., Sect. Chem.* 1956, *111*, 667-669. (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
528.2	1.000	0.000
519.7	0.903	0.097
511.2	0.805	0.195
500.7	0.698	0.302
493.4	0.606	0.394
482.9	0.505	0.495
478.4	0.472	0.528
477.2	0.445	0.555
479.8	0.396	0.604
484.7	0.347	0.653
489.6	0.301	0.699
499.2	0.200	0.800
507.5	0.108	0.892
517.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source were not specified in paper, was recrystallized before use. (2) Purity and chemical source were not specified in paper, was recrystallized before use.
	ESTIMATED ERRORS: T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]	Coon, J.E.; Auwaerter, J.E.; McLaughlin, E. *Fluid Phase Equilibr.* 1989, *44*, 305-345.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
344.7	0.9927	0.0073	495.2	0.3029	0.6971
374.8	0.9897	0.0103			
476.2	0.7113	0.2887			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Ethyl ethanoate; $C_4H_8O_2$; [141-78-6]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES:	**PREPARED BY:**
T/K = See below	W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.980	0.020

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Butyl butyrate; $C_8H_{16}O_2$; [109-21-7]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	$c_1/(mol\ dm^{-3})$
25.0	0.0994

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.

(2) Purity not given, Eastman Chemical Co., Rochester, New York, USA, was shaken with sodium hydroxide, washed with distilled water, dried over magnesium sulfate and distilled. Stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Tetrahydropyran; $C_5H_{10}O$; [142-68-7]

ORIGINAL MEASUREMENTS:

Acree, W.E., Jr.; McCargar, J.W.; Zvaigzne, A.I.; Teng, I.-L.

Phys. Chem. Liq. **1991**, *23*, 27-35.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	x_2	x_1
25.0	0.9572	0.04284

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, anhydrous, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 4 % (relative error).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Tetrahydrofuran; C_4H_8O; [109-99-9]	**ORIGINAL MEASUREMENTS:** Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES: *T*/K = See below	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.929	0.071

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source not specified in paper. (2) Purity and chemical source not specified in paper. **ESTIMATED ERRORS:** *T*/K: Unknown. x_1: ± 8 % (relative error; compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1,1-Oxybisethane; $C_4H_{10}O$; [60-29-7]	**ORIGINAL MEASUREMENTS:** Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES: *T*/K = See below	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.987	0.013

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source not specified in paper. (2) Purity and chemical source not specified in paper. **ESTIMATED ERRORS:** *T*/K: Unknown. x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,1-Oxybisethane; $C_4H_{10}O$; [60-29-7]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9870	0.0130

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was distilled from lithium aluminum hydride shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,1-Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

Phys. Chem. Liq. 1987, *17*, 123-138.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9950	0.005011

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) Gold Label, 99+ %, Aldrich Chemical Company, was stored over molecular sieves and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,1 -Oxybisbutane; $C_8H_{18}O$; [142-96-1]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(mol\ dm^{-3})$
25.0	0.0287

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.

(2) 99 %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,1 -Oxybispentane; $C_{10}H_{22}O$; [693-65-2]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	c_1
25.0	0.0182

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.

(2) Purity not given, Pfaltz and Bauer, Waterbury, Connecticut, USA, was treated with potassium permanganate, washed with distilled water and sulfuric acid solution, dried over calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,4-Dioxane; $C_4H_8O_2$; [123-91-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.964	0.036

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Methoxybenzene; C_7H_8O; [100-66-3]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.987	0.013

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Trichloromethane; $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.995	0.00478

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.

x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Trichloromethane; $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Fung, H.-L.; Higuchi, T.

J. Pharm. Sci. 1987, *60*, 1782-1788.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9963	0.0037

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for 24 hours at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with ether. Concentrations determined spectrophotometrically at 292.5 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Reagent Grade, source not specified, recrystallized from aqueous-ethanol to to give a melting point of 242-243 °C.

(2) Reagent Grade, source not specified, was washed with distilled water five times, stored overnight over calcium chloride and distilled from phosphorous pentoxide.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).

x_1: ± 3 % (relative error, compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Trichloromethane; $CHCl_3$; [67-66-3]

ORIGINAL MEASUREMENTS:

Anderson, B.D.

Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	c_1/(mol dm^{-3})
25.0	0.0468

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.

(2) Purity not given, Fisher Scientific, Pittsburgh, Pennsylvania, USA, was washed with distilled water, stored over calcium chloride and distilled shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Tetracloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

T/K = 293, 298, 313 and 333

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1	$t/^\circ C$	x_2	x_1
20.0	0.999	0.000659	40.0	0.998	0.00165
25.0	0.999	0.000899	60.0	0.996	0.00377

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1-Chlorohexane; $C_6H_{13}Cl$;
[544-10-5]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Solution Chem. 1989, *18*, 151-158.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9974	0.00255

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1-Chlorooctane; $C_8H_{17}Cl$;
[111-85-3]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Solution Chem. 1989, *18*, 151-158.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9976	0.00242

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1-Chlorotetradecane; $C_{14}H_{29}Cl$; [2425-54-9]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Solution Chem. 1989, *18*, 151-158.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9976	0.00240

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Chlorocyclohexane; $C_6H_{11}Cl$; [542-18-7]

ORIGINAL MEASUREMENTS:

McCargar, J.W.; Acree, W.E., Jr.

J. Solution Chem. 1989, *18*, 151-158.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9971	0.00291

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, calorimetric thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, recrystallized 3 times from absolute ethanol.

(2) 99 %, Aldrich Chemical Company, was treated with sulfuric acid, washed with distilled water, dried over calcium chloride and distilled before shortly before use.

ESTIMATED ERRORS:

T/K: ± 0.05.
x_1: ± 1.5 % (relative error).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Methanol; CH_4O; [67-56-1]	**ORIGINAL MEASUREMENTS:** Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* <u>1967</u>, *32*, 931-943.
VARIABLES: *T*/K = 293	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
20.0	0.998	0.00183

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Ethanol; C_2H_6O; [64-17-5]	**ORIGINAL MEASUREMENTS:** Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* <u>1967</u>, *32*, 931-943.
VARIABLES: *T*/K = 293	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
20.0	0.997	0.00332

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Ruelle, P.; Sarraf, E.; Kesselring, U.W.

Int. J. Pharm. 1994, *104*, 125-133.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9964	0.00358

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given in paper.

ESTIMATED ERRORS:

T/K: ± 0.2 (Compiler).
x_1: ± 3 % (relative error, Compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Ethanol; C_2H_6O; [64-17-5]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9886	0.0114

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1,2-Ethanediol; $C_2H_6O_2$; [107-21-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.993	0.007

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 1-Propanol; C_3H_8O; [71-23-8]

ORIGINAL MEASUREMENTS:

Ruelle, P.; Sarraf, E.; Kesselring, U.W.

Int. J. Pharm. 1994, *104*, 125-133.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
25.0	0.9963	0.00365

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given in paper.

ESTIMATED ERRORS:

T/K: ± 0.2 (Compiler).
x_1: ± 3 % (relative error, Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 2-Propanol; C_3H_8O; [67-63-0]	Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* 1967, *32*, 931-943.
VARIABLES:	**PREPARED BY:**
T/K = 293, 313 and 333	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1	t/°C	x_2	x_1
20.0	0.997	0.00277	60.0	0.991	0.00912
40.0	0.995	0.00523			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.	(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %. (2) 99 %, Commercial sample, source and purification method was not specified. **ESTIMATED ERRORS:** T/K: precision ± 0.05. x_1: ± 3 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	Anderson, B.D. Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.0493

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer. Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.	(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures. (2) puriss, 99.5 %, Fluka Chemical Corporation, Ronkonkoma, New York, USA, was stored over molecular sieves to remove trace water. **ESTIMATED ERRORS:** T/K: ± 0.1 (compiler). c_1: ± 3 % (relative error; compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1-Butanol; $C_4H_{10}O$; [71-36-3]	**ORIGINAL MEASUREMENTS:** Ruelle, P.; Sarraf, E.; Kesselring, U.W. *Int. J. Pharm.* <u>1994</u>, *104*, 125-133.
VARIABLES: $T/K = 298$	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
25.0	0.9956	0.00444

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given in paper.

ESTIMATED ERRORS:

T/K: ± 0.2 (Compiler).
x_1: ± 3 % (relative error, Compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1-Octanol; $C_8H_{18}O$; [540-84-1]	**ORIGINAL MEASUREMENTS:** Anderson, B.D. Ph.D. Dissertation, University of Kansas, Lawrence, Kansas, USA (1978).
VARIABLES: $T/K = 298$	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	$c_1/(\text{mol dm}^{-3})$
25.0	0.0515

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in glass vials and allowed to equilibrate for several days at constant temperature. Attainment of equilibrium verified by repetitive measurements. Aliquots of saturated solutions transferred through a coarse filter into tared volumetric flasks, weighed and diluted with methanol. Concentrations determined spectrophotometrically at 356 nm.

SOURCE AND PURITY OF MATERIALS:

(1) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from acetone-heptane mixtures.

(2) 99+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1-Octanol; $C_8H_{18}O$; [540-84-1]	Ruelle, P.; Sarraf, E.; Kesselring, U.W. *Int. J. Pharm.* 1994, *104*, 125-133.
VARIABLES:	**PREPARED BY:**
T/K = 298	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
25.0	0.9919	0.00806

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and an ultraviolet/visible spectrophotometer.

Excess solute and solvent placed in amber glass bottles and allowed to equilibrate at constant temperature. Concentrations determined spectrophotometrically at 292 nm.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not given in paper.

(2) Purity and chemical source not given in paper.

ESTIMATED ERRORS:

T/K: ± 0.2 (Compiler).
x_1: ± 3 % (relative error, Compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Phenol; C_6H_6O; [108-95-2]	Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* 1967, *32*, 931-943.
VARIABLES:	**PREPARED BY:**
T/K = 313	W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^\circ C$	x_2	x_1
40.0	0.994	0.00598

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1
20.0	0.976	0.0239

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2-Propanone; C_3H_6O; [67-64-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9628	0.0372

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) 2-Butanone; C_4H_8O; [78-93-3]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9576	0.0424

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Cyclohexanone; $C_6H_{10}O$; [108-94-1]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.932	0.068

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Acetophenone; C_8H_8O; [98-86-2]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES:	**PREPARED BY:**
T/K = See below	W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.959	0.041

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	(1) Purity and chemical source not specified in paper. (2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS:
	T/K: Unknown. x_1: ± 8 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Carbon disulfide; CS_2; [75-15-0]	Smutek, M.; Fris, M.; Fohl, J. *Collection Czech. Chem. Commun.* 1967, *32*, 931-943.
VARIABLES:	**PREPARED BY:**
T/K = 293	W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	x_2	x_1
20.0	0.999	0.00149

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Constant temperature bath, thermometer, and a precision balance. Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.	(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %. (2) 99 %, Commercial sample, source and purification method was not specified.
	ESTIMATED ERRORS:
	T/K: precision ± 0.05. x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Smutek, M.; Fris, M.; Fohl, J.

Collection Czech. Chem. Commun. 1967, *32*, 931-943.

VARIABLES:

$T/K = 293, 313$ and 333

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/^{\circ}C$	x_2	x_1	$t/^{\circ}C$	x_2	x_1
20.0	0.911	0.0895	60.0	0.862	0.138
40.0	0.890	0.110			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, thermometer, and a precision balance.

Excess solute and solvent placed in closed glass container and allowed to equilibrate for several hours at constant temperature. Aliquots of saturated solutions were transferred into tared constainers and weighed. Solubilities calculated from weight of solid residue that remained after solvent had evaporated.

SOURCE AND PURITY OF MATERIALS:

(1) coal tar extract, was recrystallized several times from toluene and pyridine, and then sublimed to give a final purity of 98.3 %.

(2) 99 %, Commercial sample, source and purification method was not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.05.
x_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
301.5	0.9023	0.0977	400.7	0.7376	0.2624
318.1	0.8852	0.1148	439.2	0.6167	0.3833
345.5	0.8510	0.1490			
370.3	0.8041	0.1959			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Pyridine; C_5H_5N; [110-86-1]	**ORIGINAL MEASUREMENTS:** Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES: *T*/K = See below	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.914	0.086

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source not specified in paper. (2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS: *T*/K: Unknown. x_1: ± 8 % (relative error; compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Quinoline; C_9H_7N; [91-22-5]	**ORIGINAL MEASUREMENTS:** Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES: *T*/K = See below	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.879	0.121

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source not specified in paper. (2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS: *T*/K: Unknown. x_1: ± 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Thiophene; C_4H_4S; [110-02-1]	Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E. *J. Solution Chem.* <u>1988</u>, *16*, 519-534.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
313.7	0.9893	0.0107
337.1	0.9796	0.0204
345.6	0.9746	0.0254
349.5	0.9713	0.0287

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Dimethylsulfoxide; C_2H_6OS; [67-68-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* <u>1986</u>, *52*, 41-44. (English Translation)
VARIABLES:	**PREPARED BY:**
T/K = See below	W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.861	0.139

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Nitromethane; CH_3NO_2; [75-52-5]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.996	0.004

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Acetic anhydride; $C_4H_6O_3$; [108-24-7]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.988	0.012

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) 1-Methyl-2-pyrrolidinone; C_5H_9NO; [872-50-4]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES:	**PREPARED BY:**
T/K = See below	W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.843	0.157

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) N,N-Dimethylacetamide; C_4H_9NO; [127-19-5]	Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES:	**PREPARED BY:**
T/K = See below	W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.810	0.190

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) N,N-Dimethylformamide; C_3H_7NO; [68-12-2]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.836	0.164

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS:

(1) Carbazole; $C_{12}H_9N$; [86-74-8]

(2) Tetramethylene sulfone; $C_4H_8O_2S$; [126-33-0]

ORIGINAL MEASUREMENTS:

Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I.
Sov. Prog. Chem. 1986, *52*, 41-44.
(English Translation)

VARIABLES:

T/K = See below

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.9526	0.0474

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

No experimental details were given in the paper.

Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source not specified in paper.

(2) Purity and chemical source not specified in paper.

ESTIMATED ERRORS:

T/K: Unknown.
x_1: ± 8 % (relative error; compiler).

COMPONENTS: (1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Tributyl phosphate; $C_{12}H_{27}O_4P$; [126-73-8]	**ORIGINAL MEASUREMENTS:** Chernyi, A.V.; Rubstov, V.I.; Aleksandrov, V.V.; Nazarov, V.N.; Vail, E.I. *Sov. Prog. Chem.* 1986, *52*, 41-44. (English Translation)
VARIABLES: T/K = See below	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

x_2	x_1
0.911	0.089

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE No experimental details were given in the paper. Based upon experimental values given in the paper for solvents for which independently determined values exist, compiler estimates the temperature as between 298-303 K.	**SOURCE AND PURITY OF MATERIALS:** (1) Purity and chemical source not specified in paper. (2) Purity and chemical source not specified in paper.
	ESTIMATED ERRORS: T/K: Unknown. x_1: ± 8 % (relative error; compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Carbazole; $C_{12}H_9N$; [86-74-8] (2) Dibenzofuran; $C_{12}H_8O$; [132-64-9]	Cullinane, N.M.; Rees, W.T. *Trans. Faraday Soc.* 1940, *36*, 506-514.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
355.6	354.7	1.000	0.000
401.6	356.7	0.898	0.102
439.2	360.7	0.753	0.247
469.5	368.6	0.562	0.438
492.8	382.7	0.331	0.669
510.0	414.4	0.141	0.859
519.0	518.3	0.000	1.000

[a] Phase diagram, given in the original paper, shows formation of a complete series of solid solutions. Melting points of binary mixtures lie between those of the two pure components. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	**SOURCE AND PURITY OF MATERIALS:**
Mixtures were placed in small capillary tubes. Temperature was slowly varied with ample time given for equilibration. Transition temperatures determined by visual observations. Reported temperatures verified by repetitive measurements.	(1) Purity and chemical source not given, was sublimed and recrystallized from acetone. (2) Purity and chemical source not given in paper, was sublimed and recrystallized from alcohol several times.
	ESTIMATED ERRORS:
	T/K: precision ± 0.2 (Compiler). x_1: ± 0.002 (Compiler).

CHRYSENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

benzene
naphthalene
anthracene
benz[a]anthracene
acenaphthene
fluorene
fluoranthene
pyrene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

carbazole
dibenzofuran

J. Binary Solvent Mixtures

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.0040

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
308.8	0.9979	0.0021
319.0	0.9968	0.0032
333.8	0.9948	0.0052
345.4	0.9921	0.0079

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Gesellschaft fur Teerverwertung, was passed over an alumina column with toluene eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Naphthalene; $C_{10}H_8$; [91-20-3]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
353.2	1.000	0.000
351.7	0.975	0.025
351.0	0.958	0.042
388.4	0.897	0.103
406.2	0.843	0.157
417.8	0.798	0.202
442.4	0.710	0.290
459.7	0.593	0.407
476.2	0.496	0.504
487.5	0.407	0.593
500.2	0.298	0.702
511.4	0.183	0.817
520.2	0.097	0.903
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Anthracene; $C_{14}H_{10}$; [120-12-7]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
489.7	1.000	0.000
481.7	0.897	0.103
473.7	0.798	0.202
469.7	0.740	0.260
467.2	0.697	0.303
466.2	0.635	0.365
470.5	0.598	0.402
480.4	0.504	0.496
490.9	0.397	0.603
499.7	0.307	0.693
509.5	0.212	0.788
519.2	0.104	0.896
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

ORIGINAL MEASUREMENTS:

Sturrock, M.G.; Lawe, T.

Can. J. Res., Sect. B. 1939, *17*, 71-74.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
433.2	433.2	1.00	0.00
448.2	436.2	0.90	0.10
470.2	442.2	0.75	0.25
487.2	451.2	0.60	0.40
496.2	461.2	0.50	0.50
505.2	468.2	0.40	0.60
516.2	484.2	0.25	0.75
525.2	505.2	0.10	0.90
528.2	528.2	0.00	1.00

[a] Continuous solid solutions were found in the chrysene - benz[a]anthracene system. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Melting points and freezing points were obtained by determining temperatures of incipient fusion and complete liquefaction using capillary tube method. Temperature very slowly raised and material observed through a low power microscope.

SOURCE AND PURITY OF MATERIALS:

(1) Obtained from heavy crude oil, purified by column chromatography using activated alumina and recrystallized.

(2) Obtained from heavy crude oil, and was fractionally recrystallized from alcohol before use.

ESTIMATED ERRORS:

T/K: precision ± 0.5 (Compiler).
x_1: ± 0.005 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Benz[a]anthracene; $C_{18}H_{12}$; [56-55-3]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES[a]

T_{in}/K	T_{fin}/K	x_2	x_1
431.2	430.9	1.000	0.000
435.4	431.7	0.960	0.040
438.2	432.2	0.947	0.053
446.7	434.2	0.898	0.102
451.6	436.2	0.852	0.148
459.2	438.6	0.805	0.195
473.8	445.2	0.700	0.300
483.2	453.2	0.603	0.397
493.7	461.7	0.498	0.502
502.2	474.2	0.395	0.605
508.7	486.2	0.300	0.700
514.5	499.2	0.202	0.798
522.2	513.2	0.095	0.905
528.2	528.2	0.000	1.000

[a] Continuous solid solutions were found in the chrysene - benz[a]anthracene system. T_{in} refers to the temperature at which crystallization begins; T_{fin} is the temperature at which crystallization of the solid solution concludes.

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS: (1) Chrysene; $C_{18}H_{12}$; [218-01-9] (2) Acenaphthene; $C_{12}H_{10}$; [83-32-9]	**ORIGINAL MEASUREMENTS:** Kravchenko, V.M.; Pastukhova, I.S. *Proc. Acad. Sci. U.S.S.R., Sect. Chem.* 1956, *111*, 667-669 (English translation)
VARIABLES: Temperature	**PREPARED BY:** W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
368.2	1.000	0.000
366.4	0.966	0.034
364.2	0.928	0.072
378.5	0.899	0.101
416.2	0.796	0.204
437.4	0.704	0.296
457.0	0.596	0.404
471.5	0.499	0.501
477.8	0.387	0.613
500.2	0.278	0.722
513.2	0.147	0.853
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:	**ORIGINAL MEASUREMENTS:**
(1) Chrysene; $C_{18}H_{12}$; [218-01-9] (2) Fluorene; $C_{13}H_{10}$; [86-73-7]	Kravchenko, V.M.; Pastukhova, I.S. *Proc. Acad. Sci. U.S.S.R., Sect. Chem.* 1956, *111*, 667-669 (English translation)
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
387.2	1.000	0.000
384.4	0.948	0.052
381.2	0.902	0.098
395.7	0.871	0.129
419.5	0.795	0.205
445.4	0.680	0.320
458.7	0.597	0.403
480.2	0.445	0.555
491.6	0.350	0.650
504.2	0.246	0.754
513.9	0.139	0.861
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Fluoranthene; $C_{16}H_{10}$; [206-44-0]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
383.2	1.000	0.000
378.7	0.939	0.061
378.2	0.918	0.082
387.3	0.897	0.103
403.2	0.846	0.154
418.8	0.799	0.201
442.4	0.691	0.309
457.2	0.602	0.398
474.5	0.498	0.502
486.2	0.404	0.596
498.4	0.293	0.707
510.5	0.195	0.805
519.2	0.090	0.910
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Pyrene; $C_{16}H_{10}$; [129-00-0]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
423.2	1.000	0.000
413.7	0.901	0.099
410.2	0.864	0.136
408.2	0.835	0.165
415.4	0.813	0.187
420.6	0.790	0.210
441.2	0.697	0.303
458.7	0.602	0.398
473.2	0.505	0.495
487.2	0.396	0.604
496.2	0.314	0.686
506.7	0.218	0.782
517.7	0.103	0.897
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.00200

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Carbazole; $C_{12}H_9N$; [86-74-8]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
517.2	1.000	0.000
507.5	0.892	0.108
499.2	0.800	0.200
489.6	0.699	0.301
484.7	0.653	0.347
479.8	0.604	0.396
477.2	0.555	0.445
478.4	0.528	0.472
482.9	0.495	0.505
493.4	0.394	0.606
500.7	0.302	0.698
511.2	0.195	0.805
519.7	0.097	0.903
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

COMPONENTS:

(1) Chrysene; $C_{18}H_{12}$; [218-01-9]

(2) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

ORIGINAL MEASUREMENTS:

Kravchenko, V.M.; Pastukhova, I.S.

Proc. Acad. Sci. U.S.S.R., Sect. Chem. 1956, *111*, 667-669 (English translation)

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
356.2	1.000	0.000
354.7	0.968	0.032
353.2	0.940	0.060
373.7	0.907	0.093
401.2	0.848	0.152
429.2	0.752	0.248
450.4	0.649	0.351
474.6	0.496	0.504
486.7	0.404	0.596
499.0	0.300	0.700
509.6	0.295	0.805
516.5	0.113	0.887
528.2	0.000	1.000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Phase diagram was determined using a thermal analysis method (described in detail in V.M. Kravchenko, *J. Phys. Chem. U.S.S.R.* 1939, *13*, 133), supplemented by visual observations.

SOURCE AND PURITY OF MATERIALS:

(1) Purity and chemical source were not specified in paper, was recrystallized before use.

(2) Purity and chemical source were not specified in paper, was recrystallized before use.

ESTIMATED ERRORS:

T/K: precision ± 0.2 (Compiler).
x_1: ± 0.002 (Compiler).

CORONENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:

(1) Coronene; $C_{24}H_{12}$; [191-07-1]

(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

$T/K = 293$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	$c_1/(mol\ dm^{-3})$
20.0	0.00048

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and a spectrofluorimeter.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured fluorescence emission intensity.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Coronene; $C_{24}H_{12}$; [191-07-1]

(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

$T/K = 298$

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

$t/°C$	$c_1/(mol\ dm^{-3})$
25.0	0.000386

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

DIBENZ[a,h]ANTHRACENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

n-heptane

B. Alkenes

C. Aromatic Hydrocarbons

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

1-octanol

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:

(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [53-70-3]
(2) n-Heptane; C_7H_{16}; [142-82-5]

ORIGINAL MEASUREMENTS:

Lissi, E.A.; Abuin, E.B.

Bol. Soc. Chil. Quim. 1981, *26*, 19-34.

VARIABLES:

T/K = 293

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
20.0	0.00034

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, centrifuge, thermometer, and an uv/visible spectrophotometer.

Excess solute and solvent were placed in glass vials, pre-equilibrated for several hours at 60-80 °C, and then equilibrated at 20 °C for several additional hours. After equilibration and centrifugation, concentrations determined from the measured absorbance using the Beer-Lambert law.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, commercial sample of unspecified source, was used as received.

(2) Purity and chemical source not given, purification procedure not specified.

ESTIMATED ERRORS:

T/K: ± 2.
c_1: unknown.

COMPONENTS:

(1) Dibenz[a,h]anthracene; $C_{22}H_{14}$; [53-70-3]
(2) 1-Octanol; $C_8H_{18}O$; [111-87-5]

ORIGINAL MEASUREMENTS:

Miller, M.M.; Wasik, S.P.; Huang, G.-L.; Shiu, W.-Y.; Mackay, D.

Environ. Sci. Technol. 1985, *19*, 522-529.

VARIABLES:

T/K = 298

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

t/°C	c_1/(mol dm^{-3})
25.0	0.000938

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath, rotator, thermometer, and a gas-liquid chromatograph with flame ionization detection.

Excess solute and solvent placed in glass vials and allowed to equilibrate for 24 hours with gentle agitation, and left to settle for 48 hours before analysis. Aliquots of saturated solutions were removed and concentrations were determined using a gas-liquid chromatograph equipped with flame ionization detector and on 10 % SE30 ultraphase column.

SOURCE AND PURITY OF MATERIALS:

(1) Highest available commercial purity, specific chemical supplier not given, was used as received.

(2) 99+ %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was used as received.

ESTIMATED ERRORS:

T/K: ± 0.1 (compiler).
c_1: ± 3 % (relative error; compiler).

DIBENZOFURAN SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
1,2,3,4-tetrahydronaphthalene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
327.8	0.5774	0.4226	338.5	0.3300	0.6700
330.2	0.5195	0.4805	345.1	0.1880	0.8120
334.0	0.4564	0.5436			
337.5	0.3700	0.6300			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
326.4	0.5755	0.4245	337.2	0.3553	0.6447
328.2	0.5354	0.4646			
331.5	0.4890	0.5110			
333.5	0.4248	0.5752			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from solution.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Domanska, U.; Groves, F.R., Jr.; McLaughlin, E.

J. Chem. Eng. Data 1993, *38*, 88-94.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
278.7	1.0000	0.0000
276.1	0.9365	0.0635
274.0	0.9144	0.0856
273.4	0.9066	0.0934
272.4	0.8878	0.1122
274.8	0.8761	0.1239
277.9	0.8637	0.1363
280.2	0.8537	0.1463
282.8	0.8401	0.1599
290.3	0.8022	0.1978
296.3	0.7654	0.2346
298.3	0.7520	0.2480
302.5	0.7187	0.2813
305.3	0.7005	0.2995
312.0	0.6441	0.3559
320.0	0.5514	0.4486
329.1	0.4209	0.5791
337.7	0.2955	0.7045
340.9	0.2430	0.7570
346.4	0.1654	0.8346
355.3	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) 99+ %, Aldrich Chemical Company, was fractionally distilled and stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
321.9	0.5203	0.4797	338.7	0.2776	0.7224
323.5	0.4932	0.5068			
329.4	0.4156	0.5844			
332.0	0.3778	0.6222			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
318.9	0.5479	0.4521	339.5	0.2670	0.7330
322.6	0.5093	0.4907			
326.6	0.4506	0.5494			
337.9	0.3010	0.6990			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.6 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystalfrom solution.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
323.7	0.4917	0.5083	340.8	0.2418	0.7582
326.2	0.4554	0.5446			
331.2	0.3839	0.6161			
336.3	0.3188	0.6812			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzofuran; $C_{12}H_8O$; [132-64-9]

(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
314.2	0.5780	0.4220	337.0	0.3040	0.6960
319.3	0.5243	0.4757	341.1	0.2415	0.7585
322.3	0.4917	0.5083			
332.8	0.3653	0.6347			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

DIBENZOTHIOPHENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane
decahydronaphthalene

B. Alkenes

C. Aromatic Hydrocarbons

benzene
1,2,3,4-tetrahydronaphthalene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

pyridine
thiophene

J. Binary Solvent Mixtures

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
320.6	0.9129	0.0871	343.0	0.6846	0.3154
326.6	0.8871	0.1129	343.3	0.6654	0.3346
328.2	0.8706	0.1294			
335.8	0.8001	0.1999			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]
(2) Decahydronaphthalene; $C_{10}H_{18}$; [91-17-8]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
311.3	0.8944	0.1056	333.9	0.7372	0.2628
318.9	0.8607	0.1393			
325.8	0.8141	0.1859			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from solution.

(2) 99+ %, Aldrich Chemical Company, having isomer ratio of 60.6 % cis and 39.4 % trans, stored over molecular sieves.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0] (2) Benzene; C_6H_6; [71-43-2]	Domanska, U.; Groves, F.R., Jr.; McLaughlin, E. *J. Chem. Eng. Data* 1993, *38*, 88-94.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
278.7	1.0000	0.0000
278.0	0.9770	0.0230
277.2	0.9570	0.0430
276.6	0.9468	0.0532
276.0	0.9402	0.0598
278.2	0.9337	0.0663
283.1	0.9216	0.0784
285.7	0.9133	0.0867
290.5	0.8990	0.1010
294.7	0.8842	0.1152
299.2	0.8670	0.1330
301.3	0.8571	0.1429
304.3	0.8427	0.1573
306.7	0.8301	0.1699
312.9	0.7934	0.2066
319.2	0.7884	0.2516
325.6	0.6962	0.3038
330.7	0.6399	0.3601
335.4	0.5869	0.4131
340.8	0.5267	0.4733
346.4	0.4649	0.5351
350.3	0.4142	0.5858
353.2	0.3577	0.6423
372.0	0.0000	1.0000

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE	SOURCE AND PURITY OF MATERIALS:
Constant temperature bath and a precision thermometer. Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.	(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene. (2) 99+ %, Aldrich Chemical Company, was fractionally distilled and stored over molecular sieves.
	ESTIMATED ERRORS:
	T/K: precision ± 0.1. x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. 1988, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
309.9	0.8104	0.1896	342.3	0.4856	0.5144
315.3	0.7754	0.2246			
327.8	0.6653	0.3347			
337.2	0.5638	0.4362			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]
(2) 1,2,3,4-Tetrahydronaphthalene; $C_{10}H_{12}$; [119-64-2]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Auwaerter, J.E.; McLaughlin, E.

Fluid Phase Equilibr. 1989, *44*, 305-345.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	*T*/K	x_2	x_1
308.7	0.7837	0.2163	337.8	0.5308	0.4692
318.2	0.7219	0.2781			
326.6	0.6492	0.3508			
336.3	0.5534	0.4466			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99.5 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystalfrom solution.

(2) 99.6+ %, Aldrich Chemical Company, was stored over molecular sieves to remove trace water.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]
(2) Pyridine; C_5H_5N; [110-86-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. <u>1988</u>, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
306.5	0.7857	0.2143	334.7	0.5502	0.4498
313.0	0.7448	0.2552	335.2	0.5348	0.4652
322.8	0.6687	0.3313			
327.4	0.6216	0.3784			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

COMPONENTS:

(1) Dibenzothiophene; $C_{12}H_8S$; [132-65-0]
(2) Thiophene; C_4H_4S; [110-02-1]

ORIGINAL MEASUREMENTS:

Coon, J.E.; Sediawan, W.B.; Auwaerter, J.E.; McLaughlin, E.

J. Solution Chem. <u>1988</u>, *16*, 519-534.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
309.3	0.7621	0.2379	328.1	0.6128	0.3872
315.2	0.7224	0.2776	337.0	0.5050	0.4950
322.7	0.6639	0.3361			
327.0	0.6257	0.3743			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) 99 %, Aldrich Chemical Company, Milwaukee, Wisconsin, USA, was recrystallized from toluene.

(2) Gold Label, 99.9+ %, Aldrich Chemical Company, was used as received.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003.

1,2-DIPHENYLBENZENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

cyclohexane

B. Alkenes

C. Aromatic Hydrocarbons

benzene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

tetrachloromethane

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:

(1) 1,2-Diphenylbenzene; $C_{18}H_{14}$; [84-15-1]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 3854-3857.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
296.0	0.6463	0.3537
303.2	0.5004	0.4996
313.6	0.2927	0.7073
322.8	0.1045	0.8955

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Eastman Kodak, Rochester, New York, USA, was passed over an alumina column with light petroleum ether as eluant.
(2) Purity, source, and purification method were not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) 1,2-Diphenylbenzene; $C_{18}H_{14}$; [84-15-1]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1
301.2	0.4148	0.5852
305.6	0.3558	0.6442
318.0	0.1898	0.8102
323.6	0.0987	0.9013

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Eastman Kodak, Rochester, New York, USA, was passed over an alumina column with light petroleum ether as eluant.
(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) 1,2-Diphenylbenzene; $C_{18}H_{14}$; [84-15-1]
(2) Tetrachloromethane; CCl_4; [56-23-5]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 2485-2488.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
302.0	0.4257	0.5743	323.0	0.1125	0.8875
308.0	0.3293	0.6707			
314.8	0.2507	0.7493			
318.6	0.1814	0.8186			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, Eastman Kodak, Rochester, New York, USA, was passed over an alumina column with light petroleum ether as eluant.
(2) AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

1,3-DIPHENYLBENZENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. <u>Saturated Hydrocarbons (including cycloalkanes)</u>

cyclohexane

B. <u>Alkenes</u>

C. <u>Aromatic Hydrocarbons</u>

benzene

D. <u>Esters</u>

E. <u>Ethers</u>

F. <u>Haloalkanes and Haloaromatic Hydrocarbons</u>

tetrachloromethane

G. <u>Alcohols</u>

H. <u>Ketones</u>

I. <u>Miscellaneous Pure Solvents</u>

J. <u>Binary Solvent Mixtures</u>

COMPONENTS:

(1) 1,3-Diphenylbenzene; $C_{18}H_{14}$; [92-06-8]
(2) Cyclohexane; C_6H_{12}; [110-82-7]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1960, 3854-3857.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
311.4	0.9230	0.0770	333.4	0.5925	0.4075
320.6	0.8368	0.1632			
325.5	0.7579	0.2421			
329.9	0.6669	0.3331			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with light petroleum ether as eluant.
(2) Purity, source and purification method not specified.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:

(1) 1,3-Diphenylbenzene; $C_{18}H_{14}$; [92-06-8]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
310.0	0.7173	0.2827	347.4	0.2429	0.7571
320.2	0.6162	0.3838	350.8	0.1656	0.8344
334.0	0.4534	0.5466			
340.6	0.3593	0.6407			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with light petroleum ether as eluant.
(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) 1,3-Diphenylbenzene; $C_{18}H_{14}$; [92-06-8] (2) Tetrachloromethane; CCl_4; [56-23-5]	McLaughlin, E.; Zainal, H.A. *J. Chem. Soc.* 1960, 2485-2488.
VARIABLES:	**PREPARED BY:**
Temperature	W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
312.6	0.7937	0.2063	343.2	0.5750	0.4250
318.2	0.7391	0.2609			
328.6	0.6282	0.3718			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with light petroleum ether as eluant.

(2) AnalaR grade, source not given, was dried over anhydrous calcium chloride and distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.

x_1: ± 0.0003 (compiler).

1,4-DIPHENYLBENZENE SOLUBILITIES IN PURE AND BINARY SOLVENT MIXTURES

A. Saturated Hydrocarbons (including cycloalkanes)

B. Alkenes

C. Aromatic Hydrocarbons

benzene

D. Esters

E. Ethers

F. Haloalkanes and Haloaromatic Hydrocarbons

G. Alcohols

H. Ketones

I. Miscellaneous Pure Solvents

J. Binary Solvent Mixtures

COMPONENTS:

(1) 1,4-Diphenylbenzene; $C_{18}H_{14}$; [92-94-4]
(2) Benzene; C_6H_6; [71-43-2]

ORIGINAL MEASUREMENTS:

McLaughlin, E.; Zainal, H.A.

J. Chem. Soc. 1959, 863-867.

VARIABLES:

Temperature

PREPARED BY:

W.E. Acree, Jr.

EXPERIMENTAL VALUES

T/K	x_2	x_1	T/K	x_2	x_1
311.2	0.9929	0.0071	350.8	0.9721	0.0279
333.4	0.9844	0.0156			
337.4	0.9822	0.0178			
341.2	0.9796	0.0204			

AUXILIARY INFORMATION

METHOD: APPARATUS/PROCEDURE

Constant temperature bath and a precision thermometer.

Mixtures of known concentrations sealed in glass ampoules and placed in constant temperature to equilibrate. Samples were rotated while bath temperature slowly increased. Solubility determined by noting the temperature at which the last trace of solid solute disappeared.

SOURCE AND PURITY OF MATERIALS:

(1) Purity not given, British Drug Houses, United Kingdom, was passed over an alumina column with benzene as eluant.

(2) "AnalaR", was dried over sodium wire and freshly distilled before use.

ESTIMATED ERRORS:

T/K: precision ± 0.1.
x_1: ± 0.0003 (compiler).

SYSTEM INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

REGISTRY NUMBER INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

AUTHOR INDEX

In this volume there is a general evaluation of the compiled data in the introductory material. There are a few individual critical evaluations. Most page numbers below refer to compiled tables.

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